

JULY TO SEPTEMBER 1990

AD-A242 111

VOL. 15 NO. 3

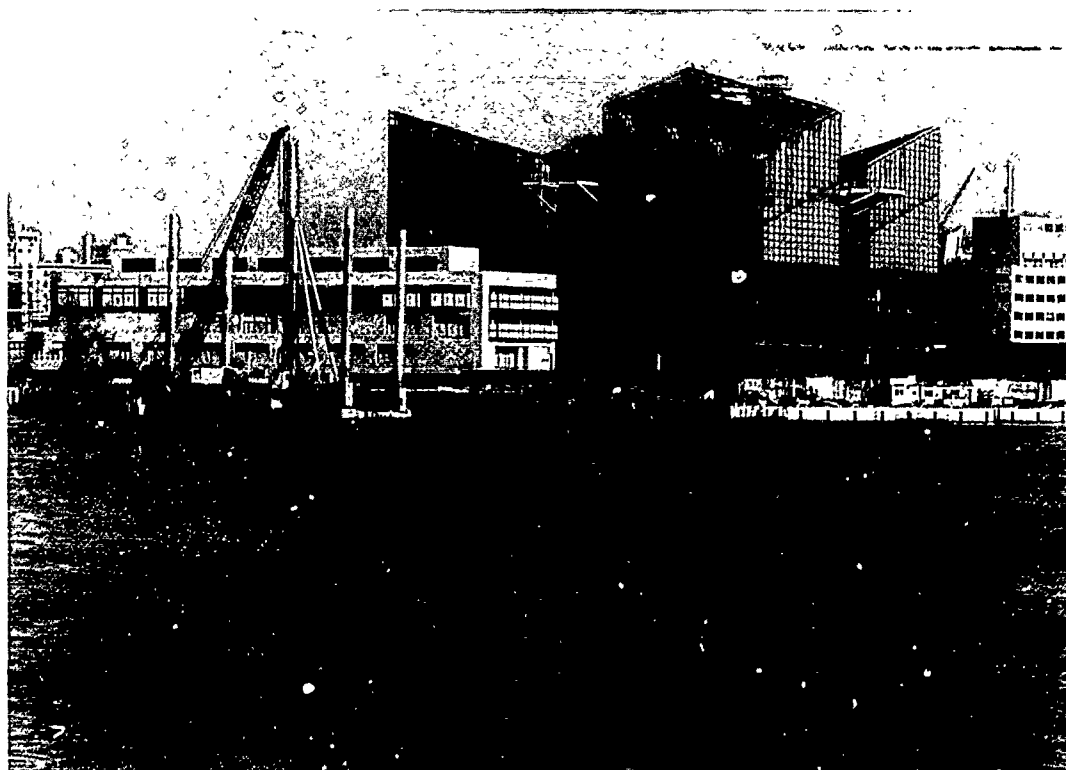
# SCIENTIFIC INFORMATION BULLETIN



1

DEPARTMENT OF THE NAVY OFFICE OF NAVAL RESEARCH FAR EAST  
DEPARTMENT OF THE AIR FORCE OFFICE OF SCIENTIFIC RESEARCH FAR EAST  
UNITED STATES ARMY RESEARCH OFFICE FAR EAST

DTIC  
ELECTE  
OCT 29 1991  
S B D



91-14115



APPROVED FOR PUBLIC RELEASE. DISTRIBUTION UNLIMITED

NAVSO P-3580

91 10 25 024

# REPORT DOCUMENTATION PAGE

Form Approved  
OMB No. 0704-0188

Public reporting burden for this collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden, to Washington Headquarters Services, Directorate for Information Operations and Reports, 1215 Jefferson Davis Highway, Suite 1204, Arlington, VA 22202-4302, and to the Office of Management and Budget, Paperwork Reduction Project (0704-0188), Washington, DC 20503.

1. AGENCY USE ONLY (Leave blank)		2. REPORT DATE Jul-Sep 1990		3. REPORT TYPE AND DATES COVERED	
4. TITLE AND SUBTITLE  ONR FAR EAST SCIENTIFIC INFORMATION BULLETIN				5. FUNDING NUMBERS	
6. AUTHOR(S)  Glenn W. White, Administrator; Sandy Kawano, Editor					
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)  ONR/AFOSR/ARO Liaison Office, Far East APO San Francisco 96503-0007				8. PERFORMING ORGANIZATION REPORT NUMBER  ONRFE Vol 15, No. 3	
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)				10. SPONSORING/MONITORING AGENCY REPORT NUMBER	
11. SUPPLEMENTARY NOTES  ISSN: 0271-7077					
12a. DISTRIBUTION/AVAILABILITY STATEMENT  APPROVED FOR PUBLIC RELEASE; DISTRIBUTION UNLIMITED.				12b. DISTRIBUTION CODE	
13. ABSTRACT (Maximum 200 words)  This is a quarterly publication presenting articles covering recent developments in Far Eastern (particularly Japanese) scientific research. It is hoped that these reports (which do not constitute part of the scientific literature) will prove to be of value to scientists by providing items of interest well in advance of the usual scientific publications. The articles are written primarily by members of the staff of ONR Far East, the Air Force Office of Scientific Research, and the Army Research Office, with certain reports also being contributed by visiting stateside scientists. Occasionally, a regional scientist will be invited to submit an article covering his own work, considered to be of special interest. This publication is approved for official dissemination of technical and scientific information of interest to the Defense research community and the scientific community at large. It is available free of charge to approved members of the DOD scientific community. Send written request describing DOD affiliation to: Director, Office of Naval Research, Liaison Office Far East, APO San Francisco 96503-0007.					
14. SUBJECT TERMS Supercomputers, Nanocomposites, Magnetostriction Parallel processors, Superhard materials, Thin films Fine ceramics, Magneto-optics, Amorphous films				15. NUMBER OF PAGES 160	
				16. PRICE CODE	
17. SECURITY CLASSIFICATION OF REPORT Unclassified	18. SECURITY CLASSIFICATION OF THIS PAGE Unclassified	19. SECURITY CLASSIFICATION OF ABSTRACT Unclassified		20. LIMITATION OF ABSTRACT	

# CONTENTS

	Page
Scientific Information Briefs .....	1
Magneto-Optical Materials: Translations from the Japanese .....	9
Earl Callen	
<i>These are summaries of reports to the Ministry of Education on research on magneto-optics aimed toward recording media and optical waveguide devices.</i>	
The ERATO Program .....	27
Aharon Gibor	
<i>The ERATO program was created to foster research in basic sciences toward development of advanced future technologies.</i>	
Second International Workshop on Software Quality Improvement: Summary and Assessment .....	31
David K. Kahaner	
<i>The major conclusions drawn from this conference are that some Japanese companies are better at managing the software development process than comparable U.S. companies and that more interaction is needed between numerical and nonnumerical software developers.</i>	
French-Japanese Seminar on Composite Materials .....	39
Michael J. Koczak	
<i>This seminar provided a unique opportunity to compare the materials development of two world-class composite research groups.</i>	
First International Conference on Supercomputing in Nuclear Applications .....	57
David K. Kahaner	
<i>This paper summarizes the significant presentations and vendor exhibits associated with Japanese software and hardware.</i>	
Performance of Japanese Supercomputers vis-a-vis Cray Computers .....	65
Hideo Yoshihara	
<i>This article reviews the performance of Japanese supercomputers.</i>	



Availability Codes	
Dist	Avail and/or Special
A-1	

	Page
Reactive Polymer Processing .....	75
J. Thomas Lindt	
<i>Reactive processing is expected to play an important role in the development of new advanced composite materials in Japan and in the ongoing efforts to continuously improve the performance of existing polymers through chemical modifications.</i>	
Century Research Corporation (CRC), Tokyo .....	83
David F. Kahaner	
<i>This report illustrates the breadth of applications and research areas in which this "service bureau" type organization is involved.</i>	
Research on Various Electronic Thin Films in Japan .....	89
Robert F. Davis	
<i>This article describes research on thin films at Nagoya and Kyoto Universities.</i>	
The Sixth International Symposium on Passivity .....	95
Clive R. Clayton	
<i>Recent research efforts on passivation of metals, including passive film characteristics, influence of the electric field, passive film breakdown, and new advances in passive film research, are described.</i>	
Molecular Recognition in Japan .....	101
Cynthia J. Burrows	
<i>Molecular recognition is a strong area of research interest in both universities and government institutes in Japan. This article gives a few highlights of organic and inorganic chemical aspects of this area in Japan.</i>	
Advanced Scientific Computing in Japan .....	109
Edward F. Hayes	
<i>This article focuses on the current status of advanced scientific and engineering computing in Japan.</i>	



	Page
Chemical Research Institutes in Taiwan ..... Cynthia J. Burrows	129
<p><i>With the recent boom in the Taiwanese economy, the Government is investing more money in scientific research and technology. This article describes some of the chemical research institutes in Taiwan.</i></p>	
Marine Biology in Okinawa ..... Aharon Gibor	135
<p><i>This article describes the marine biological research being conducted at three Okinawan research facilities.</i></p>	
The Stabilization Step in the Fabrication of Pitch-Based Carbon Fiber ..... Sin-Shong Lin	141
<p><i>The chemical and structural changes associated with stabilization are reviewed and the parameters affecting this process are examined.</i></p>	
Process Diagnostics on Plasma Chemical Vapor Deposition of Hydrogenated Amorphous Silicon and Related Materials ..... Nobuhiro Hata	155
<p><i>This paper reviews Japanese activities in process diagnostics by laser spectroscopy on plasma CVD of hydrogenated amorphous silicon and related materials and discusses the future scope of process diagnostics as an important part of materials science.</i></p>	

---

Cover: All over Japan, cities with the resources and the vision--Tokyo, Yokohama, Osaka, Kobe, Fukuoka--are making plans to revitalize their waterfronts. These cities are holding international architectural competitions and asking major companies to lend their support, and thus are providing a rallying point for a new Japanese interest in urban design. Osaka is the first city to show results. On 20 July, Osaka will open to the public Tempozan Harbor Village, a ¥21.5B bid to establish the City of Osaka as the leader among Japanese cities in urban water edge planning for the delight of its citizens. The photograph was taken by Mr. Yoshiharu Matsumura and is reprinted with permission from the Osaka Waterfront Development Co., Ltd.

---

---

# SIBRIE<sub>Fs</sub>

## Scientific Information Briefs

---

### MATHEMATICAL MODELS OF PHYSICAL PROCESSES

A Visit to Professor Masayasu Mimura's Laboratory at Hiroshima University

Professor Masayasu Mimura has a vision that mathematical scientists should be working together with physical scientists and computer scientists to study real problems. He has several small groups of the first two kinds of people working on problems related to physics and biology. In the lecture I gave on ordinary differential equations, I mentioned the "chemical oscillator" or Belousov system, and Mimura was quick to point out that they have been studying that too, and in fact at a deeper level. This problem concerns the periodic fluctuations of certain chemical solutions. This in itself is interesting and the aspect that I have been modelling. But Mimura has been considering the spatial as well as temporal description of this phenomenon, in my work I have assumed that the solution is uniform in space. Mimura first showed me a videotape of a careful experiment associated with this. In a laboratory a beaker of solution is "tweaked" by slow insertion of a drop of appropriate reactant. Waves begin to radiate from the source, taking on fascinating shapes, crescents, etc.. He then ran another tape displaying the results of a computer model of this reaction. The agreement was fairly good, especially considering that the mesh was only 100x100. Another tape showed the results of modelling crystal structure, perhaps ice. This is known to exhibit chaotic and intricate patterns, many of these were also visible in the computer output.

Mimura's laboratory is well equipped. Plots of the solution at each time step are generated and stored on a laser disk. This is then used off line to make video tapes. Most of the programming is done by graduate students.

Mimura has been concentrating on developing good mathematical models of the physical processes he is studying. For this he collaborates heavily with physicists and chemists, who are often coauthors of research papers. His analysis is careful and thorough, with a strong emphasis on understanding and mathematical rigor. A colleague of Mimura's, Professor Yasumasa Nishiura, showed me some of his papers on reaction diffusion systems published in U.S. SIAM mathematical journals. They showed similar care and mathematical sophistication. Thus far Mimura's computational projects have been limited mostly to two-dimensional spatial models, but he has promised to have some three-dimensional results for a meeting this summer. This will be a substantial undertaking. Thus far, the computations have been performed on a one-processor Alliant that is in his department. I doubt if this will have the horsepower to crank out three-dimensional results on a fine enough mesh without using a tremendous amount of time. Via a terminal, researchers at the university can get to a Cray or other large computer at the University of Tokyo, but currently they have no real experts in its use as part of their team. Further, it is not clear how they will generate the graphics that they want except in their own laboratory. On the other hand, the Alliant is free and close at hand, and it can be run for days at a time if necessary.

Mimura asked me what kind of physical problems I was interested in

building software for, and he was not very familiar with general purpose software. I asked him if he had ever heard of IMSL, an extremely well known commercial software library probably available at Hiroshima's central computer facility, but he had not. Although the equations that Mimura has been studying are well tied to the physical problem, their numerical solution techniques could be improved. Solving time dependent partial differential equations in two space dimensions can be done "from the ground up" numerically, but in three dimensions it is best to use the wealth of numerical research that already exists. The linear systems that arise are special and correspondingly there are special techniques for dealing with them. There are experts in these matters in both the United States and Japan. I did not meet any in Mimura's group, although they may have been absent during my visit. Mimura is aware of these needs and will likely focus on them more in the future.

I was very impressed with the problems that are being studied here, the analysis being performed, and the way results are visualized via video tape. The finished product is professional looking, with color, sound, and titles. Mimura has been to the United States several times, most recently to the Math Department at the University of Arizona, and he speaks good English. He has a solid idea of the work that is going on in related departments. One of his recent Ph.D. graduates, Xu-Yan Chen, will be going to Georgia Tech this spring for a 2-year postdoctoral program. He will certainly come back full of knowledge about both visualization and chaotic physical systems. Mimura's work is well regarded both in Japan and in the United States and his Japanese colleagues think

highly of his idea of larger groups of researchers. Judging from the facilities and equipment available he has a reasonable budget with which to work. Because the group is now getting into three-dimensional models, the project would benefit from someone who is specifically interested in computing, that is, algorithms, numerical techniques, parallel processing, and software. It would also benefit from the input of a computational physicist who has experience in developing large scale codes for solving fluid problems.—*David K. Kahaner, ONRFE*

\* \* \* \* \*

## EHIME UNIVERSITY

Ehime University is in Matsuyama, which is 1 hour by fast ferry from Hiroshima, on the island of Shikoku. The math and computer science departments are in different buildings, but the faculty who are interested in scientific computing are well aware of each other's activities. Professor Tetsuro Yamamoto is in the Department of Mathematics. His primary research activities are concerned with convergence questions related to iterative algorithms such as Newton's method when applied to nonlinear equations. Yamamoto speaks excellent English and most of his papers are published in English language journals. He is well known outside Japan and has a long and distinguished research record.

Professor Takashi Kitagawa is new on the faculty (Computer Science Department). His thesis, from Nagoya University in 1983, was on regularization techniques for ill posed problems. Solving such problems have occupied scientists for years, they occur in all branches of science where the "input" is to be determined by observation of some "output" that has been smoothed, averaged, or smeared. Typical applications are inverse transforms, computerized tomography, reconstruction of turbulent or degraded

images, inverse gravimetry, etc. These problems are difficult because the numerical solution is usually very sensitive to noise; often a small change in the solution algorithm can dramatically alter the "solution." A typical approach to solving ill posed problems is via "regularization", one forces the computed solution to be "smooth" even if it means giving up some of the solution detail (accuracy). Balancing accuracy and smoothness is tricky and Kitagawa's work has been aimed at minimizing the solution error while maximizing its smoothness. His thesis and papers are all in English. Since writing his thesis Kitagawa has been busy extending it and trying the method on realistic problems. It is too early to tell if his research will have a major impact on this field, but many other extremely clever people have also been working on these problems.

Professor M. Noda has been working on an interactive differential equation solver similar to the work I've been doing but with an eye to developing symbolic rather than numerical solutions. He calls this area "hybrid computation," i.e., the use of symbolic computation in a numerical environment. One interesting application has been to the approximate solution of algebraic equations, a problem that can be very ill conditioned if treated from a totally numerical perspective. Noda has also been interested in "interfaces" for numeric computation and has attended meetings on this topic at Purdue University. Most numerically oriented scientists accept that engineering and scientific computing problems can often be posed and solved without resorting to traditional programming techniques. There are many examples of such systems, but there has been precious little work in the general development of tools to make the "next" application easier to write. Noda is also interested in many other aspects of computing, he is the author of the most popular Japanese word processor, used on virtually every PC.

Professor Kaname Amano is another member of the Department of Applied Mathematics. He recently joined the faculty at Ehime after working in the computing center at Hokkaido University. He heard Kitagawa lecture on fundamental solutions of the Dirichlet problem (this is sometimes called the charge simulation method in electrical engineering) and began to wonder if it could be applied to problems in conformal mapping. The conformal mapping problem is one of the most famous in applied mathematics, it relates to a theorem stating that it is possible to map most two-dimensional regions onto a circle in a way that preserves local orthogonal axes. Solving this problem is equivalent to solving Laplace's equation in the plane, i.e., to solving the problem of electrostatic potential. It has many other applications as well and numerical techniques have been proposed since the early days of computers by Zarantanello, Birkhoff, and others. There is still an active research group centered at ETH in Zurich under Gutknecht working in this area. Amano has a method that is a clever application of fundamental solution techniques and generates either the map into the circle or its inverse, from the circle to a given region. He calls the method "bidirectional." (This work was given an award last year by the Information Processing Society of Japan.) Unfortunately, his papers are all in Japanese, and consequently the method has not received the attention that it deserves. This method still requires quite a lot of testing to prove itself and there are obvious enhancements that suggest themselves, but he has already run many examples in which it compares very favorably to published results. He has implemented the method for computing mappings of both interior and exterior regions, simply and multiply connected regions, and computing the transfinite diameter of a given region. I strongly urge all those interested to contact Amano. Some of Amano's other work

relates to scientific databases. This is an important topic but I am not able to judge the quality of this research or evaluate it relative to other similar work.--David K. Kahaner, *ONRFE*

\*\*\*\*\*

## QUANTUM MAGNETO FLUX LOGIC (QMFL) PROJECT

This project is supported by the ERATO program. For a description of the program, see the article by Aharon Gibor later in this issue. The QMFL project (known as the Goto project after its proposer) has two more years to run. The essence of QMFL is to design a computer using flux quanta as a bit of information rather than voltage. The project is in two distinct parts: (1) a hardware or device portion that attempts to perform the research necessary to develop Josephson hardware and (2) a software portion that attempts to develop a computer architecture to take advantage of the hardware. The first part is primarily research in superconductivity, the second in computer organization and software. My interest is in the software issues, and for that I visited the software group and spent the day with Mr. Paul Spee, who is a researcher on the project. Spee claims that they have designed a new computer architecture specifically for these devices. He also claims that aspects of this design also represent improvements in conventional silicon computer design. They are having a silicon version built and will have it running in March 1990. They have already written Fortran and C compilers for the new machine, and I lent them a tape containing a great many Fortran subroutines to test the compiler. I am planning to revisit Spee to see how things are progressing and to get more details. At that point I hope to be able to make an assessment of the project's progress.--David K. Kahaner, *ONRFE*

\*\*\*\*\*

## HITACHI CENTRAL RESEARCH LABORATORY

This laboratory is about 45 minutes from central Tokyo. It has about 1,300 employees. I visited Dr. Chisato Konno, who has been working on the DEQSOL project for almost 10 years. DEQSOL is a software package that allows scientists to set up and solve complicated nonlinear, time dependent partial differential equations (real engineering problems) using a natural mathematical like notation. The DEQSOL "language" is converted to Fortran. The language translator (written in Pascal) is specially tuned to generate code that will vectorize easily. This project has a U.S. counterpart in the ELLP-CK project centered at Purdue University, initiated by Professor John Rice. Very little about DEQSOL is known outside of Japan because most of the papers are in Japanese. DEQSOL only runs on Hitachi computers. A more comprehensive article on DEQSOL will be published in a future issue.--David K. Kahaner, *ONRFE*

\*\*\*\*\*

## NATIONAL RESEARCH LABORATORY OF METROLOGY

This laboratory is one of seven in Tsukuba run by the Ministry of International Trade and Industry (MITI). My primary contact was Dr. Walter Liggett, another colleague from the National Institute of Standards and Technology (NIST), who is there on a 1-year guest researcher program. He is working in the Information Mathematics Section, under Dr. Masayoshi Koike, who also spent a year in the Statistics Division at NIST. This group works primarily on developing methods for increasing the quality and decreasing the variability of manufactured assembly line products, and they showed me a videotape of their

work applied to a plastic molding process. This laboratory was discussed in a recent *Scientific Information Bulletin* article [K.O. Bowman, T.H. Hopp, R.N. Kacker, and R.J. Lundegard, "Statistical quality control technology in Japan," 15(1), 57-73 (1990)], so I was mostly interested in learning how they make use of computers and what kind of software they use. Koike's group owns several Sun workstations and a number of Japanese PCs. The Suns are used to run canned application programs, primarily engineering software such as PATRAN. Any programming, as such, is done in Basic, on the PCs. Basic is the language of choice here because it has built-in access to graphics, something that is, unfortunately, not available in Fortran. On the other hand, Basic is not standardized, and Liggett has been forced to learn an entirely new version of Basic in order to get any programs to run.

The main computer center is called RIPS, Research Information Processing Section, and is run by Dr. Masafumi Kito. We saw the Cray XMP 2/16, which was installed in 1987. This runs UNICOS, the Cray version of Unix, but it is not accessible in interactive mode, only batch. They also have an IBM 3090, but this is used only to run smaller jobs and to front end the Cray. There are no plans to add any vector facility capabilities to the 3090. There is also a large FACOM M780 mainframe that is used for nonscientific computation. The computer center supports all the MITI laboratories, so use is dependent on interest and application, in fact, Koike explained that he has never used the Cray. Kito gave me a long list of software that is supported, again mostly engineering analysis packages such as ANSYS, FLOW-3D, PATRAN, SPICE, etc., and explained that GAUSSIAN is one of the most heavily used. He also explained that one of the reasons they chose the Cray rather than a Japanese supercomputer was that very few of the application packages they were

interested in ran on the Japanese machines. I asked about consulting assistance for users and Kito explained that for systems help they rely on vendor-provided system analysts and that for scientific assistance they rely on the support provided by the package vendors. They do not have any scientific support group nor any group engaged in research related to such activities. There is a very large and modern "terminal" area containing a tremendous variety of small computers, workstations, graphical devices, digitizers, etc. All of them are interfaced to one of the three networks that are currently in use. Of course, to take advantage of the specialized equipment, users must be at Tsukuba or have an assistant there. It is not clear how scientists at more remote MITI laboratories feel about that. Currently electronic mail is not universally available but will be brought up during the spring to the remaining MITI laboratories.--David K. Kahaner, ONRFE

\*\*\*\*\*

## MEETING ON PARALLEL PROCESSING

A 1-day meeting on parallel processing, "Parallel Processing in Scientific Computation," was held at Keio University. The papers presented were:

1. "Fuzzy Control for PDE Systems and Parallel Processing," H. Imai and I. Natori (Tsukuba Univ.) & H. Kawaharada (Chiba Univ.).
2. "Fast Fourier Transforms Methods for Partial Differential Equations," K. Oda and T. Torii (Nagoya Univ.).
3. "Complexity of Parallel Matrix Computations," R. Rai (Hirosaki Univ.).
4. "Numerical Solution of Ordinary Differential Equations Using a Parallel Algorithm," A. Goto and T. Mitsui (Nagoya Univ.).

5. "Dialogonalization of Large Scale Matrix by Jennings' Method," U. Nagashima (Okazaki National Res. Inst.).

6. "Parallel Processing of Chemical Program ATOMCI," A. Hasegawa and N. Motoshiro (Japan IBM) & K. Ohtsuki and M. Sekiya (Hokkaido Univ.).

7. "Error Behavior of Finite Element Numerical Solution with Repeating Method Applied to 3D Potential Problems," S. Kurata and T. Ushijima (Univ. of Electro Communications).

8. "Operation Processing Mechanism of the LAMAX-S Language for Matrix Operations on a Supercomputer," T. Uchida and K. Noma (Aoyama Gakuin Univ.); N. Yatsumaki, M. Inoue, and K. Tanaka (Systems Plan Lab); S. Hongo (Senshu Univ.).

9. "A Vectorizable Algorithm for the PCG Method for the Solution of Large Systems of Banded Anti Symmetric Linear Equations," K. Taguchi (Fuji Sogo Kenkyujo Inc.).

10. "Theory of ILU Decomposition Ordering and Applications of Multiprocessors," S. Dohi (A NEC C&C Info Lab) & A. Lichnewsky (INRIA).

11. "Japanese TeX and Matrix Computation," T. Nodera (Keio Univ.).

The above presentations were all in Japanese, so it was difficult to get more than a general sense of their content. But it was clear that Japanese researchers do not yet have much access to really new parallel computers to practice with, such as hypercubes, transputers, etc., and even multiprocessor supercomputers are not readily available. There may be many experimental computers being built, but the algorithmic research, i.e., numerical and applications software, is focused on using supercomputers such as Cray,

Hitachi, etc. to solve engineering problems.--David K. Kahaner, ONRFE

\*\*\*\*\*

## NEC's NEW SUPER-COMPUTER, THE SX-3

At a recent visit to the NEC factory, the SX-3, NEC's new top-of-the-line computer, was presented. In 1989 NEC had sales of around \$25B in 145 countries and currently supports a workforce of 125,000 people. The corporate logo is now C&C, for Computers and Communications, and I believe that NEC really means business about integrating these technologies. The SX-3 has been described several times before, including once by its principal architect Tadashi Watanabe at Supercomputing '89 last November in Reno. Watanabe was introduced as the "Seymour Cray of Japan," and he again summarized the SX-3's main features. Here I will briefly mention a few of the more important aspects of this computer.

The SX-3 is a followup to the NEC SX-2. One SX-2 is in Houston at the Houston Area Research Center (HARC); another is in the Netherlands. Several others are in Japan, for example, at Mazda and Sumitomo Metal Industries. The new SX-3 can be purchased with four processors. Each processor can have four independent functional arithmetic units, two "adds" and two "multiplies." The machine has a very fast cycle time of 2.9 ns. If all the arithmetic units are kept busy, the SX-3 has a maximum peak performance of 22 GFLOPS. For comparison, peak performance of a Cray YMP-8 or Hitachi S-820/80 is around 3 GFLOPS. But by now we all appreciate that peak performance is not a good measure of an application's performance except in very special situations. Other factors are also important, such as the rate at which data can be pumped between memory and the arithmetic units and the length of time necessary to access a

memory element. For the SX-3, as with every other supercomputer, it is very unlikely that peak performance will be achieved in practical applications because there are simply not enough pipes from memory to the arithmetic registers. Further, the time from an issue of a load to the appearance of a value in the register (latency) is 70 cycles, very long, and this is certainly going to degrade performance on problems with short vectors. A realistic expectation for performance on real problems is in the range of 4 to 7 GFLOPS. Hideo Yoshihara, a former colleague in this office, who has also been studying and benchmarking computational fluid dynamics codes on Japanese supercomputers, also estimates performance for a specific code of interest to him at around 7 GFLOPS. The British Meteorological Service has estimated performance on one of its codes at between 3 and 4 GFLOPS. At the present these are all educated guesses and assume that all four processors can be used--a sophisticated programming task at which Cray has more experience. But all the estimates are greater than the performance for a Cray YMP and as good or better than a Cray 3, although the latter is much less further along in its development and performance figures are even more speculative. Thus, with 256-MB control processor memory (CPM), 2-GB main memory, and 16-GB extended memory, the SX-3 looks like a winner if NEC can deliver the applications software.

The SX-3 clearly takes advantage of NEC's long experience in chip technology. NEC's philosophy is to reduce circuit distance and wiring delay. To do this sophisticated insulation techniques as well as a great deal of automated chip assembly have been used, each pack of chips has about 12,000 pins and is quite fragile. The chips are cooled by chilled pure water. Each package dissipates about 3 kW of heat. We had an opportunity to visit the factory floor where three SX-3s are being worked on. One is up and

running for software development and testing. It has two processors, but its cabinet setup allows for a complete four-processor configuration. Benchmarking has begun this spring with programs from potential customers and will continue through the end of the year; apparently NEC has had a great many requests for benchmarking information but now needs all the machine time it can get for its own system work. Two other machines were on the assembly floor; one is going to Houston to replace the SX-2, but NEC would not say where the second is to be shipped. The SX-3 is a large machine and its length accounts for a portion of the long latency time. NEC is also developing a 10-MB/s disk drive that will be available with the SX-3, as well as an automated archival store based on tape cartridges. While the SX-3 has dominated the spotlight, these peripheral devices are important as well. Among the others on the tour were Dr. Bill Buzbee (National Center for Atmospheric Research), Dr. Jack Dongarra (Univ. of Tennessee), Dr. John Levesque (Pacific Sierra Research), and Mr. Peter Zidek (Zidek Inc). We were all impressed with the engineering and manufacturing know-how that has gone into this product.

Watanabe also made rather confident predictions that by 1995 NEC would have the one-processor peak performance in the range of 10 to 20 GFLOPS, largely through a reduction of cycle time to about 1 ns, and multiprocessor performance of around 100 GFLOPS, with 8 to 16 processors. He also stressed that NEC feels that there are still performance gains to be wrung out of silicon.

The SX-3 will run Super UX, which is based on System V Unix version 3.1, but has been enhanced to take advantage of the parallelism and other special hardware such as fast I/O. NEC is committed to development of an assortment of software tools to make programmers' jobs easier. Drs. Katayama and Ikumi, speaking about software, emphasized that three main points guide the software

development program: performance, ease of use, and portability. Ikumi gave a few performance figures for  $c_i = a_i + b_i$ . For an SX-3/14 (one processor with four functional units), 5.5 GFLOPS maximum,  $n_{1/2}$ , vector length at which half the maximum performance is achieved, between 80 and 160, and vector-scalar crossover about 7 (the vector length below which it is faster to use scalar code). The main difficulty I see getting near maximum performance from the SX-3 will be that with eight arithmetic multiply units, keeping all eight busy with long enough vectors will require that the original problem have arrays that may be longer than are desired for other reasons--longer vectors imply more memory, more iterations for convergence, etc.

One important piece of software that NEC has been developing is SXview, for visual simulation. While we did not have an opportunity to learn many of its details, SXview will have several important features such as an interactive command processor so that figures and scientific graphs can be drawn with simple commands; 2D, 3D, and rendering via simple commands, and enlargement, shrinkage, and rotation of figures with local viewing options. SXview also supports recording of each graphics frame on videocassette tape. The software is claimed to be for general use but mainly to be applied to structural analysis, fluid dynamics, and molecular science.

NEC is developing various specialized software libraries and will support commercial libraries such as IMSL and engineering analysis software. A vector analyzer to determine how efficiently a program is using the vector hardware and another to evaluate the effectiveness of any parallelizing are both under development, as is an enhanced debugger and automatic parallelizer. Automatic vectorization, in-line expansion of vectorizing calls, loop unrolling, etc. are also being worked on. Multitasking both at the macro level via subroutine calls

and at the micro level such as Parallel DO is also planned. At the present moment, though, only the automatic vectorizer is actually working. Release 1.1 of the Fortran compiler is expected in December 1990 and release 2.1 by December 1991. The latter will allow parallel processing and provide automatic file archiving. Fortran will not only support standard Fortran 77 but, of course, vectorizing and parallelizing extensions, both those that are unique to NEC and some that are used by Cray, such as Pointer and Buffer. In addition, a source code converter will automatically convert either Cray or CDC Fortran to the SX equivalent. Also Fortran 8X work is being followed and NEC plans to support this within 18 months after some agreement on standardization is finally worked out. All the usual network interfaces will be supported as well as TCP/IP. It is clear that NEC realizes that the SX-3 will ultimately be determined by its software base. This is an area in which Cray has a tremendous lead, so they have a lot of work yet to do. —David K. Kahaner, ONRFE

\*\*\*\*\*

## COMMERCIALIZATION OF PAX BY ANRITSU

In an earlier *Scientific Information Bulletin* article ["The PAX computer and QCDPAX: History, status, and evaluation," 15(2), 57-65 (1990)], I mentioned that the MIMD computer PAX, developed at the University of Tsukuba by Professor Hoshino and colleagues, was being considered by the Anritsu Corporation for commercialization. On 1 April 1990, Anritsu announced that a 16-processor version of this machine is available. Anritsu already markets a scientific workstation, called DSV6440A, which has a 30-MFLOP peak performance. This is a Unix machine built around the MC68030 chip. An attached vector processor speeds up floating point computations. The standard DSV6440A has

a 320-MB disk and 123-MB cartridge tape unit. It comes with a 21-inch color monitor with a resolution of 1280x1024 dots. It can be networked via the usual networking interfaces.

The vector processor is built into one triple height VME board. Users write programs in CorFortran that run on the 68030, called "main programs," and other programs called "calculation programs" to describe algorithms to be performed on the vector processor. Programs for the latter are written in "FAUST-C." The calculation program is loaded into the vector processor memory by the main program. Data for calculation programs can come from vector registers (2 MB) or from main memory. The vector processor has a maximum claimed performance of 30 MFLOPS and scalar performance of 1.7 MFLOPS in 32-bit single precision. In addition to arithmetic operations, the vector processor has built-in trig, exponential, square root, and logarithm functions.

Only one vector processor board is mounted in the DSV6440A, but a parallel computer can be configured by connecting to a separate device in which a number of these boards are mounted. The board itself has an independent processing unit and a four-channel interface for connecting other 32-bit data channels. A parallel computer can be configured by connecting via this route to a neighboring processing unit with data switching. If 16 such boards are connected the peak performance is thus 16\*30 or 480 MFLOPS. This additional collection of 16 boards has now been packaged by Anritsu. The ensemble unit is named DSV6450.

Below is a simple example of programming in FAUST-C for the core portion of an SOR (Successive Over Relaxation) calculation. It is very close to the program that I displayed in describing QCDPAX and illustrates the vector instructions.

```
for (iter=0, iter<ITERMAX, iter++){
  for (rb=0, rb<2, rb++){
```

```
    getorg();
    vfor (k=orgnw; k<MSEE; k+=2){
      u[k]=omg4*(u[k-1]+u[k+1]+u[k-M12]+
        u[k+M12]+q[k])+omg1*u[k];
    } with;
    vfor (m1=orgc; m1<M1; m1+=2){
      u[m1+1]=ZERO;
      u[m1+MSWS]=ZERO;
    } with;
    vfor (m2=orgc; m2<M2; m2+=2){
      u[M12*m2+M12]=ZERO;
      u[M12*m2+MNEE]=ZERO;
    } with;
  }
}
```

This is one of the first entirely Japanese parallel processors. It has all the capabilities that I reported on in Hoshino's PAX computer plus, now, the backing of a substantial company. Anritsu has arranged for demonstrations of the machine in several Japanese cities. However, Anritsu is not well known as an advanced computer manufacturer, and there is speculation here that the responsibilities for building this machine were subcontracted out. At this time I have no pricing information. Anritsu can be reached at 10-27, Minamiazabu 5-chome, Minato-ku, Tokyo 106, Japan; phone: 81-3-446-1111; fax: 81-3-442-0235. —David K. Kahaner, ONRFE

\*\*\*\*\*

## "FINE CERAMICS—CHALLENGING THE UNKNOWN"

This was the theme of the Third International Forum on Fine Ceramics held in Nagoya on 12-14 March 1990. More than 150 scientists from around the world gathered to discuss fine ceramics from a global point of view as an important class of materials of the 21st century.

Professor Hiroshige Suzuki of Tokyo University reviewed the status of fine ceramics in Japan. He stated that Japanese research on structural ceramics started

later than in the United Kingdom, the United States, or West Germany. However, Japan has succeeded in the industrialization of some automobile ceramic parts. More than one million rotors for turbochargers have been sold, and quality control is good. Under a new initiative, large-scale efforts to industrialize ceramic gas turbine engines have started. Active studies include preparation of raw materials, homogeneous shaping, sintering with control microstructures, highly efficient machining, oxidation resistance, coatings, improvement of fracture toughness, and proof testing. It is expected that within the next two years or so a prototype gas turbine engine will be developed. The objectives of this program are to produce (1) silicon nitride for rotors with a fracture strength higher than 600 MPa at 1,250 °C and with a delayed (1,000-h) fracture strength of 250 MPa at 1,250 °C and (2) silicon carbide with a delayed (1,000-h) fracture strength of 400 MPa at 1,400 °C.

Some significant advances were reported in several areas of fine ceramics.

**Ceramic Powder Processing.** The past decade has seen great progress in powder synthesis. Dr. G. Onada of IBM, in his paper titled "Ceramic Powder Processing--Challenging the Unknown," reviewed both the traditional technology and recent developments in the area of fine monodispersed powders. He stated that there was considerable room for improvement in the traditional forming processes such as binder removal from injection-molded parts. He also believes that to challenge the unknown in ceramic processes it will be necessary to depart from traditional methods. New methods such as solvent-based binders and sol-gel type solutions are being developed. As the trend is toward finer particles, new forming methods need to be developed to take advantage of the colloidal nature of the powders, now a problem in most existing methods. Electrophoretic deposition of particles for forming beta alumina

tubes and porcelain coatings, coatings of high  $T_c$  superconducting oxides on silver metal wires, and alternating or graded composition in coatings are being studied. Other methods of forming from colloidal suspensions include "centrifuge shape forming" and colloidal filtration. In the coming years fine particle processing may involve the use of ultrasonic, magnetic, electrostatic, and optical (including lasers) energy sources, gases that permeate the body, and catalyst-enhanced reactions. At the same time advances in sintering and other high temperature reactions must also occur.

**Functionally Gradient Materials.** Functionally gradient materials (FGMs) are novel engineered composites designed to optimize material properties for use in real environments by spacial control of composition and microstructure. In Japan research in this area was prompted by the "Space Plane Project," which was initiated in 1987. It was necessary to develop high temperature materials to protect the spacecraft from thermal damage during reentry. Professor Koizumi of Ryukoku University described one such material, the  $TiB_2$ -Cu system. In this material the  $TiB_2$ -Cu ratio decreases from the exterior to the interior of the surface layer placed on the exterior surface of the spacecraft. The material has been tested successfully in Government laboratories. Similar concepts have been applied to develop new bio-optical materials and superior actuators and tools. Professor Ryuzo Watanabe of Tohoku University summarized the work of a number of companies involved in FGM research. Systems discussed included  $ZrO_2$ -W,  $Si_3N_4$ /steel, and PSZ/molybdenum or steel. Fabrication processes mentioned included direct high temperature bonding, hot isostatic pressing (HIPing) of layers with different compositions, and sintering. For example, PSZ304SS was made by first preparing a suspension of the two powders in alcohol and spraying the suspension on a heated surface. Sheets with different compositions were thus prepared.

They were stacked in a sequence designed to give graded properties from one side to the other. The stack was hot pressed under controlled conditions to achieve predetermined microstructure and finally HIPed.

A national program on FGM began in 1986 and is in its second phase. A symposium to discuss the progress in this field is scheduled to be held in Sendai in October 1990. The Science and Technology Agency of Japan has also initiated a program to develop composite materials capable of adapting to the environment through self-protection and self-restoration. These concepts have potential application in aerospace systems and medicine. Such novel processes have enabled scientists to challenge the realm of well-controlled heterogeneous ceramics, which until recently was relatively unknown.

**Nanocomposites.** There is a strong interest in both the United States and Japan in developing ceramics with high strength and high fracture toughness. The main emphasis in research and development efforts has been on incorporating short fibers and whiskers in the matrix; the results have been very encouraging. A newer concept that originated in the United States is to incorporate the second phase in the grains of the matrix as fine nano-sized particles or precipitates. Professor Koichi Nihara from Osaka University reported the results of his study on the preparation of both oxide and nonoxide based nanocomposites.  $Si_3N_4$ /SiC powders were made from a hexamethyl silazane ammonia-nitrogen system by chemical vapor deposition. The C/N ratio was controlled by changing the ammonia gas flow rate. Alumina, yttria or yttria alone was used as a sintering aid. In the final product silicon nitride appeared as elongated grains containing up to 10 percent silicon carbide particles. Such composites had a bend strength approaching 1,200 MPa and a fracture toughness two to three times that of the conventional composites.



---

*New Hybrid Metal Matrix Composites for Diesel Engine Pistons.* Japan so far leads in the application of ceramic fiber reinforced metal matrix composites (MMC) in automobile engines. Since 1982 aluminum-based MMC have been used in Toyota diesel engine pistons to improve the wear resistance of the top ring groove of the piston. The composite contains 4 to 8 vol % of aluminum oxide-silica (KAWOOL, SAIFIL, or ALSILON) short fibers as reinforcement in JIS ACSA-T7 aluminum alloy. The composite is manufactured by the squeeze casting process, in which the molten matrix is infiltrated under pressure into the preform of the reinforcement. Dr. Tetsuya Suganama, of the Technical Center, Toyota Motor Corp., reported a new metal matrix composite that is more wear resistant and can perform at relatively higher temperatures than the conventional composite material. It is a hybrid composite consisting of aluminum nitride intermetallic particulates (20 vol %) and ALSILON short fibers (7 vol %) dispersed in the aluminum alloy matrix. Aluminum alloy is pressure infiltrated into a preform of the ALSILON fibers mixed with 4 percent nickel powder. Aluminum nitride forms in situ by the interaction of nickel and aluminum.

*Superhard Materials.* There has been considerable activity in the design and fabrication of superhard materials in Japan. Professor Osumu Fukinaga of Tokyo University reviewed the P-T phase equilibria of diamond-graphite and hBN-cBN. He described some ongoing work in his laboratory on the preparation of polycrystalline or sintered cBN with high thermal conductivity at 5.5 GPa and 1,500 °C using 2.5 wt. % Mg-B-N as a catalyst. He also reported an extraordinary rapid rate of hBN to cBN phase transformation when a low catalyst content was used.--*Iqbal Ahmad, AROFE*

\* \* \* \* \*

---

---

# MAGNETO-OPTICAL MATERIALS: TRANSLATIONS FROM THE JAPANESE

---

Earl Callen

---

*These are summaries of reports to the Ministry of Education on research on magneto-optics aimed toward recording media and optical waveguide devices.*

---

## INTRODUCTION

We have about 700 pages on *Advanced Materials: Development and Properties of Magneto-Optical Materials*, Tokyo Monbusho Tokutei Kenkyu (research reports funded by the Ministry of Education (Monbusho), 1988 grants, under the Science Research in Special Projects). These reports are publicly available in Japanese. They were translated because they are deemed to illuminate Japanese programs and to contain some information that has not been circulated in English. For example, some reports describe incomplete, exploratory screening of new materials, and some describe research efforts that proved unfruitful and were not reported in the published professional literature or at international meetings but are nonetheless useful to know about. The ensemble of reports gives a picture of the scope and thrust of Ministry of Education-supported programs of research on magneto-optics at Japanese universities. The perhaps-twice-as-large industrial effort--at Hitachi, NEC, Fujitsu, NTT, Mitsubishi

Electric, Matsushita Electric, Matsushita Communications, Sony, Sanyo Electric, KDD, TDK, and others--is not represented here.

## SUMMARY AND COMMENTS ON REPORTS

### Electronic Structure and Magnetic Properties of Metallic Superlattice Multilayer Films

*Takeo Fujiwara, Dept. of Physical Engineering, University of Tokyo*

**Summary:** Band structure calculation of Mn/Al superlattice.

### Magnetic Anomaly of Transition Metal Microclusters

*Tsuyoshi Yamaguchi and Nobuhisa Fujima, Faculty of Engineering, Shizuoka University*

**Summary:** DV-X alpha-LCAO calculation of shell model and magic numbers for Ni clusters.

---

## Structure and Properties of Microclusters

*Shigeru Sugano, Institute for Solid State Physics,  
University of Tokyo*

**Summary:** Molecular dynamic computer simulation of small clusters of alkalis and of transition metals; temperature dependence of cluster moment.

## Magneto-Modulation Vacuum Ultraviolet Spectroscopy of Bismuth-Substituted Iron Garnet

*Akira Misu, Masaaki Kobayashi, and  
Katsuhiko Yamaguchi, Dept. of Physics, Tokyo  
Science University*

**Summary and Comments:** As the garnets absorb strongly in the vacuum ultraviolet, the researchers perform reflectivity measurements by means of the Cotton-Mouton effect using a synchrotron source. Reflectivity spectra are interpreted in terms of electron transfer transitions. The intent is to understand how Bi enhances the Faraday rotation of the garnets, since it is nonmagnetic.

## Magneto-Optical Effect of Rare Earth Iron Garnets and Rare Earth Iron Amorphous Alloys

*Tatsuro Tsushima, Kimishige Shinagawa,  
Toshiaki Shinagawa, Ken Tamanoi, and  
Junichiro Maedomari, Faculty of Science, Toho  
University*

**Summary and Comments:** Measurements of Faraday rotation and Cotton-Mouton effect by partially Co-substituted GdIG (with Ge to compensate). Transitions responsible for Faraday rotation are identified. Co increases the Faraday rotation. Cotton-Mouton optical delays are also rationalized.

Ce-substituted YIG single crystal films were grown on GGG (111). Ce, though present only in minute quantities, increases the Faraday rotation. Magnetization, Hall effect, and Kerr rotation were measured on amorphous Gd-Fe thin films. This is a ferrimagnetic random anisotropy (in the film plane) correlated spin glass with a compensation temperature (in an aligning field) and uniaxial anisotropy with easy axis perpendicular to the film plane. The measurements are explained on this model.

## Studies on Magneto-Optical Effects in Transition Metal Chalcogenides and Compositionally Modulated Multilayer Films

*Katsuaki Sato, Hiroyuki Kida, Yasutomo  
Aman, and Masakazu Hirai, Tokyo Univer-  
sity of Agriculture and Mechanics*

**Summary and Comments:** Measurements of reflection (0.2-25 eV), photoelectron, and magneto-optic spectra of single crystals of  $\text{Fe}_7\text{Se}_8$ ,  $\text{Co}_7\text{Se}_8$ ,  $\text{Cr}_3\text{Te}_4$ ,  $\text{Cr}_2\text{Te}_3$ , and  $\text{Cr}_2\text{Se}_3$ . Magnetic and optical properties of the NiAs-structured Fe and Co selenides are explained qualitatively by appeal to the band structure calculated for FeSe. In multilayer films of Co/Cu and Fe/Cu there is a promising peak in the Kerr rotation at light energies near the Cu absorption edge. This report explains the mechanism in terms of interband transitions and the virtual (i.e., effective) optical constant of the multilayer.

## Magneto-Optical Effects in Magnetic Fluids

*S. Chikazumi, H. Miyajima, S. Taketomi,  
N. Inaba, H. Takahashi, S. Ogawa, and  
M. Mizukami, Physics Dept., Keio University  
and Matsumoto Oil, Fat, and Pharmaceutical  
Company*

**Summary and Comments:** Thin films of magnetic fluid (100 Å particles of magnetite or Mn-Zn ferrite suspended in paraffin or other solvents) were investigated optically and magnetically in a magnetic field in the film plane and perpendicular to the direction of propagation of laser light (normal to the film plane). Magnetic dichroism and magnetic birefringence are observed--the light is linearly polarized, and the transmitted intensity and phase angle of the transmitted light depend upon the magnetic field strength and upon the angle between the polarization and field (ordinary and extraordinary rays). Chikazumi et al. show that the effects have a Curie-Weiss temperature dependence and are therefore related to the paramagnetic moment induced in the magnetic fluid by the applied field. They confirm that microclusters of suspended particles grow into macroclusters and chains along the field direction as the field is increased in strength. Anisotropic optical properties are a consequence of these clusters and chains.

### Formation and Magnetism of Superlattices

*Teruya Shinjo and N. Hosoi, Institute for Chemical Research, Kyoto University*

#### Summary and Comments:

1. Introduction
2. Fe/Mg Superlattices: Monolayers of iron are ferromagnetic, and in these atomically planar superlattices, with the Fe layers one and two angstroms thick, Curie points are 35 K and 55 K. Magnetic moments are normal to the film planes. As Fe layers are increased in thickness above 13 Å their structure changes from amorphous to crystalline (bcc Fe). But for those thicknesses for which the Curie point is above room temperature the structure is crystalline and the moment lies in the film plane.

3. Mn/Sb Superlattices: In laminating Mn and Sb, an MnSb compound layer at the interface grows epitaxially on the Sb layer. Neither Mn nor Sb is ferromagnetic, but the MnSb layer of the superlattice is ferromagnetic. The moment is normal to the film plane.

4. Au/Co Superlattices: Others have shown that when the Co thickness is less than 8 Å its moment is normal and its Curie point is above room temperature. Shinjo et al. confirm this. For magneto-optics a difficulty yet to be overcome is the chemical instability of exposed Co. A thick Au surface layer stabilizes the structure, but its opacity prohibits magneto-optic applications.

5. Fe/Nd Superlattices: Fe layers are amorphous when less than 20 Å thick and bcc above; Nd layers also shift from amorphous below to crystalline above about 20 Å thickness. When both the Fe and Nd thicknesses exceed 20 Å, the Fe moment lies in the film plane at room temperature and rotates to the perpendicular at 4.2 K. When the Fe thickness exceeds 20 Å but the Nd layers are less than 20 Å, the Fe moment is vertical at both room temperature and at 4.2 K. Irrespective of Nd layer thickness, when the Fe layers are less than 20 Å thick the Mössbauer spectrum is that of amorphous Fe, with the Fe moment vertical. Nd contiguous to Fe layers apparently contribute magnetization parallel to the Fe. Magneto-optic studies are underway.

### Magnetostriction of 3d Transition Metal/Noble Metal Compositionally Modulated Multilayer Films

*A. Itoh, H. Kurino, and O. Taniguchi, Nihon University, T. Katayama, Electrotechnical Laboratory*

**Summary and Comments:** The authors examine Young's modulus, magnetostriction, and stress of 3d transition metal/noble metal compositionally modulated multilayer films; they evaluate their induced anisotropy constants ( $K_u$ ) and compare with their perpendicular magnetic anisotropy constants. The magneto-optical Kerr effect increases near the light absorption edge of the noble metals. In multilayers with thin magnetic layers the magnetization can be oriented perpendicular to the film surface. Dissimilar atomic layers at the interface cause a magnetostrictive stress that induces uniaxial anisotropy, making the perpendicular direction easy. This study reports the magnetostriction of multilayer films of noble and other metals with magnetic layers: Fe/Cu, Co/Cu, Co/Ag, Co/Pd, Fe/Au, and Co/Au. Others have reported that Young's modulus increases abnormally at a modulation period of around 20 Å, but the authors' data show no evidence of this. They do confirm the general finding that Co/Pd multilayers are perpendicularly magnetized when the Co layers are less than 8 Å thick. Using bulk Young's moduli and estimated magnetostrictive stress at the interface, say  $10^5$ , the induced anisotropy should be significant. But what the real Young's modulus is within the thin magnetic layer is difficult to determine; the authors measure the total Young's modulus, stresses, and magnetostriction of the multilayer package. Films are produced by sputtering and magnetostriction measured by a cantilevered capacitance bridge, in a field of 7 kOe. Young's modulus of the multilayers is independent of magnetic layer thickness and is close to that of the noble metal. With regard to stress, Co/Cu and Co/Ag have small stress at small Co layer thickness, increasing to the tensile stress of pure Co as the Co layers are made thicker. In Fe/Cu multilayers the stress changes little with

Fe layer thickness, lying between that of pure Fe and pure Cu, up to Fe layer thickness of 100 Å. In single layer films of Cu and Ag, stress increases with film thickness. Ag films have small stress and only small increase as the film is made thicker. Next, the magnetostriction was measured. In Co/Cu, Co/Ag, and Co/Au multilayers, as the Co is thickened the magnetostriction changes from negative to positive at about 10 Å of Co. There is a maximum positive magnetostriction whose size depends upon the other metal of the multilayer (as does the Co layer thickness at which the maximum occurs). At large Co layer thickness the magnetostriction reverts to the negative value of pure Co. The goal of the study is understanding the stress-induced anisotropy. This is the magnetostriction times the stress. It is practically zero and independent of magnetic layer thickness in Co/Cu, Fe/Cu, and Co/Ag. It has some thickness dependence but is small in Fe/Au and Co/Au. In Co/Ag the uniaxial surface anisotropy is also small, but far larger than the stress contribution. In Co/Cu and Fe/Cu the room temperature uniaxial surface anisotropy grows rapidly with magnetic layer thickness, reaching about  $-30 \times 10^5$  ergs/cm<sup>2</sup> at 60 Å of magnetic layer, and saturating. The authors state that  $K_u$  of Co/Au multilayers is great compared to that of other films. These multilayers become perpendicularly magnetized through annealing (their figure 10 seems to be mislabelled). Stress-induced anisotropy in all cases appears to be negligible and independent of surface uniaxial anisotropy, which is evidently of different origin. The authors also report on Co/Pd multilayers. For fixed Pd layer thickness (36 Å), as Co layer thickness increases,  $K_u$  changes from large and positive to large and negative.  $K_u$  is significant and, in fact, dominant only when the Co thickness is about 13 Å and  $K_u$  is reversing sign.

---

## Study of Artificial Lattice Magneto-Optical Films

*H. Fujimori, H. Takanashi, T. Wakiyama, and K. Takahashi, Tohoku University*

**Summary and Comments:** The study consists of three parts: magnetism and Kerr effect in PtMnSb and its superlattice films, 3d transition metal/rare earth amorphous films and superlattices, and NiAs type  $\text{Mn}(\text{Sb}_{1-x}\text{Bi}_x)$  thin films.

1. Magnetism and Kerr rotation in PtMnSb superlattices: Since the discovery of the large magneto-optical rotation in the Heusler alloy PtMnSb, many studies have been done on its films. The present study went back to the bulk material to lay the foundation. They investigated the effect of annealing on the Kerr angle and reflectance. Annealing has little effect on reflectance. Kerr rotation is a maximum at a wavelength of about 700 nm. Annealing does not shift the location of the maximum but almost doubles the Kerr angle of polished PtMnSb, from about  $-1^\circ$  to  $-2^\circ$ . Kerr angle versus field plots show that annealing makes the material easier to saturate magnetically; the knee of the field curves of the annealed material is at 5 kOe while the polished sample saturates at about twice that field strength. Annealing appears to change the surface magnetic anisotropy, making saturation easier to achieve. Sputtered ferromagnetic/antiferromagnetic superlattices of PtMnSb/CuMnSb were then investigated at fixed thickness (100 Å) of PtMnSb and various thicknesses of the antiferromagnetic layer from 10 to 100 Å. All films contained 35 periods. The results are strange. All multilayers have about the same Curie point as has a single layer PtMnSb film. The multilayer with 10 Å of antiferromagnet has a saturation magnetization curve like that of

the single layer material. The 50- and 100-Å antiferromagnetically layered multilayers have magnetization curves that are similar to each other but have a saturation magnetization at 0 K which is about 25 percent larger than that of the unadorned ferromagnet. A ferromagnetic moment is presumably induced in the antiferromagnetic layers. Zero kelvin saturation moment of the multilayers, for fixed amount of ferromagnetic material, but varying the thickness of the antiferromagnetic layers, has a maximum when the CuMnSb is between 500 and 1,000 Å thick. At the maximum the moment is twice that of the single layer PtMnSb film. Kerr rotation angle depends upon wavelength. Curves for the multilayers are broader than for the single layer film, location of the maximum is shifted to longer wavelengths as the antiferromagnetic layers are made thicker, and the magnitude of the maximum rotation decreases with thicker antiferromagnetic layers.

2. Magnetism and Magneto-Optical Properties of 3d-Rare Earth Amorphous Thin Films: The focus is on magneto-optical recording media, on perpendicular magnetization for perpendicular recording, and on compensation point thermomagnetic recording. Figures show the temperature dependence of perpendicular anisotropy in  $a\text{-Co}_{1-x}\text{R}_x$  for various  $x$ , and for  $\text{R}=\text{Pr}, \text{Gd}, \text{Dy}, \text{and Er}$ . For the light rare earth Pr, in which the sublattice moments are parallel, there is a simple monotonic drop-off with increasing temperature. For the heavy rare earths the apparent perpendicular anisotropy goes to zero at the compensation point because there is no moment to get a handle on. The authors report the concentration dependence of perpendicular anisotropy and of magnetostriction at fixed temperature (77 K) for Fe and Co with varying concentrations of light and heavy rare earths in

amorphous films. Kerr rotation has only a weak wavelength dependence but drops markedly with increasing rare earth concentration. This is explained as being due not merely to the loss of Co but to the reduction of moment on Co atoms in the alloy. The authors also make superlattices of cobalt with rare earths and report on their magnetizations, perpendicular anisotropies, and Kerr angles. In Co/Pr superlattices, when the thickness of the Co layer is held constant and that of the Pr is varied, there is a maximum in the saturation magnetization at about 50 Å of Co per layer, exceeding the bulk moment of Co. There appears to be diffusion and mixing at interfaces; in a 10-Å-thick layer at the interface a ferromagnetic moment is induced on the Pr. Sign and behavior of perpendicular magnetic anisotropy depend upon layer thickness. When Co/Pr superlattice period exceeds 110 Å the anisotropy is small and negative at low temperature and becomes more negative as the temperature is increased. For superlattice period less than 50 Å the anisotropy is positive (magnetization normal to film plane) at all temperatures, decreasing to zero with increasing temperature. Down to a 10-Å period, the thinner the layers the greater the (positive) anisotropy. Saturation magnetization of the multilayers is small for thin layers but approaches that of bulk Co for periods in excess of 100 Å.

3. Magnetic and Magneto-Optical Properties of NiAs Type  $\text{MnSb}$  and  $\text{Mn}(\text{Sb}_{1-x}\text{Bi}_x)$ :  $\text{MnBi}$  has large crystal anisotropy, easy c-axis, and large magneto-optical rotation.  $\text{MnSb}$  is chemically more stable than  $\text{MnBi}$ , but it has easy plane anisotropy. This report is a summary of research on  $\text{Mn}(\text{Sb}_{1-x}\text{Bi}_x)$  two-layered thin films, with  $x$  up to 0.3. In  $\text{Mn}_x\text{Sb}_{1-x}$ ,  $K_u$  is negative and maximum in magnitude at  $x=0.5$ —easy plane and very large anisotropy. Bi is not very effective in inducing positive surface

anisotropy. In an insufficiently large aligning field, Kerr angle has a broad maximum between 0.5 and 0.7 micrometer for all concentrations.

### **Magneto-Optical Properties of Artificial Lattice Films and Rare Earth/Transition Metal Amorphous Films**

*S. Uchiyama, S. Tsunashima, and S. Iwata, Nagoya University*

**Summary and Comments:** Magnetization and Kerr rotation in multilayers of (1) Fe/Si, (2) Co/Pd, and (3) amorphous rare earth/transition metals.

1. Fe/Si Multilayers: Magneto-optical properties are studied at wavelengths near 1,100 nm, the Si bandgap (1.1 eV). Both Fe and Si seem to be amorphous, since no x-ray peaks due to crystallinity are seen. Magnetization lies in plane. Perhaps due to Si diffusion causing loss of Fe moment, thin Fe layers show a much-reduced moment. Thick layers appear to have greater moment than bulk iron; the authors suspect that this is evidence only of their incorrect measurement of layer thickness. Kerr rotation measurements are described. A transverse field is employed to obtain perpendicular magnetization. For fixed Fe layer thickness, as the thickness of the Si layers is increased the maximum in the Kerr angle shifts to longer wavelengths and the maximum Kerr angle increases. Calculation shows that multiple internal reflection is not the cause of the dependence of Kerr angle and reflectance on period and layer thickness. The authors argue that alloy formation at interfaces is occurring and affecting magneto-optical behavior.

2. Pd/Co Multilayers: Magnetostriction is probably the origin of the perpendicular magnetic anisotropy of PdCo. Magnetization and uniaxial anisotropy are measured

as layer thicknesses are varied and as the composition of the Co layers is changed by alloying with Pd. Addition of Pd decreases Co moment and the anisotropy switches to planar. For all compositions the Kerr angle peaks at a wavelength of about 400 nm. Kerr rotation is large and largest when the Co layers consist of Co undiluted by Pd. The smaller the superlattice period the larger the Kerr rotation. Smaller superlattice period also increases magnetization because of Pd polarization. But the increase of Kerr rotation in the thinner layered multilayers is because of PdCo alloy formation at interfaces.

**3. Magneto-Optical Effects of Rare Earth-Transition Metal Alloy Amorphous Films:** The authors measure and compare Kerr rotations in Fe and Co to those in YFe and YCo. The purpose of the Y is to make the transition metal amorphous. Presumably it does little. Yet the Kerr spectrum is quite different, particularly at higher energies. Broadening and smearing of peaks in the Kerr spectrum is reasonably attributed to smoothing of the electron energy band structure in the amorphous material. The report contains figures of the wavelength dependence of Kerr angle and ellipticity of a-GdCo, a-GdFe, and a-GdNi. Kerr spectra of the former two are like those of a-YCo and a-YFe. (Polarities are reversed because of the dominant Gd moment.) Kerr spectra are presented for numerous rare earths alloyed with Fe and Co.

#### **Magneto-Optical Effects of $\text{Cd}_{1-x}\text{Mn}_x\text{Te}$ Monolayered and Multilayered Films Produced by Ion Cluster Beams**

*K. Matsubara and T. Koyanagi, Yamaguchi University*

**Summary and Comments:** CdMnTe is a dilute magnetic semiconductor with extremely large

Faraday rotation in the visible. The authors grow their epitaxial thin films of CdMnTe on sapphire substrate by ion cluster beam deposition. By alternating barrier layers of a composition such as  $\text{Cd}_{0.5}\text{Mn}_{0.5}\text{Te}$  with layers of  $\text{Cd}_{0.9}\text{Mn}_{0.1}\text{Te}$  (for example), they make quantum well multilayers and superlattices and explore their optical properties in magnetic and electric fields. First, they discuss the epitaxial thin film results. Absorption coefficient as a function of photon energy was measured for various compositions in  $\text{Cd}_{1-x}\text{Mn}_x\text{Te}$ . The absorption edge shifts to higher energy with increasing  $x$ , from 1.5 eV at  $x=0$  to 2.6 eV at  $x=.77$ . Because of the onset of the d-d transition of  $\text{Mn}^{2+}$  at 2.2 eV, the short wavelength limit for magneto-optical application of  $\text{Cd}_{1-x}\text{Mn}_x\text{Te}$  is 2.2 eV, or 560 nm. Faraday rotations in the thin films are similar to those of the bulk material. Verdet constant displays dispersion at the band edge as expected. But the height of the dispersion peaks increases with increasing  $x$ . The investigators next report on their studies of the effects of an electric field on the magneto-optical response of  $\text{Cd}_{1-x}\text{Mn}_x\text{Te}$  thin films (not multilayers or superlattices). Electric fields were both normal and parallel to the film surface. To impress normal (perpendicular) fields the films are deposited on an indium tin oxide transparent conducting substrate over glass and an Al electrode is placed against the upper surface. In vertical fields the absorption edge shifts to longer wavelength with increased electric field. Birefringence, the difference in refractive indices in double refraction, goes up as the square of the electric field strength. For each composition  $x$  there is a dispersion peak in the birefringence at the gap energy. The electro-optical effect is far greater in  $\text{Cd}_{1-x}\text{Mn}_x\text{Te}$  than in other II-VI semiconductors of the same structure.



---

## High Density Magneto-Optical Memory and Recording Medium

*H. Kobayashi, J. Akedo, Y. Shirai, K. Tsutsumi, and Y. Hosoda, Faculty of Science and Engineering, Waseda University*

### Summary and Comments:

1. Introduction: Magneto-optics promises to raise memory capacity by two orders of magnitude. This report deals with reduction of beam spot size, now 1.6 micrometers and reaching the diffraction limit of light. The report then discusses the use of magnetic oxides--cobalt spinel-- as an alternative to the intensely developed amorphous rare earth-transition metal films, which are vulnerable to oxidation. A shift to oxides, which are chemically stable, also helps with the beam spot size problem because the oxides have high transmissivity in the neighborhood of the shorter wavelength (0.78 micrometer) emitted by semiconductor lasers.

2. Flying Head for Magneto-Optical Memory: The proposal of the authors is to place the port from which the semiconductor laser beam is emitted close up against the recording medium, with the slider about 0.4 micrometer from the medium as with a conventional head. This would enable the beam to penetrate the recording medium before it is diffracted and diffused. Coupled with going to shorter laser beam wavelengths and the authors' proposal to reduce the emission aperture to a size less than the laser wavelength, the researchers argue that it would be possible to significantly reduce spot size and increase bit density. By computer simulation they arrive at an optimum arrangement, with the distance from the light source being 0.5 times the laser wavelength and the bit size being 0.75 times that

wavelength (based on a point source). The authors, of course, recognize that their approach relinquishes one of the major advantages of optical technology. With conventional magnetic recording, head crash is a serious problem. (Yet to realize the potential benefits of perpendicular magnetic recording, head flying heights will have to move down from 0.4 to 0.1 and to an unbelievable but talked about 0.01 micrometer.) One of the great advantages of magneto-optics is that it takes off the pressure for lower flying heights.

3. Fabrication of Magnetic Thin Films of Oxides for Use in Magneto-Optical Memories: Magnetic oxides have two advantages over rare earth-transition metal films for magneto-optics. Since the former are optically transparent, large Faraday rotations can be obtained rather than the small Kerr rotations within the skin depth on reflection from metals. Also, the oxides are chemically stable while the rare earth-transition metal films oxidize in air and deteriorate. The authors attempted deposition of the hexagonal ferrite, Ba ferrite, but were unsuccessful because of the large difference in evaporation rates between Ba and Fe. They did succeed in depositing the cubic spinel cobalt ferrite,  $\text{CoFe}_2\text{O}_4$ . But because of demagnetization and the very large magnetocrystalline anisotropy conferred by Co, even with large perpendicular aligning fields the degree of saturation normal to the film was small, and Faraday rotations were consequently small.

### Garnet Thin Films Having Magneto-Optical Effects

*Masanori Abe and Manabu Gomi, Tokyo Institute of Technology*

---

**Summary and Comments:** This is important research.

1. Introduction: Garnet thin films are grown by sputtering. Polycrystalline and epitaxial films were produced. Bi substitution has long been known to increase Faraday rotation. This is because Bi increases electronic transition between the Fe and O ions. The researchers produce garnet films with a high degree of Bi substitution. They explore the effect of other substitutions and discover that Bi-substituted garnet with Ce is a superior magneto-optical material. The properties of films of this material are demonstrated.

2. Growth of Garnet Films by Sputtering Method and Establishment of the Film Forming Conditions: The authors describe their method for sputtering Bi-substituted garnet epitaxial single crystal films. Because it is weakly bonded to O, Bi is easily resputtered and lost; to attain stoichiometry a target with a much larger ratio of Bi is needed.

3. Characteristics of Garnet-Sputtered Films: X-ray diffraction reveals a shift toward larger lattice constant. This is in part due to a larger density of lattice imperfections than in single crystal bulk samples. Curie temperatures of the garnet films are also lower than those of bulk material. Curie points go up linearly with increasing substitution of Bi for Y in both bulk and sputtered films, but the film Curie temperatures lie about 25° below those of bulk compositions.

4. Nature of Bi-Substituted Garnet Polycrystalline Films: The polycrystalline films grown on glass substrates show no preferential orientation. Saturation magnetization can be lowered by substitution of nonmagnetic ions such as Al or Ga for Fe. Vertical magnetization can then be easily induced. These films are promising as a

magneto-optical recording medium, but a major barrier, medium noise, remains to be overcome. Being polycrystalline, they suffer large medium noise due to two mechanisms discovered and attacked in this research: optical (refractive index) nonuniformity and distortion of bit profiles. Lattice defects segregate at crystal boundaries and scatter light. Imperfections at grain boundaries are confirmed by etching; etching first occurs in the grain boundaries. The authors cleverly compensate for this by intentionally introducing imperfections into grain interiors. This smooths out the refractive index and demonstrably reduces light scattering! The second cause of medium noise, irregularity of bit shapes brought about by domain wall motion and grain moment rotation when bits cross grain boundaries, could be mitigated if grain boundaries could be made small with respect to bit size. Distortion of bit profiles at grain boundaries on bit borders would then be small. But unfortunately, Bi substitution markedly increases crystal grain size up to several tens of micrometers at large Bi concentration. A remedy that has some success is raising the coercive force in the interior of the grains by adding a small amount of tungsten. Faraday rotation is unaffected.

5. Formation of Bi-Substituted Garnet Epitaxial Films and Their Properties: Crystallinity of sputtered epitaxial films depends upon lattice mismatch with substrate. Films grown on GGG (111) substrate ( $\text{GGG} = \text{Gd}_3\text{Ga}_5\text{O}_{12}$ ) are subject to a large compressive stress. They grow unevenly, have a rough surface, and their magnetic domain patterns are irregular and discontinuous. In contrast, films grown on NGG (111), with a lattice mismatch of less than 0.1 percent, and small tensile stress, are smooth and uniform, and their magnetic

domains are of smooth and continuous shape. Faraday rotational hysteresis curves of the films on the two substrates are also quite different. The coercive force, a few Oersteds, of films grown on NGG is as good as that of a liquid phase epitaxy film. In sputtered epitaxial films the magnetization lies perpendicular to the film plane. The cause of this is not growth-induced anisotropy, as in liquid phase epitaxy films, but is stress-induced anisotropy.

**6.1 Development of New Magneto-Optical Materials:** Since Bi increases Faraday rotation in the garnets, why not go all the way to  $\text{Bi}_3\text{Fe}_5\text{O}_{12}$ ? This has been done successfully by others by liquid phase epitaxy, and Abe and Gomi show that epitaxial films of that composition can also be grown by sputtering onto NGG. Faraday rotation is intrinsically enormous, 100 times that of YIG, but the magnetization lies in the film plane.

**6.2 Ce-Substituted Garnet Films:** It is difficult to get Ce into the garnets. Ce is a  $3+$  ion, it has a large radius, and it tends to form  $\text{CeO}_2$ . Previous researchers have attained only  $x=0.06$  Ce substitution in bulk garnets and in liquid phase epitaxial films, but by sputtering Abe and Gomi reach  $x=1.5$ . The magnetization is perpendicular on GGG (111). Coercive force is less than 10 Oe. Curie temperature rises  $12^\circ$  per Ce ion substituted (per formula unit). At a wavelength of 633 nm the Faraday rotation of Ce-substituted films is about the same magnitude as that of Bi-substituted films, at each composition  $x$ , but while the rotation of the Bi is negative, that of the Ce films is positive. Faraday rotation is proportional to Ce concentration, being  $+2 \times 10^4$  deg/cm/Ce ion/formula unit. At a wavelength of 1,150 nm, Ce ions, like Bi, cause a negative rotation, but are five times as effective per ion as Bi.  $\text{Y}_2\text{Ce}_1\text{Fe}_5\text{O}_{12}$  is an excellent candidate as a magneto-optic medium.

## Research on Magneto-Optical Properties of Amorphous Magnetic Oxide Films

*Nobuyuki Hiratsuka and Mitsuo Sugimoto,  
Faculty of Engineering, Saitama University*

### Summary and Comments:

1. Foreword: The research concerns itself with conditions for the growth of films of amorphous spinel  $\text{CoFe}_2\text{O}_4$  and the magneto-optical properties of these ferrite films.

2.1 Forming Methods of Amorphous Cobalt Ferrite Films: Phosphorous pentoxide vapor pressure determines whether the films are crystalline or amorphous.

2.2 Dependence of Kerr Rotation Angle on Wavelength: Samples prepared under different  $\text{P}_2\text{O}_5$  partial pressures show strikingly different curves of Kerr angle versus wavelength. With increasing  $\text{P}_2\text{O}_5$  in the film the Kerr angle shifts from negative and large to positive at small wavelengths, changing sign at about 500 nm. Kerr angle also depends upon annealing conditions. This is associated with the polycrystal-amorphous transition.

2.3 Dependence of Kerr Angle on Wavelength: Crystalline and amorphous  $\text{CoFe}_2\text{O}_4$  films have quite different Faraday spectra. Where the crystalline film has a large negative peak at about 500 nm, changes sign at 625 nm, and has a large positive peak at 700 nm, a- $\text{CoFe}_2\text{O}_4$  causes positive rotation at all wavelengths measured, with a broad, low maximum of about  $2 \times 10^4$  deg/cm between 700 and 800 nm. The absorption coefficient of a- $\text{CoFe}_2\text{O}_4$  falls with increasing wavelength, but not markedly. This causes a maximum in the figure of merit (Faraday angle/absorption coefficient) between 700 and 900 nm.

---

3. Perpendicular Magnetic Anisotropy in Amorphous Cobalt Ferrites: Uniaxial anisotropy and perpendicular magnetization of the films are linked to phosphorous take-up; as  $P_2O_5$  partial pressure is increased, uniaxial anisotropy changes from negative to positive. Saturation magnetization decreases with increasing P.

4. Composition and Structure of Amorphous Cobalt Ferrite Films: Scanning electron microscope (SEM) photographs of the cross-sectional structure of an amorphous cobalt ferrite film with perpendicular magnetization reveal a columnar structure, with columnar diameter of about 0.2 micrometer. The anisotropy of the columnar structure, coupled with the large single ion anisotropy of the Co ion, is believed to be the cause of perpendicular easy axis in these amorphous films.

#### Changes in Absorption in Ca-Substituted Rare Earth Iron Garnet Thin Films by Etching

*Yoshiyuki Naito and Tetsuya Mizumoto, Faculty of Engineering, Tokyo Institute of Technology*

**Summary and Comments:** Rare earth garnet (RIG) films are useful in nonreciprocal devices in the infrared because of their large Faraday rotation and low loss. But optical absorption is sensitive to treatment, and particularly to impurities of valence 2+ and 4+, which cause the Fe to compensate by shifting from  $Fe^{3+}$  to 4+ and 2+. Fe in these valence states absorbs in the infrared. The authors show that the introduction of bivalent Ca and reduction in  $Fe(OH)_2$  produce high quality, low loss films suitable for optical waveguides.

---

#### Waveguide Nonreciprocal Optical Devices

*Sadahiko Yamamoto and Yasayuki Okamura, Faculty of Engineering, Osaka University*

##### Summary and Comments:

1. Forward: Stable, small, lightweight optical waveguides are fabricated by depositing on dielectric substrates thin films whose thickness is of the order of the wavelength. Usual substrates are ceramics, such as glass, electro-optical material, lithium niobate or, in some instances, acousto-optically active materials. Such devices are not unidirectional. With the burgeoning use of optical fibers in communications, of optical disk memories, and of all sorts of integrated optical technologies, lasers emitting ever shorter wavelength radiation will be utilized as light sources. To minimize interference, noise, and alteration of the laser oscillating modes, optical isolators will be needed. Optical isolators will allow light to pass out of the laser but will prevent reflected light from entering the laser. Nonreciprocal optical devices will be needed for high quality optical communication, computers, and signal processing systems of various kinds. This comprehensive report describes research focused on the theory, design, construction, and performance of nonreciprocal optical waveguides, made possible by the use of magneto-optical media. Isolators, circulators, magic tees, phase shifter circulators, and a guided wave branch interferometer were constructed and are described.

2. Magneto-Optical Waveguide Materials: Rare earth iron garnets, and in particular Bi-substituted RIGs, have large Verdet constant and are transparent in the near infrared, at about 1.15 micrometers

where a He-Ne laser is a convenient light source. Furthermore, to function as waveguides the film material must have a larger refractive index than the substrate. By good fortune this is the case for RIG films on GGG, the usual and convenient substrate. Epitaxial RIG films on single crystal GGG are uniform, and the thickness can be controlled as desired.

3. Magneto-Optical Effect in Optical Waveguides; 4. Orthogonal Polarized Wave Mode-Coupled Phenomenon; 5. Nonreciprocal Phase Shift Phenomenon: For a two-dimensional waveguide with uniform magnetization, the authors work out a simple and clear perturbative analysis that exposes the nature of the magnetized medium on the waveguide characteristics. To the isotropic (diagonal) dielectric tensor is added a small off-diagonal, hermitean, purely imaginary (if there is no loss) term. In the absence of magnetization and its off-diagonal manifestation, the modes of the waveguide are the usual horizontally polarized TE mode (with no component of electric field in the direction of propagation and only one component of electric field in a transverse direction) and the vertically polarized TM mode (with no component of magnetic field in the propagation direction and electric field components in the transverse directions). In a magneto-optically active medium these are no longer pure modes; they couple. The authors analyze the coupled mode problem. Mode conversion and phase shifts depend upon magnetization in a rather complicated way. One of the solutions is of particular technological importance. It involves an alteration of the TM mode alone, but its phase is shifted from that of the uncoupled TM mode when there is no magnetization. Yamamoto and Okamura graph nonreciprocal phase shift versus film thickness for typical circumstances and parameters--GGG

substrate,  $(\text{LaY})_3(\text{GaFe})_2\text{O}_{12}$  waveguide layer, and air above, with indices of refraction 1.945, 2.175, and 1, respectively. The maximum nonreciprocal phase shift occurs when the film is about 0.4 micrometer thick (for 1.15-micrometer wavelength light). This is advantageous regime of single mode operation.

6. Waveguide Nonreciprocal Optical Devices; 7. Fabrication of Magneto-Optical Waveguides; 8. Measurement of Mode Coupling Characteristics; 9. Amount of Nonreciprocal Phase Shift; 10. Characteristics of Magneto-Optic Guided Wave Branch Interferometer: The authors describe what is required in two classes of devices, those such as isolators and circulators utilizing the unidirectional mode conversion feature and those utilizing the nonreciprocal phase shift feature, such as the phase shift circulator. Yamamoto and Okamura demonstrate that their analysis can be reduced to practice; they grow RIG single crystal epitaxial films on GGG single crystals, etch channels by ion beam etching to make rib channel waveguides, and produce multi-mode and single-mode waveguides. They have formed guided wave branch interferometers. This reviewer is impressed.

#### Nonreciprocal Optical Thin Film Devices

*Yasumitsu Miyazaki, Faculty of Engineering,  
Toyoashi University*

Summary and Comments: The author analyzes mode conversion in a "single domain" optical isolator. The isolator consists of an isotropic substrate, a thick gyrotropic (magneto-optic) intermediate layer, a thin magneto-optic guide layer, and an isotropic top layer. Mode selectors of metal cladding on top of the thin isotropic film of the top layer form the front and back input

and output sections of the isolator. In the central mode converter section the magnetizations in the intermediate and guide layers are uniform, parallel to each other, but tipped from the direction of propagation down the guide and (about 85°) from the film plane by the magnetic field of an external magnet. Thus in the central region there are two magnetized layers with different anisotropic dielectric tensors. In the central region the top layer can be air. Miyazaki numerically analyzes propagation and optimizes unidirectional mode conversion with respect to a number of parameters—guide layer thickness and length, difference in dielectric constants, and direction of magnetization. Having a thick magneto-optically active intermediate layer makes it possible to shorten the device and reduces loss in the forward direction. With the values of the numerous parameters assumed, an isolation ratio of 30 dB can be obtained. In practice the author so far achieves only 13-dB forward/backward isolation, but development of the device had only just begun at the time of the report.

#### Deterioration with Age of TbFe Amorphous Films

*Yoshifumi Sakurai, Hikaru Hankyu, Kazumasa Furukawa, Tetsuya Hattori, and Yasutsugu Onishi, Setsunan University and School of Basic Engineering, Osaka University*

**Summary and Comments:** Adoption of TbFe, TbFeCo, GdCo, GdTbFe, and TbCo amorphous films as optical magnetic memory media has been seriously impeded by their propensity to oxidize and deteriorate. The authors study effects on deterioration of various deposition circumstances and protective coatings.

**TbFeCo Films:** The authors examine Kerr rotation, looking at both the top surface and at the substrate sides, of TbFeCo films on many substrates. The films were held for 700 hours at 60 °C and 90 percent relative humidity. While Kerr angle does not degrade on the substrate side, on glass, it suffers major change on the film face side. Of the substrates tested, PC is best. As a protective coating, Si<sub>3</sub>N<sub>4</sub> is better than SiO<sub>2</sub>.

**TbFe Films:** The best substrate is glass, but PC and PCHA can be used if a protective coating is applied. Cr is superior to Mo and C as a protective coating. Auger analysis shows that the film is passivated by formation of a TbFeCr alloy interface layer.

**TbFe Films Produced by Binary Electron Beam Vapor Deposition:** Sputtering is the usual and convenient method of producing films, and the films studied above were produced in this way. But sputtering causes resputtering, embeds O and Ar, reduces film density, and fosters deterioration. Vapor deposition produces purer denser films, but it is difficult to vapor deposit alloys because of the difference in vapor pressures of the components. So the authors tried a binary electron beam vapor deposition approach to see if this would improve stability of the RE-TM film. It does. With no protective coating, films kept for 1 year on the shelf at room temperature showed no deterioration of Kerr rotation. But films heated to 60 °C in a 70 percent relative humidity environment degraded in time.

#### Properties of a Dy-Fe (Co) Amorphous Alloy Film

*Yoshifumi Sakurai and Shunsuke Matsushita, School of Engineering, Setsunan University; Yasutsugu Onishi, School of Engineering, Osaka University*

---

**Summary and Comments:** The authors measure Kerr angle and Hall angle of Dy-Fe and Dy-Co amorphous sputtered films and find the relationship between these angles. They then apply a bias voltage to the substrate during deposition and produce major changes in the magnetic and galvanomagnetic properties. They interpret their results as being in part due to a change in the Dy resputtering rate in the electric field and in part due to structural changes in the amorphous alloy induced by the electric field.

#### **Magnetic Inspection Using a Magneto-Optical Device**

*Yoshifumi Sakurai, School of Engineering, Setsunan University; Takuhisa Numata and Toru Okaya, School of Engineering, Osaka University*

**Summary and Comments:** This study is aimed at developing a magneto-optical device for nondestructive inspection of the surface of steel plates. In magnetized plates, surface flaws, defects, or inclusions can disrupt the magnetization pattern and create leakage magnetic flux in their vicinity. Other techniques, such as Bitter patterns, inductive pickup, and Hall measurements, have been developed, but magneto-optics offers the possibility of high sensitivity, real time detection, and point localization of very small defects. Imagine a fine surface crack or channel in a magnetic steel plate. An impressed field in the plane of the plate but perpendicular to the long axis of the groove will align the magnetization, but there will be some small bulging of the magnetic field out of the plane of the plate as the field traverses the crack. The vertical component of this leakage flux can be detected by a magneto-optical sensor, a rare earth garnet magnetic slab with a reflecting Al layer on one side, laid flush on top of the steel slab

to be inspected. Polarized light normally incident on the garnet is rotated by the leakage flux, and its distortion of the magnetization in the garnet, and detected by visual inspection of the display of a photodetector or electronically. Spatial resolution by this device is found to be far superior to that of a conventional detector, a magnetic diode. A scratch of width 100 micrometers can be detected.

#### **Manufacturing of Ferromagnetic Glass and Magnetism**

*Toshitaka Fujii, Kazuhiro Yamaguchi, Yosuke Asahara, Shinichi Kuranouchi, and Yasunori Yamanobe, Toyohashi University of Technology; Atsushi Kashima, Kitakyushu Industrial Academy*

**Summary and Comments:** The report describes efforts to develop new transparent ferromagnetic glasses (amorphous ferromagnetic iron-group oxide compounds).

**Sputtered Thin Films and Bulk Materials:** This group had previously reported that amorphous Fe-B-O thin films and  $\text{Bi}_2\text{O}_3\text{-Fe}_2\text{O}_3\text{-ABO}_3$  ( $\text{ABO}_3$ =ferroelectric perovskite such as  $\text{BaTiO}_3$ ,  $\text{PbTiO}_3$ , or  $\text{PbZrO}_3$ ) reaction sputtered thin films exhibit simultaneous ferromagnetism and ferroelectricity. Ferromagnetic and ferroelectric ordering temperatures are above room temperature so that at room temperature simultaneous B-H and D-E hysteresis loops can be traced. Films several microns thick transmit well (>90 percent) in the near infrared. Such behavior is found in films of nonstoichiometric composition containing excess iron. Films of  $\text{Bi}_2\text{O}_3\text{-Fe}_2\text{O}_3\text{-PbTiO}_3$ , with other 3d ions--Ti, V, Cr, Mn, Co, Ni, Cu--partially substituted for the Fe, were also investigated. Besides films the authors have experimented with preparing bulk materials by the sol/gel method. Films have

---

been prepared on many kinds of substrates: glasses ( $\text{SiO}_2$ ,  $\text{TiO}_2$ ,  $\text{RO}_2$ ), piezoelectric ceramics ( $\text{BaTiO}_3$ ,  $\text{PbTiO}_3$ ), and high  $T_c$  superconducting ceramics.

**$\text{Bi}_2\text{O}_3$ - $\text{Fe}_2\text{O}_3$ - $\text{ABO}_3$  Sputtered Thin Films:** Films were magnetron sputtered onto glass, (100) silicon, and mica. For material of composition  $(\text{BiFeO}_3)_{1-x}(\text{BaTiO}_3)_x$ , neither the  $x=0$  nor  $x=1$  compositions are ferromagnetic (at room temperature, at which the experiments were conducted). Saturation magnetization peaks at an intermediate composition but is nowhere large (about 1 kG). The authors report the composition dependence of the Curie temperature, which decreases monotonically with increasing  $x$  (decreasing iron constituent) and reaches room temperature at  $x=0.5$ . Films are simultaneously ferromagnetic and ferroelectric, but the ferroelectric properties are not reported on here because the capacitive measurement technique has not yet been perfected. Color and translucency of these films are unchanged by the substitution of other transition metal ions for the Fe. Best annealing temperature varies from one composition to another, but saturation moments remain low.

**Fe-B-O and Fe-P-O Ceramics Produced by Sol/Gel Method:** With the addition of B and properly adjusted annealing temperature, a higher saturation magnetization, 49.5 emu/g at 20 percent B, is attained. This material, with its reasonably high magnetic moment and transparency, may be useful for some mixed ferromagnetic/ferroelectric transducer device if its ferroelectric response proves out. The magnetic characteristics of the phosphorous glasses are different from those of the boron glasses. Saturation magnetizations are reduced by half, to about 20 emu/g, depending upon composition. Coercive force is much lower.

**Characteristics of an Fe-B-O Thin Film:** A firm, unflakable, semitransparent Fe-B-O film was prepared by drying gel. Saturation magnetization is sensitive to annealing conditions. At 0.2 B composition a saturation magnetization of 3.1 kG was attained.

**Synthesis of  $\text{Bi}_2\text{O}_3$ - $\text{Fe}_2\text{O}_3$ - $\text{BaTiO}_3$  Ceramics by the Sol/Gel Method:** Because the  $\text{Bi}_2\text{O}_3$ - $\text{Fe}_2\text{O}_3$ - $\text{ABO}_3$  films were found to be ferromagnetic and ferroelectric, the authors were encouraged to make bulk materials of the same composition. They did this by sol/gel and selected  $\text{BaTiO}_3$  as the ferroelectric component. The report gives details of the process and of the various annealing conditions tried. There is a range of compositions and annealing temperatures in which the bulk material is both ferromagnetic and ferroelectric at room temperature.

#### **Production of Magneto-Optical Films by Ion Implantation and Their Properties**

*Yasuo Gondo, Hideo Kogure, and Jun Aoyagi, School of Engineering, Yokohama National University; Yoshitaka Suezawa, Teikyo University of Science and Technology*

**Summary and Comments:** Ion implantation is a powerful and versatile way of altering surfaces and films. This report describes efforts to produce amorphous rare earth-transition metal films by implanting rare earths (R) in transition metal (TM) films. The transition metals studied were Fe and Ni. Tb and Dy were implanted, and Bi and Ge were added, to increase the Kerr angle. Ar was also implanted. A dosage range of  $10^{13}$  to  $10^{17}$  ions/cm<sup>2</sup> was implanted in films between 200 and 3,000 Å thick. Depending upon bombarding energy, implantation concentration, and film thickness, multilayer



structures can be formed. For example, at low implantation concentrations, in a TM film thicker than the (voltage-controlled) energy of the bombarding R ions allows them to fully penetrate, there will be on the bottom an unaffected TM layer on the substrate. Above this lies a TM layer unreached by the R ions but compressed by the bombardment pressure. On top of this lies the gaussian-distributed layer of embedded R in TM, and at the surface lies a TM layer that the R ions have traversed. But when the implantation concentration is high, the high density of lattice defects introduced by ions bombarding the surface layer can no longer be ignored. The thickness of the fully traversed surface layer is reduced, and with heavy ions in large concentrations the maximum of the implanted density moves toward and actually peaks at the surface, dropping monotonically into the film. This is demonstrated with Bi and Ge implantation. Amorphous and other metastable phases can be formed. Ion implantation causes changes in structure and composition that alter the magnetic properties. At high dosage of 50 keV Ge ions, there is a large reduction in the magnetization of both Fe and Ni films. This can be in part due to alloy formation and in part due to resputtering loss of TM ions from the film. For a 190-Å-thick Tb-implanted Fe film, and at a wavelength of 633 nm, the Kerr angle at first increases with dosage and then decreases with continued implantation. The maximum occurs at about 1.6 at. % Tb, and a 30 percent increase is attained. This is consistent with other measurements and techniques. Ge implantation also initially increases Kerr rotation. Strangely, Bi is not very effective in increasing magneto-optical rotation when introduced by ion implantation. This is explained as due to resputtering and loss of transition metal by the heavy Bi ions.

## Study of Alloy-Metal Compound and Rare Earth/Transition Metal Magneto-Optical Films and Multilayers

*Tetsuzo Kusuda, Shigeo Honda, and Masatoshi Ogoe, School of Engineering, Hiroshima University*

**Summary and Comments:** The report comprises two subreports, one on Co-CoO and one on TbFe.

I. Magnetic Characteristics and Structure of a Co/CoO Multilayer Sputtered Film by Substrate Potential Modulation: Previous studies by the authors had shown that introducing oxygen into the Ar in sputtering Co created a film with a mixture of ferromagnetic hcp Co and antiferromagnetic fcc CoO and vertical magnetization. Attempts to periodically modulate composition by modulation of O partial pressure were hampered by the need to close the shutter in the chamber each time the O pressure was altered. This research describes an alternate method: at constant O and Ar pressures, a negative voltage applied to the substrate reduces the O concentration in the film. Multilayer films are produced by substrate bias modulation. Saturation magnetization, coercive force, and in-plane and out-of-plane anisotropy were investigated as functions of the thicknesses of the Co and CoO layers.

II. Magnetic and Magneto-Optical Characteristics of a Tb/Fe Compositionally Modulated Film and of a Dy/Fe Laminated Film: The same technique, periodic variation of the bias voltage on the substrate during deposition (but in this case during RF bipolar sputtering of compound targets), was used to produce compositionally modulated Tb/Fe and Tb/FeCo films. Targets of various proportions of Tb, Fe, and Co were investigated, as were the effects of layer

thickness on saturation magnetization, perpendicular magnetic anisotropy, and Kerr angle. Negative substrate bias reduces Tb concentration because of selective resputtering of Tb. Cross-sectional transmission electron microscope (TEM) photographs show that both Tb/Co and Tb/Fe compositionally modulated films produced in this way can have sharp interfaces. For reasons unknown, at the same bias voltage, Tb concentration is lower for thin layers (small period). This changes the saturation magnetization and other magnetic properties. The authors graph the dependence of perpendicular magnetic anisotropy energy ( $K_u$ ) on period.  $K_u$  has a minimum at a period of about 30 Å, rises to a maximum at a period of about 50 Å, and thereafter drops monotonically. Beyond the maximum  $K_u$  is well fitted by a curve of the form of a constant (the volume anisotropy energy) plus  $2K_i/\text{period}$ .  $K_i$  is the surface anisotropy energy at an interface. The larger the period the less effect of the interface.

**Dy/Fe Laminated Film:** Dy and Fe layers of equal thickness were alternately deposited. For periods greater than 50 Å the saturation magnetization is independent of period.  $M_s$  drops sharply below a period of 50 Å. As possible causes of the sudden drop in  $M_s$  at low period, the authors suggest antiferromagnetic coupling between Dy and Fe (but why would this cause a precipitous drop?) and a change in the crystal structure of the Fe in thin layers. Gondo et al. report that the Kerr angle shows the same sharp drop at a 50-Å period. Above that period the Kerr angle is about that of pure Fe. The drop in Kerr angle reflects the reduction in  $M_s$ . As in the voltage-modulated Tb/Fe films, the perpendicular magnetic anisotropy energy of the laminated Dy/Fe films falls off with increasing period, and in the same inverse fashion. It may be worthy of note that at low

temperatures (80 K),  $K_u$  is positive for periods between 40 and 80 Å (perpendicular magnetization).

### Development of New Magneto-Optical Recording Materials Produced by Gas-Phase Quenching

*K. Sumiyama and Yoji Nakamura, School of Engineering, Kyoto University*

**Summary and Comments:** Metastable phases--amorphous and nonequilibrium crystal structures, homogeneous alloy compositions and concentrations far outside the equilibrium boundaries, layered and modulated distributions--can be stable. Like diamond, their time scale for decay to the true equilibrium state, the state of absolutely lowest Gibbs free energy, can be infinite, or effectively so at room temperature. Thus many new materials, some of which will have interesting and useful new properties, are being synthesized and explored. At one extreme, mechanical alloying--ball milling a mixture of powders (which normally may have no solid solubility, for example)--is interesting because ball milling is such a gentle, low energy process. At the other extreme, sputtering is interesting because of the high energy and effective temperature of the impacting particles [see "Japanese Research on Metastable Phases of Metals and Alloys," by E. Callen, F. Pettit, and P. Shingu, *Scientific Information Bulletin* 14(2), 1-40 (1989)]. By sputtering, the Kyoto University Metal Science group (formerly headed by Y. Nakamura, now retired) has made stable, high concentration, homogeneous solid solutions of Ag, Cu, and La in several transition metals, combinations that show up only as a two-phase, separated region in equilibrium phase diagrams. Fe-Ag, for example, in equilibrium, does not

even have any liquid miscibility. The group has directed some attention toward making new magneto-optical materials. Kerr rotation is large in heavy ions, with large spin-orbit coupling, and in ions with large magnetic dipole moment. Atoms on the right side of the periodic table have larger radius, and their injection into transition metals increases the interatomic distance. Moments of transition metals tend to go up when their electronic charge has more room to spread out. Such concepts focus the researcher's efforts. Sumiyama et al. report here on the Fe-Cu-Ag ternary range, on  $\text{La}_y\text{Fe}_{1-y}$ , and on sputtered Fe. In the phase diagram of the bipolar sputtered film of Fe-Cu-Ag, Sumiyama finds ranges of homogeneous composition extending from the terminal bcc Fe, fcc Ag, and fcc Cu. In the center is a single-phase amorphous region. Connecting this with the crystalline regions, and separating the single-phase crystalline regions from each other, are two-phase and three-phase crystalline plus amorphous domains. As anticipated, at fixed Fe concentration, as Ag is substituted for Cu, the lattice constant, moment, and hyperfine field all increase. This is not the case with the binary-sputtered film of  $\text{La}_y\text{Fe}_{1-y}$ . The large La ion increases the atomic separation, but the moment saturates and is constant beyond about  $y=0.3$ . The Kyoto group finds an interesting and potentially important result on the sputtered Fe and Fe-Cu alloy films. As with Co-Cr, a perpendicularly magnetized film can be synthesized by developing columnar structure, with coexisting paramagnetic Cu-rich and ferromagnetic Fe-rich regions, or with

oxidized interfaces. This imposes a form anisotropy on the ferromagnetic columns that aligns the magnetization perpendicular to the film.

## FINAL COMMENTS

This concludes our summaries (and comments) on all reports submitted to the Ministry of Education describing progress on 1988 grants to universities on magneto-optics. Monbusho holds equally impressive portfolios in other fields of magnetism with immediate and large device, computer, and high-tech commercial impact -perpendicular magnetic recording,  $\text{R}_2\text{Fe}_{14}\text{B}$  permanent magnets--and far more portfolios outside magnetism, in semiconductors, superconductivity (conventional and high  $T_c$ ), optical communications and laser science, ceramics, surface modification, and composite materials.

Where Monbusho stops, the Ministry of International Trade and Industry (MITI), the Science and Technology Agency (STA), and other Ministries (Transportation, Post and Telecommunications) pick up. Professor Susumu Uchiyama, a highly regarded scientist, was one of the authors of the report from the Nagoya University Department of Electrical Engineering on multilayer films. MITI is paying for construction of buildings on the campuses of all the major national universities of Japan to house programs in university/industry cooperation. Industry will pay project costs. The new director of the MITI Nagoya University Institute is Professor Uchida.

---

Earl Callen was a member of the staff of the Office of Naval Research Far East from June 1987 to June 1990. He is a Professor Emeritus of The American University. He has been active in the physics of magnetoelastic phenomena and amorphous magnetism.

---

---

# THE ERATO PROGRAM

---

Aharon Gibor

---

*The ERATO program, initiated in 1981 by the Research and Development Corporation of Japan, was created to foster research in basic sciences toward development of advanced future technologies.*

---

## INTRODUCTION

ERATO stands for Exploratory Research for Advanced Technology. It is an innovative research and development (R&D) program that was initiated in 1981 by the Research Development Corporation of Japan (JRDC).<sup>\*</sup> JRDC is a government-owned corporation that organizes R&D projects at nonprofit public laboratories, universities, and private sector research laboratories. JRDC is one of the branches of the Science and Technology Agency (STA). STA is a ministerial agency reporting directly to the prime minister's office.

The stated objective in the creation of the ERATO program was to "generate advanced technologies while promoting the development of Japan's activities in basic research." The ERATO program supports lavishly a few carefully selected research projects. At present 14 ERATO projects are in progress and 7 have been completed. Each project is supported for 5 years at a cost of about \$10 million. A cluster of new projects is expected to be inaugurated every year, each with a term of 5 years.

## ACTIVITIES AND DEVELOPMENT

Annual symposia on the ERATO program were held in Tokyo in late November and early December 1989. In each session (held on four afternoons) researchers from four different projects presented the progress in their respective projects. I was impressed by the titles and subjects of the projects, especially those in the biological realm, and subsequently I made an effort to meet with some of the principal investigators. The completed projects as well as the ongoing ones proved to be more successful than anticipated, and JRDC is now organizing groups of private companies for fostering the research results and confirming the feasibility for utilization. Also in line with political pressure for internationalization, plans are being drawn for expanding ERATO or similar programs to include foreign institutions. In the 26 October 1989 issue of *Nature* (Volume 341, 1989, Classified, pages 26-27), JRDC advertised its international program. This program includes: (1) joint international research projects, (2) the STA fellowship program, (3) a sup-

---

<sup>\*</sup> A panel report on ERATO was published in December 1988 by the Japanese Technology Evaluation Program (JTECH), which is coordinated by the Science Applications International Corp., 1710 Goodridge Dr., McLean, VA 22102.

---

port program to facilitate exchange of personnel, and (4) an information program to provide foreign researchers with information on Japanese research activities.

To further discuss the operations of the ERATO program as well as the new international research activities, I arranged to visit the JRDC offices and speak to Mr. Genya Chiba, a vice president of JRDC. Mr. Chiba was a graduate student in particle physics at Columbia University in New York in the 1950s. I told him that I was most impressed by the choice of ERATO projects, which indicated to me a very imaginative outlook on the potential of these projects. I asked him how projects are chosen. Apparently they do not solicit applications from the scientific community. According to Chiba the subjects of the projects originate at the ERATO organization. JRDC is continuously searching for suitable project directors. Once one is identified, a series of discussions takes place between the selectee and the JRDC committee in order to develop the research subject and strategy. Chiba considers the choice of the director to be the most important and difficult task. They seek a charismatic, dynamic personality, eminent in his scientific field, who is capable of attracting and inspiring his coworkers. Such a person, when found, is offered funds to acquire the necessary equipment and to recruit a working team. JRDC prefers to use rented laboratory facilities since each project lasts for 5 years only. Some projects become subdivided, with the various segments located at different places. For example, the project on molecular dynamic assembly, headed by Professor Hotani, is carried out in Kyoto, where they are studying the assembly of membranes and microtubules, and at Tsukuba, where they are studying the assembly of bacterial flagella. The details of the execution of the project are left to the director.

The chosen director, usually but not always from the academic community, determines in his way how to contribute his time to ERATO as well as to his home institution. Members of the team are recruited by the director from both academic as well as private sectors. There is strong encouragement to hire foreign scientists to make ERATO teams as heterogeneous as possible with individuals from a variety of different backgrounds and cultures. In those projects that have already been terminated, members of the teams that were recruited from industry usually returned to their companies; others found employment in industry, academic institutions, and government laboratories.

Chiba says that the specific subjects of the projects result from young, emerging generations, reflecting their enthusiasm gained by working with leaders of their fields. Many young JRDC staff members circulate among scientific meetings and elsewhere while trying to identify unique young scientists who can be successful project directors. Attention is also paid to new and interesting topics. From conversations I had with Dr. Hotani and Dr. Horikoshi, who were chosen leaders for ERATO projects, Chiba himself is probably "the brains" behind many of the choices. As is the case with many other decision making policies in Japan, I suspect that the "fraternal cliques" of their "alma mater" are a great influence in choosing research subjects for support.

The accomplishments of the ERATO research projects can be judged by using several criteria. First is the standard academic scale of research success: the publication of research results in scientific journals. The bibliography of the ERATO projects is ample evidence for its academic productivity. A different indicator of the success of a project is its fate after the expiration of ERATO support. I did not

investigate the nonbiological projects, but the vitality of some of the biological projects became evident. The Bioinformation Transfer Project, headed by O. Hayaishi, grew to become the Osaka Bioscience Institute, a magnificent research facility constructed by the City of Osaka. Professor Hayaishi and his team continue to expand their research on the physiology and biochemistry of brain function. The new institute also houses other related projects, including that of Professor Tsuji on bioluminescence. Another project, the "Superbugs" Project, headed by Professor Horikoshi, was terminated in 1989. In cooperation with several private industries and JAMSTEC, a public agency, Horikoshi will move part of his team to a new institution, now under construction, which will be dedicated to the biology of deep ocean organisms. Facilities are being planned for the cultivation of deep sea organisms under high pressures and at different temperatures. Thus a viable research project becomes self-evident by its capacity to perpetuate itself.

## LIST OF ERATO PROJECTS

- Ultra-Fine Particle Project (1981-86); Project Director: Dr. Chikara Hayashi, president, ULVAC Corp.
- Amorphous & Intercalation Compounds Project (1981-86); Project Director: Dr. Tsuyoshi Masumoto, professor, Research Institute for Iron, Steel and Other Metals, Tohoku University
- Fine Polymer Project (1981-86); Project Director: Dr. Naoya Ogata, professor, Sophia University
- Perfect Crystal Project (1981-86); Project Director: Dr. Jun'ichi Nishizawa, professor, Research Institute of Electrical Communication, Tohoku University; director, Semiconductor Research Institute
- Bioholonics Project (1982-87); Project Director: Dr. Den'ichi Mizuno, professor, Teikyo University
- Bioinformation Transfer Project (1983-88); Project Director: Dr. Osamu Hayaishi, president, Osaka Medical College; director, Osaka Bioscience Institute
- Superbugs Project (1984-89); Project Director: Dr. Koki Horikoshi, professor, Tokyo Institute of Technology; chief scientist, Institute of Physical & Chemical Research (RIKEN)
- Nano-Mechanism Project (1985-90); Project Director: Mr. Shoichiro Yoshida, managing director, Nikon Corp.
- Solid Surface Project (1985-90); Project Director: Dr. Haruo Kuroda, professor, University of Tokyo
- Quantum Magneto Flux Logic Project (1986-91); Project Director: Dr. Eiichi Goto, professor, University of Tokyo; chief scientist, RIKEN
- Molecular Dynamic Assembly Project (1986-91); Project Director: Dr. Hirokazu Hotani, associate professor, Kyoto University
- Biophoton Project (1986-91); Project Director: Dr. Humio Inaba, professor, Research Institute of Electrical Communication, Tohoku University

- 
- Terahertz Project (1987-92); Project Director: Dr. Jun'ichi Nishizawa, professor, Research Institute of Electrical Communication, Tohoku University; director, Semiconductor Research Institute
  - MorphoGenes Project (1987-92); Project Director: Dr. Mitsuru Furusawa, deputy general manager, Research Institute, Dai-ichi Seiyaku Co., Ltd.
  - Molecular Architecture Project (1987-92); Project Director: Dr. Toyoki Kunitake, professor, Kyushu University

## CONCLUDING REMARKS

The ERATO concept appears to me to be very productive. I think highly of the National Science Foundation (NSF) project

of career development grants; these are designed to promote the development of highly promising young individuals, and we certainly can use geniuses. The ERATO program, on the other hand, is designed to enhance and promote the development of a specific area of scientific research. Each one of the supported projects can be seen as a mini "Manhattan project." It is the focusing of the best available brains and facilities on the research of a specific scientific objective. From what I gather the program is successful. Of course, not all the supported projects will prove equally successful and rewarding, but if a fraction proves to be successful it will justify the whole program, and from what I was told the success so far exceeds the early expectations.

---

Aharon Gibor began a 1-year assignment at the Office of Naval Research Far East in August 1989. Dr. Gibor is a professor of biology at the University of California, Santa Barbara and is now on a leave of absence from that institution. He received a B.A. degree in 1950, his M.A. degree in 1952 from the University of California, Berkeley, and his Ph.D. degree in 1956 from Stanford University. His thesis research was done at the Hopkins Marine Station. Dr. Gibor was involved in research on the genetic autonomy of cytoplasmic organelles of eukaryotic cells, especially chloroplasts and flagella. His present research is on the growth and development of algal cells and tissues and the role of cell walls of these plants in controlling their development.

---

# SECOND INTERNATIONAL WORKSHOP ON SOFTWARE QUALITY IMPROVEMENT: SUMMARY AND ASSESSMENT

---

David K. Kahaner

---

*The Second International Workshop on Software Quality Improvement was held in Kyoto, Japan, from 22-24 January 1990. The workshop was jointly organized by Professor Torii (Osaka University) and Professor Basili (University of Maryland). The workshop is summarized from the perspective of a numerical analyst. The major conclusions are that some Japanese companies are better at managing the software development process than comparable U.S. companies and that more interaction is needed between numerical and nonnumerical software developers.*

---

## INTRODUCTION

In 1990 the U.S. Navy will spend approximately \$10B on computer software. In the future this figure will go higher. It is essential to conduct research in methods that can lead to reductions in the rate of increase of these costs. All large technology organizations face a similar challenge. The Office of Naval Research supports a number of programs within its Computer Science Division that address software productivity. In support of that effort I attended this workshop. Sponsored jointly by the Ministry of International Trade and Industry (MITI), the Joint System Development Corporation (JSD), and the Research Institute for Software Engineering (RISE), this workshop brought together almost 60 scientists: about a dozen from the United States, one from Italy, and the remainder from Japan. The

Appendix provides a list of the papers presented. My own invitation to this workshop came from Professor Victor Basili [University of Maryland (UMD)], who played an important role in organizing the workshop and who participated very actively in many of the discussions. The official goal of the workshop was to use quantitative and qualitative evaluation to understand the effects of various software processes and how to improve software measurement techniques.

## KYOTO RESEARCH PARK AND JOINT SYSTEM DEVELOPMENT CORPORATION

The workshop was held at the Kyoto Research Park (KRP), a new and spectacularly modern facility about 15 minutes by taxi from the Kyoto train station. KRP bills itself as a "self-contained laboratory complex with all the benefits of a modern city."



---

Apparently with help from the city of Kyoto KRP is constructing and managing this large facility, which commenced operation in the fall of 1989. KRP has "members" including:

- The Kyoto Prefectural Comprehensive Center for Small & Medium Enterprises
- The Kyoto Municipal Institute of Industrial Research
- The Advanced Software Technology & Mechatronics Research Institute of Kyoto
- The Japan Institute of Invention and Innovation, Kyoto Branch

The building in which the workshop was held was the public center of KRP. It contains meeting rooms, dining facilities including a cafe and separate restaurant, and a large lecture hall that was used for the workshop sessions. The sessions had simultaneous translation in Japanese and English so participants could use their natural language. (The wireless receivers were German.) Last year's workshop was conducted entirely in English and this proved to be a deterrent to many of the Japanese participants.

The Joint System Development Corporation (JSD) was founded by 19 major information processing companies and about 100 related businesses in 1976. Its objective is to improve technical standards and to strengthen the Japanese information processing industry. It functions somewhat like the U.S. American Federation of Information Processing (AFIP). JSD focuses on

(1) "National Projects"

- Formal Approach to Software Environment Technology

- Simple Input & Retrieval Information Utility System
- System Integration Fundamental Technology
- Computer Assisted Instruction
- Survey and Research on Software Engineering
- Network Center for Information Processing Industry
- Software Maintenance Engineering Facility
- User Support Engineering Facility

- (2) Development of paperless system for Japanese Patent Office
- (3) Distribution of the SPIDER image processing package
- (4) Cooperation with the Small Business Promotion Corporation
- (5) Software sales promotions

## WORKSHOP OBSERVATIONS

As a scientist who has been developing software throughout my career, I realized after listening for 2 days that the issues addressed here apply to a very different class of problems than those faced by myself and my peers. The best sense of this came to me while listening to the speaker from Mitsubishi, who claimed that his company produces more than 34 million lines of software (code) each year. Most of this is developed to run industrial processes such as

---

manufacturing production lines. The main questions associated with this software are not if the algorithm is clever, efficient, or creative, but rather how to reduce the number of potential errors that large, multiperson software projects can produce. In fact the most important parameter discussed at this workshop was BKLOC, bugs (errors) per thousand lines of code. In this community there appears to be little place for the traditional questions about numerical methods that physicists, chemists, and engineers raise when thinking about computer programs. Thus, my attendance at this workshop was as an educated observer. I attended all the formal presentations but did not attend the working group sessions during the last 2 days. Nevertheless, it was possible to draw some very interesting conclusions.

FIRST, there was general perception that the Japanese (companies) were doing a better job than their U.S. counterparts in reducing error rates. Basili claimed that Japanese BKLOC rates were about one order of magnitude less than those in the United States, down below 1 BKLOC, and that Japanese software productivity was from 2 to 20 times that in the United States. He claimed that a major reason was that Japanese companies used better management techniques and were better at motivating people. (After listening to several talks by representatives of Japanese industry I concurred with this assessment.) Nevertheless, the gap between industry and research was greater in Japan than in the United States. Basili felt that entry level Japanese software developers are less well prepared than their U.S. counterparts, but it's the other way around after about 5 years of work. There was no disagreement to his statement that Japanese companies are doing a good job of training and retraining workers, so perhaps this accounts for part of this effect. (On a personal

level I have been amazed to discover courses in Unix, mathematics beyond calculus, statistics, etc. on the educational channel of our home TV during prime time.) Professor Koji Torii (Osaka University), a co-host of the workshop along with Basili, echoed the remarks about the narrow pipeline between Japanese university research and industry. Incidentally, the excellent facilities at the workshop site, KRP, contrast strongly with the mildly threadbare look of some Japanese universities I have seen.

SECOND, I was surprised by the meager attendance and intellectual presence of U.S. industry, even considering the distance to Kyoto. The U.S. industrial participants who gave papers were from Mitre, Hughes Aircraft, NASA, CTA, and MCC. Agresti (Mitre) discussed how to assure quality in software being developed by others. Deutsch (Hughes) discussed an after-the-fact analysis he did of some of Hughes' projects while he was on sabbatical at CMU. McGarry (NASA) discussed work done to a large extent in collaboration with Basili at Maryland. CTA is a small contractor in Rockville, MD, and MCC is an Austin, TX, software think tank. Some other American companies attended but presented no papers. Representatives from AT&T Bell Labs (Columbus, OH, office only) and GenRad (Concord, MA) were there, but mostly to learn more about Quality Function Deployment (QFD), a method developed by Professor Tadashi Yoshizawa of Tsukuba University. QFD is well known and has been promoted by Yoshizawa since the 1970s. In his talk he indicated that a symposium on QFD was held in Novi, MI, in June 1989. Ohba (IBM Japan) gave a talk, but only about modeling the errors that were discovered after software was delivered. (I questioned his use of linear differential equations as being simplistic.)

---

On the other hand, Japanese industry was well represented. Papers presented by Oki Electric, NEC, Mitsubishi, Fujitsu, Nippon Steel, Sharp, and JSD gave very clear evidence that these companies are trying hard to learn how to improve software productivity. Papers by university researchers from both countries were mostly excellent, but I was struck by the fact that the Japanese are really working at reducing software errors. There was a strong emphasis on user requirements driving the design process (natural in any company that produces a product), a team approach to solving problems, developing methods that assure quality at every step of the software process, and quality control involving all departments including top management. The speaker from Nippon Steel said it very well, "We put stress on human motivation as well as machine's automation."

## DETAILS OF SELECTED PAPERS

A paper by Professor Tetsuo Tamai (Tsukuba University) on Japanese-based programming tools was a substitute but generated a substantial amount of discussion anyway. Essentially, Tamai studied the existing programming languages that utilize Japanese in some direct way and attempted to compare them. The discussion centered not so much on his results, which were very tentative and modest, but on the general usefulness of a Japanese programming language. Basili pointed out earlier that he had been impressed with the strides that had been made in the use of Japanese syllabic input (hiragana) with resulting conversion to kanji. I have watched this process, too, and although it is slower than using an ordinary alphabet it is perhaps only a factor of two slower and it allows Japanese speakers more natural access to computers. One of my noncomputer colleagues remarked that

kanji, which is pictographic, permits experienced readers to grasp the essence of a page more quickly than alphabetic languages. (I do not read kanji.) Other icon-based software, vis Sun, Macintosh, etc., are also pictographic and clearly very successful. Professor Jun Murai (Keio University) wrote recently that Japanese network traffic is almost all in kanji, so perhaps Japanese prefer to communicate this way. In any case it was admitted that Japanese language programming would be unmarketable outside of Japan; consequently research in this direction has never been a priority project. My assessment is that Japanese language software would provide improved productivity and open the door to amateur software developers in much the same way that the PC did in the United States. Further, the lessons learned developing Japanese software can then be applied to other Asian languages for countries whose markets are just now opening for computer technology. Even the current wave of Japanese word-processors has already fueled very good display technology; a Japanese PC on a secretary's desk has much better graphics capability than the U.S. counterpart.

The paper on the FASET project by scientists from JSD was interesting to me because it represented one on the major projects undertaken by this group. I was disappointed with the progress they have made. Some other listeners seemed to feel similarly, questioning the use of inefficient LISP as an output language, wondering why logic programming (PROLOG) was not used, and why the tools were not better integrated. This work strikes me as being so high level that it suffers from a lack of concrete focus.

Professor Basili's work (UMD) on packaging software experience was very well received. His collaborations with NASA have apparently been jointly productive. Professor John Knight (University of Virginia) is a

---

recognized expert on safety critical software, such as those used in nuclear power facilities, avionics systems, or dangerous medical appliances. He discussed the problems associated with designing software with failure rates of  $10^{-9}$  per event or per hour. For extremely reliable hardware systems the usual approach is redundancy. This has been shown both by analysis and experiment to be effective. For software the same technique is often used, i.e., having different contractors develop software with identical specs. Unfortunately, Knight's research shows that the usual assumption of independence between failures of redundant systems is often invalid for software, because difficult parts of the design are likely to lead to errors whoever codes them. He concluded very succinctly, that he was "scared to death" when he thinks about some of the places such safety critical software are used.

McGarry's paper (NASA) was particularly relevant to me because he provided comparisons between software projects done using Fortran and Ada. He showed that, surprisingly, the percentage of time spent in the design, test, and code stages of a big project was about the same with either language. Further, the error profiles were also about the same, although Ada programs had fewer interface errors. The NASA approach to improving software quality lies in "understanding" many of the measures of software quality that have been developed over the past 15 years, "analysis" or defining relationships between the software process and software product, and "automation" or the development of software tools to improve quality. Much of the research has been done within the Software Engineering Laboratory (SEL) jointly supported by NASA, the University of Maryland, and Computer Sciences Corp.

Yamazaki (Nippon Steel) represented his company view that employee motivation

and technology are like two wheels on the same axle--both must be equal diameter or straight line motion toward the company's goal cannot occur. A similar view was expressed by Masanori Teramoto (NEC). He estimated that NEC has approximately 15,000 people in 2,500 groups associated with software development. They have production design meetings, software quality control meetings, and evaluation and self-help groups. These involve all levels of company employees, including top management, and are very goal oriented. NEC estimates that in 1991 they will write 140 million lines of code and that BKLOC will be less than 0.1. Further, their reuse percentage (code that can be utilized in other applications without rewriting) will go from 50 percent in 1987 to 60 percent in 1991. As a side remark, he noted that Unix has helped increase their productivity because the same system is used across a wide variety of computers and hence less relearning was needed. My own experience is that Unix is a wonderful system for software hackers who love its flexibility and abbreviated command syntax and an awful system for the inexperienced who are easily confused by these same features.

The paper by Hino from Fujitsu seemed particularly useful for me, but did not generate much interest from most of the participants. The NAIVE language he discussed is higher level than C or Fortran but still has the flavor of "programming." As such it does not represent much new when viewed as a technique for assuring program correctness. It was pointed out during the discussion that it was still possible to write programs in NAIVE that were illogical and that it had no mechanism to insure that changes made in one section were propagated to other sections. I see NAIVE as an incremental improvement in the process of writing programs. Nevertheless, these are

---

just the small steps the Japanese have proved to be very good at making.

There also did not seem to be much interest in formal methods, such as proof of correctness. Gerhart's paper struck me as rather defensive and the first question asked was if it was not hopeless to try to apply these techniques to large systems. My own experience is that formal methods have worked only on very small core sections of big programs and never have provided me with any new insights.

## MISCELLANEOUS

I participated in a coffee-time discussion between a few of the U.S. researchers and their Japanese colleagues about supercomputing. I had been querying many of these people individually about the relevance of their work to the scientific computing community that I represent and had concluded (see above) that there was not much overlap at this time. Some of the Americans expressed the opinion that the National Science Foundation supercomputing centers were bad news for computer science because they cost too much and left precious little money for other types of

computer science research. What is interesting is that I also have heard individual members of the supercomputing community make similar comments about the Gore bill, which focuses on networks. Officially, the computer science community through the Computing Research Board supports this legislation. The Japanese researchers at this meeting do not use much high performance computing either, but I did not hear any complaints about lack of funding from them.

## CONCLUSION

There is not enough interaction between the sorts of computer scientists who would naturally attend meetings of this type and physical scientists who develop large scale engineering software. Both groups could benefit from closer contacts. On the basis of the talks presented here, some Japanese companies that write a great deal of software are ahead of those in the United States in managing the software development process. Managing and motivating people are important factors as are clear signals from the top that productivity enhancement tools are to be taken seriously.

---

**David K. Kahaner** joined the staff of the Office of Naval Research Far East as a specialist in scientific computing in November 1989. He obtained his Ph.D. in applied mathematics from Stevens Institute of Technology in 1968. From 1978 until 1989 Dr. Kahaner was a group leader in the Center for Computing and Applied Mathematics at the National Institute of Standards and Technology, formerly the National Bureau of Standards. He was responsible for scientific software development on both large and small computers. From 1968 until 1979 he was in the Computing Division at Los Alamos National Laboratory. Dr. Kahaner is the author of two books and more than 50 research papers. He also edits a column on scientific applications of computers for the Society of Industrial and Applied Mathematics. His major research interests are in the development of algorithms and associated software. His programs for solution of differential equations, evaluation of integrals, random numbers, and others are used worldwide in many scientific computing laboratories. Dr. Kahaner's electronic mail address is: kahaner@xroads.cc.u-tokyo.ac.jp.

---

---

## Appendix

### PAPERS PRESENTED AT THE WORKSHOP

- Agresti, W., "Quality Projection for Risk Assessment" (MITRE)
- Basili, V., "The Experience Factory: Packaging Software Experience" (University of Maryland)
- Deutsch, M., "Predicting Project Success From the Software Project Management Process: An Exploratory Analysis" (Hughes Aircraft Co.)
- Gerhart, S., "Back to Basic Principles--What Do Formal Methods Contribute to Software Construction?" (MCC)
- Hino, K., "Software Quality Improvement by the Specification Language NAIVE" (Fujitsu)
- Howden, W., "Verification of Complex Systems Using Incremental Operational Specifications" (University of California, San Diego)
- Kawasaki, Y., T. Miyoshi, and T. Oishi, "The FASET Project, Construction of the New Software Development Environment" (Joint System Development Corp.)
- Knight, J., "Software Quality Where it Really Counts, Safety-Critical Systems" (University of Virginia)
- Masuda, M., "Software Quality Target Control, Target and Evaluation" (Mitsubishi Electric Corp.)
- Matsumoto, Y., "Introducing KyotoDB-1: A Computer-Aided Software Requirements Engineering Environment" (Kyoto University)
- McGarry, F., "The Role of Measurement in Software Quality Improvement" (NASA)
- Miyamoto, M., "Database Support for Software Quality Improvement" (Sharp Corp.)
- Ohba, M., "Applying Software Reliability Growth Models" (IBM Tokyo Research Laboratory)
- Sacchi, W., "A Framework for Modeling Software Evolution" (University of Southern California)
- Tamai, T., "Japanese-Based Programming as a Means for Enhancing Software Quality" (University of Tsukuba)
- Teramoto, M., "Evaluation of Management Process" (NEC)
- Tohma, Y., R. Jacoby, Y. Murata, and M. Yamamoto, "Hyper-Geometric Distribution to Estimate the Number of Residual Software Faults" (Tokyo Institute of Technology)
- Tokutsu, H., "Software Quality Assurance System" (Oki Electric Industry Co.)
- Torii, K., "A Measurement Environment and Some Results at Class Experiments" (Osaka University)
- Velez, C., and S. Balin, "An ADA Design and Implementation Toolset Based on Object-Oriented and Functional Programming Paradigms" (CTA Inc.)
- Yamazaki, T., "Software Quality Improvement Activities at a User" (Nippon Steel)
- Yoshizawa, T., "Quality Function Deployment for Software Development" (University of Tsukuba in Tokyo)

---

# FRENCH-JAPANESE SEMINAR ON COMPOSITE MATERIALS

---

Michael J. Koczak

---

*The French-Japanese Seminar on Composite Materials provided a unique opportunity to view the materials development of two world-class composite research groups. The French have developed expertise in aerospace structures, high strength fibers, and ceramic and carbon/carbon composites. The Japanese have strong efforts in carbon fibers, polymer and metal matrix composites, monolithic ceramics, and carbon and silicon carbide fiber reinforced systems. In addition, a summary of the composite research topics in the European Community and Japan is provided.*

---

## INTRODUCTION

French and Japanese composite specialists met at Le Bourget, Paris, on 13 and 14 March 1990 to discuss the recent activities in composite materials research and development. From the author's perspective, it was a unique opportunity to view the materials developments of two world-class composite research groups. The French have developed expertise in aerospace structures [i.e., Societe Europeenne de Propulsion (SEP), Aerospatiale (Ariane and Hermes)], high strength fibers (e.g., Rhone Poulenc), as well as ceramic and carbon/carbon composites (i.e., SEP). The Japanese research efforts have been highlighted by strong efforts in carbon fibers and national future industries (Jisedai) programs in polymer and metal matrix composites coupled with a strong monolithic ceramics program. In addition, fiber development programs are notable, particularly in carbon and silicon carbide fiber reinforced systems (i.e., Toray, Ube, Nippon Carbon).

The conference organization provided the following four sessions over a 2-day period with a balance of speakers from both nations:

- New Materials
- Processing and Fabrication
- Databases
- Evaluation and Modeling

The conference was jointly sponsored by Japan's Agency for Industrial Science and Technology (AIST) (a Ministry of International Trade and Industry (MITI) agency), Japan's Science and Technology Agency, and Japan's Industrial Technology Association. French sponsorship was provided by CODATA, the Ministries of Education, Foreign Affairs, Research and Technology, and Energy. The conference proceedings can be obtained from:

Bernard Marx  
Ministere de l'Education, de la  
Jeunesse et des Sports  
Direction de la Programation et du  
Development Universitaire  
61-65 rue Dutot  
75015 Paris, France  
Tel: 40.65.60.97  
FAX: 40.65.60.93

---

or

Claude Bathias  
Department Materiaux Industrielles  
CNAM  
292, rue Saint-Martin  
75141 Paris, Cedex 03 France

In addition, there will be a follow-on, bilateral Japan-France conference on composites in Tsukuba, Japan, from 1-3 October 1990. During October there are the following Japanese conferences in high performance materials:

1-5 Oct  
New Materials '90 Japan, Osaka, Japan

8-9 Oct  
First International Symposium on Functional Gradient Materials\* (FGM), Sendai, Japan

24-25 Oct  
Jisedai-First Symposium on High Performance Materials for Severe Environments, Tokyo, Japan

## KEYNOTE ADDRESSES

One of the two keynote speakers was Professor Hayashi, Professor Emeritus from the University of Tokyo, who spoke on "Research and Development in the R&D Project of Basic Technologies for Future Industries" in Japan. These composite programs have been reviewed in a *Scientific Monograph* [M.J. Koczak et al., "Inorganic composite materials in Japan: Status and trends," ONRFE M7 (November 1989)].

His French counterpart, Dr. J. Odorico of Aerospatiale Research Center, discussed "The Use of Composite Materials for Aeronautical Structures." The similar themes

reflected the desire of both countries to enter and/or gain a larger sector of the aerospace market. Both nations have excellent directed research and emerging aerospace programs, e.g., France's Airbus, Ariane, and Hermes programs and Japan's Future Industries Programs (i.e., Jisedai) and HOPE (High Orbiting Plane Experimental), as well as their satellite, commercial aircraft, and engine developments.

Odorico cited three composite development areas: (1) organic matrix composites with use temperatures to 100/120°C and 200/300 °C; (2) metal matrix composites, e.g., aluminum, magnesium, and titanium; and (3) materials for thermal structures from 500/600 °C to 2,000 °C. In the first area of organic matrix composites, the weight saving realized on the A320 Airbus is 1,100 kg, or a structural weight saving of 25 percent. The application of composite structures in aircraft applications is shown in Table 1 with possible future weight savings to be anticipated from carbon fiber wing spars and fuselage.

Aerospatiale has stressed the requirements for the development of outer wing structures at or near the competitive cost of aluminum wing structures. In order to achieve these objectives, automated industrial technologies of automatic tape laying, water cutting, and stacking are required, particularly for high curvature shapes. Research and development is proceeding on a graphite/epoxy central wing box that will permit the production of a carbon epoxy wing for a 100-passenger aircraft. The critical materials property requirements focussed at compressive strength after impact for structures with a through hole. This need echoes the lower compressive properties of several fiber systems, e.g., carbon, Kevlar®, and the design limiting features that result, particularly after impact damage.

---

\*A list of papers of the last Japanese FGM conference is provided in the Appendix.



Table 1. R&D at Aerospatiale for Weight Savings Via Composite Use

Year	Aircraft	Applications	% Weight Savings
1969	Vantour	carbon nacelle doors	5
1972	Concorde	carbon elevators carbon wing fillets Kevlar® cabin trim <sup>a</sup> Kevlar® fairings <sup>a</sup>	5
1974	Corvette	carbon cargo doors	6
1977	A300	carbon air brakes carbon links	8
1979	A310	carbon air brakes <sup>a</sup> carbon LS ailerons Kevlar® fairings <sup>a</sup>	10
1981	A300-600	carbon air brakes <sup>a</sup> Kevlar® fairings <sup>a</sup>	11
1988	A320	carbon fiber wing spar fuselage	20

<sup>a</sup>Applied in production.

For metal matrix composites, utilization is focussed in thicker section structures where the resin composite systems do not have the required through thickness properties. The combination of low coefficient of expansion coupled with good thermal conductivity provides for good structural stability during thermal excursions. Applications for aluminum metal matrix composites include casings, helicopter gear box covers, and satellite tank fittings. The third area of thermal structural composites refers primarily to ceramic matrix and carbon/carbon (C/C) composites, where the development is intimately tied to national and international space programs.

## DEVELOPMENT OF NEW MATERIALS

An excellent and comprehensive review of the development of fibers in Japan was provided by Junichi Matsui of Toray in terms of utilization and production as summarized in Table 2. The major polyacrylonitrile (PAN) and pitch-based carbon fiber producers are detailed in Table 3. It would be very informative to distinguish between production capacity versus actual production and utilization. A recurring theme is the relative compressive strength of the carbon fibers. Three different trends are noted for pitch high strength (HT) and high

modulus (HM) graphite fibers. For pitch-based fibers, compressive strength is reduced with increased tensile strength. For HM fibers, compressive and tensile strengths

increase, while for HT graphite fibers, the compressive strength remains constant with increased tensile strengths. The data suggest that the ratio of tensile/compressive strength can range from 2 to 6.

Table 2. Consumption of Fiber Reinforced Plastics

Reinforcement Fiber	Matrix Resin	Consumption (tons)	Application
Glass	unsaturated polyester	323,000	Building, construction, vessels, boats
Glass	thermoplastics	130,000	Automotive, business machines
Glass	epoxy	25,000	Printed circuits
Paper	phenolics	78,000	Printed circuits, insulation
Carbon	epoxy	1,300	Sporting goods, aircraft, x-ray equipment
Aramid	epoxy	700	Sporting goods, machinery parts

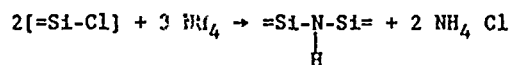
Table 3. Carbon Fiber Manufacturers and Capacity

Precursor	Manufacturer	Capacity (tons)		Strength	Modulus
		1989	1990		
PAN	Toray	1500	2250	high	high
	Toho Rayon	1420	2020	high	high
	Mitsubishi Rayon	150	500	high	high
	Asahi Kasei Carbon Fiber	450	450	high	high
Pitch, petroleum	Kureha Chemical	900	900	low	low
	Nippon Petrochemical	50	50	high	high
	Tonen	12	12	high	high
	Petoca	12	12	high	high
Pitch, coal	Donac	250	250	high/low	high/low
	Mitsubishi Chemical	500	550	high	high
	Nippon Carbon	36	36	high	high
	Nippon Steel	12	12	high/low	high/low

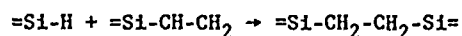
Developments in aramid fibers involve the production of Technola T240 by Teijin. Technola T240 has comparable strength but lower moduli and higher strains to failure than Kevlar®. The silicon carbide fiber systems include two Japanese and one French fiber products, i.e., Nippon Carbon, Ube, and Rhone Poulenc. In this regard the French SiC fiber is the newest and compares favorably with the Nippon Carbon Nicalon SiC fiber.

The new silicon carbide ceramic fiber, Fiberamic, from Rhone Poulenc was reviewed by Gerard Perez. The goal was to retain good properties in oxidative environments up to temperatures of 1,300 to 1,400 °C. The fiber reactions in the production of the silicon oxycarbide fibers involve thermal treatments in inert and oxidative environments. In addition, the French development of polysilazane precursors allows for the minimization of the oxygen-carbon reaction. Precursor synthesis requires three stages. The following three reactions are involved in the synthesis, curing, and pyrolysis stages:

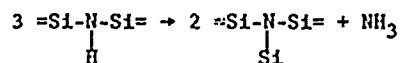
#### SYNTHESIS:



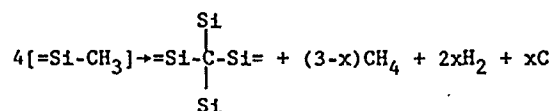
#### CURING:



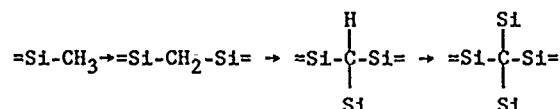
The reactions are activated by using a catalyst or photochemical techniques. Following precuring, complete curing by silylation of N-H groups can be thermally activated (up to 450 °C).



#### PYROLYSIS:



The curing transition is very complex since it involves different steps of silylation:



As a result, the chemistry of the fiber has a lower free carbon and oxygen content than Nicalon with a significantly higher nitrogen level. It would be useful to compare the Dow Corning SiC fibers with the French Fiberamic systems (see Table 4). It was claimed that the structure remains amorphous up to 1,400 °C in nitrogen atmospheres. The stability in vacuum and oxidative environments is for only short term exposures, e.g., 900 seconds at 1,000 to 1,500 MPa. In general, the Rhone Poulenc SiNC fiber appears to retain a significantly higher strength after the nitrogen short term exposures. The future development of thermally stable SiC type fibers is dependent on interfacial control via fiber and matrix chemistry. As a result, a microstructural stability comparison of the Tyranno (Ube), Nicalon (Nippon Carbon), Dow Corning, and Fiberamic (Rhone Poulenc) fibers should be an interesting assessment with regard to glass-ceramic and ceramic matrix systems (SiC/SiC). If the combination of modulus and strength is considered for the Nicalon and the Fiberamic, the SiNC Rhone Poulenc fiber has a wider range of moduli while the Nicalon has a higher strength level. In addition to the long fiber SiC systems, a 17-micron-diameter, 0.7-mm-long short fiber is also available. This should prove an interesting fiber for reaction-bonded silicon nitride

(RBSN) systems in the assessment of the effects of fiber aspect ratios and the effect on fracture toughness. Hercules has signed an agreement with Rhone Poulenc to supply the SiC fiber in the United States.

## JAPANESE AND EUROPEAN COMMUNITY (EC) GOVERNMENTAL COMPOSITE PROGRAMS

Several talks concerned the general trends of composite processing in Japan and France. However, they were disappointing, especially with regard to discussing new programs and predicting future composite materials efforts and application trends. Recently, a new intermetallic and high temperature composite program was announced; however, the details of the program were not discussed at the conference. The following excerpt is from an article from the *Nihon Kezai Shinbun* (2 May 1989) that described Japan's new intermetallics and high temperature composite materials program:

A new Japanese initiative involves a Joint R&D Plan for Ultra-High Temperature Materials. MITI's Agency of Industrial Science and Technology (AIST) has formulated a basic program for "Super Environmentally Resistant Advanced Materials" which will be taken on next fiscal year as a new topic within the Next Generation Industrial Base Technology R&D System. The

program will focus on the development of materials which can withstand temperatures as high as 2,000 °C and will deal with six types of research topics such as niobium-aluminum system metallic compounds and composite materials with carbon and silicon carbide fibers. Contingent on the establishment of a FY89 budget, initially the program will be started at five research centers under AIST and then in July a joint government/private sector system will be established by calling for the participation of businesses.

According to the plan, the materials to be developed are: (1) metallic compounds with 1,800 °C heat resistance combining niobium, molybdenum, aluminum, silicon, etc.; (2) titanium-aluminum metallic compounds that can withstand 1,300 °C; (3) carbon fibers embedded in ceramics in such a way that oxidation does not occur; (4) high strength silicon carbide fibers; (5) carbon fiber/carbon composite materials that can withstand 2,000 °C; and (6) metallic compounds strengthened by silicon carbide fibers.

The AIST research centers in charge of the research are the National Research Laboratory of Metrology, the Mechanical Engineering Laboratory, the Government Industrial Research Institute-Nagoya, the Industrial Products Research Institute, and the Government Industrial Research Institute-Kyushu. Foreign companies will also be sought for the participation of private sector businesses. Plans call for a capital investment of more than ¥5 billion (\$32 million @ ¥155 = \$1) by FY97.

Table 4. The Chemistry of Nicalon and Fiberamic SiC Fibers

Fiber	Composition		Equivalent Phase	
	Element	at. %	Component	wt. %
Nicalon	Si	58	SiC	55
	C	30	SiCO	30
	O	12	free C	15
Fiberamic	Si	57	SiCNO	95
	C	13	free C	5
	N	22		
	O	8		

---

In Europe several composite programs have been initiated under joint EC support under the BRITE/EURAM and EUREKA programs. Table 5 lists the funded metal, ceramic, and polymer matrix composite programs in the BRITE/EURAM program. Further information on the BRITE/EURAM programs can be obtained from:

UNIPUB  
4611 - F Assembly Drive  
Lanham, MD 20706-4391  
Tel: 800-274-4888  
FAX: 301-459-0056

EUREKA program information:

EUREKA Secretariat  
Avenue des Artes 19H  
B1040 Brussels, Belgium  
Tel: 32-2-217-00-30  
FAX: 32-2-218-79-06

## PROCESSING AND APPLICATIONS

A presentation by Philippe Beutin of AFME (French Agency for Energy Management) described the requirements of advanced materials for the automotive industry. The priority targets involve improved lifetime, i.e., corrosion resistance, reduction in noise and vibration, design considerations to facilitate new model changes, reduction of costs, and improved safety. Table 6 shows the motivations for the automotive industry and the immediate implication to materials processing. In addition, the automotive industry needs to convert from using two-dimensional materials (i.e., sheet steel) to integrated structures.

## Multimaterials

A view of "multimaterials" was presented by B. Ullmann of BIPE (Bureau d'informations et de Previsions Economiques) industrial consultancy department. They consider the materials market as divided into three sectors with associated technologies. The traditional materials are treated as commodities with an annual world market growth rate of 2 percent. New materials are basically high performance materials systems with growth rates of 6.5 percent, while emerging materials have growth rates in excess of 20 percent with dependent developing technologies. The technology of the commodity materials can be considered mature. The intermediate category of new materials is shown in Table 7.

Ullmann's theme reflects the use of cost effective multimaterials that are spawned by the development of emerging high performance materials. In the composites market, three areas of competition can be visualized: the high performance aerospace market and large scale automotive and recreational markets. Ullmann considered three areas: polymer, metal, and ceramic matrix composites.

**Polymer Matrix Composites.** As a result of the demands of the large scale market, cost effective alternative composite materials meet these requirements, e.g., semilong fiber composites, glass mat reinforced thermoplastics, thermoplastic matrix composites, and resin transfer molding products. In an optimistic projection, Ullmann forecasts that the high performance composite market shall increase to 25 percent of the total by 1995. A market summary is provided in Tables 8, 9, and 10 for thermosets and thermoplastic composites with regard to general use and high performance composites in Europe.

Table 5. BRITE/EURAM Programs in Composite Materials

Composite Type	Program	Research Institute
Metal matrix	* Optimization of ceramic fiber reinforced aluminum alloys	Renault
	* Prepregs and composite materials made of aluminum alloys reinforced with continuous fibers	DLR
	* Development of fiber reinforced aluminum metal matrix composites for applications in aerospace primary components using powder metallurgy techniques	Agusta SPA
	* Novel metal matrix composites based on hyper eutectic aluminum/silicon alloys	Univ. of Sheffield
	* Development of novel automotive piston/rod components and aerospace gearboxes from long fiber/metal matrix composites	ICI
Ceramic	* Improvement of the reliability of different silicon carbide grades for automotive applications	ISMRA
	* Ceramics based on doped boron carbide	Coating Development SA
	* X-Sialon mullite ceramics--precursors, powders, and cost effective components with improved microstructure and properties	Tech. Univ. of Denmark
	* Micro defect-free ceramic components	Inst. Guido Donegani SPA
	* Comparison of short fiber and particulate method for reinforcement of glass-ceramic materials	GEC-Alsthom
	* Ceramic-ceramic composite materials--a modelling of the CVI process	Univ. of Bordeaux
	* Fabrication and joining of graded cermets by a technique of metal infiltration	British Ceramic Research Ltd.
	* Metal reinforced ceramics	Krupp Widia GMBH
	* Ceramic/metal bonding by HIP	Armines-Ecole des Mines de Paris SEP
	* Reliability, thermomechanical, and fatigue behavior of high temperature structural fibrous ceramic composites	
	* Development of technology to produce 2- and 3-D carbon reinforced graphite structures for high strength and high temperature applications	New Metals & Chemicals Ltd.
		continued

Table 5. Continued

Composite Type	Program	Research Institute
Ceramic (continued)	* Development of ceramic and ceramic composite materials for structural applications at high temperatures with improved creep resistance, chemical stability, and reliability	Vetrotex International
	* Organometallic precursors for the preparation of high performance nonoxide ceramics and ceramic matrix composites	Fairey Tecramics, Ltd.
	* Improved high temperature corrosion resistant silicon nitride, silicon carbide composites	Univ. of Limerick
	* Industrial production process for silicon carbide whiskers for composite materials reinforcement	Pechiney
Polymer matrix	* New reinforced thermoplastic materials	Eniricerche
	* Development of alternative thermoplastic material forms for use of high performance thermoplastic composites	MBB
	* High performance reinforced thermoplastic for aerospace structural applications processed by injection molding	Aerospatiale
	* Mechanical and physical properties for new products made of polymers--the sulcated spring	Disc Computer Services, Ltd.
	* Development of CFRC materials with partially reduced carbon fiber content for use in car brake systems	Daimler-Benz
	* Development and characterization of high temperature performance, semicrystalline, thermoplastic matrix polymers for carbon fiber composites	ICI
	* Optimizing structural fiber composites by hybridization	Loughborough Univ.
	* The role of the fiber-matrix interface on the mechanical behavior and damage development in carbon fiber reinforced plastic composites	Univ. of Surrey
	* Advanced composite materials based on carbon fibers modified by plasma or electropolymerization	Univ. Notre Dame de la Paix
		continued

Table 5. Continued

Composite Type	Program	Research Institute
Polymer matrix (continued)	* Development of thermostable new high performance composites based on bismaleimide modified siloxanes matrix and continuous carbon fibers	Rhone Poulenc
	* Development of continuous carbon fiber reinforced thermoplastics and their processing for composite components	Dornier Luftfahrt
	* Lightweight mirrors made of carbon fiber compound for optical application	Ruhr Univ.
	* Lightweight reflectors of carbon fiber reinforced plastic	Fried. Krupp
	* Development of high temperature polyimide composite systems	BP International
	* Fiber reinforced plastic composite engine	Ford-Werke
	* Development of improved damage tolerant carbon fiber matrix composites	Aerospatiale
	* Development, characterization, and utilization of novel modified amorphous polyaromatics for use as composite matrices	ICI
	* Improving durability and performance of thermoplastic based composites using novel adhesion promoting polymer interfaces	Ecole des Mines
	* Lightweight hybrid composites with improved damage tolerance based on high modulus polyethylene and glass fibers	Univ. of Leeds
	* Simulation, detection, and repair of defects in polymeric composite materials	Agusta SPA
	* Numerical and experimental techniques for composite material, structural design, and validation in advanced industrial applications	Thompson Sintra
	* Design methodology for the improvement of damage tolerance within composite structures	British Aerospace
	* Composite material for marine structures and components	Cetena SPA

The potential benefits of these cost effective processes involve the use of large panels and components and the capability of producing complex shapes with relatively short cycle times. Matte or "paper" style technology is used for 12-mm-thick panels

using recyclable thermoplastics. The limitations of the process remain the relative materials cost, the requirements of a "class A" surface finish, and hot handling of the components.



Table 6. The Generic Material Drivers of Automotive Technology

Generic Drivers of Automotive Technology	Implication for Materials R&D
Need for reliability	<p>Emphasis on production of materials with minimal variation in properties and dimensions.</p> <p>Development of sensors and control systems of materials fabrication processes.</p> <p>Development of materials databases.</p>
Need for low cost	<p>Emphasis on 'net shape' processes for complex components.</p> <p>Development of high productivity processes (including energy).</p>
Need for functional improvement	<p>Emphasis on weight saving materials.</p> <p>Development of functional characteristics and design studies simultaneously with materials and process choice.</p>
Need for durability	<p>Research on durability-related failure mechanisms (wear, fatigue, and corrosion).</p> <p>Research on methods of predicting durability.</p>
Need for reusability	<p>Research on technical and economic factors in recycling.</p>

**Metal Matrix Composites.** For automotive applications, three classes of products were considered: (1) billets produced by powder metallurgy or spray forming processes for wrought powder metallurgy and SiC composite materials applications, (2) ingot types of materials using traditional casting approaches, and (3) direct squeeze casting of products. The ability to use the squeeze casting approach is limited by the

need for integrated manufacturing systems that can mass produce components at competitive costs. The developmental investment cost and engine material redesign, however, can limit applications. The technical issues involve the understanding of melt fluidity as a function of reinforcement and temperature coupled with manufacturing consolidation or injection pressure limitations of 7 to 14 MPa.

Table 7. New Materials as Drawn by BIPE

Basic Materials	New Materials
Technical thermoplastics	<ul style="list-style-type: none"> <li>* Polyamides (PA)</li> <li>* Polyacetals (POM)</li> <li>* Polycarbonates (PC)</li> <li>* Modified PPO</li> <li>* Thermoplastic polyesters (PET/PBT)</li> <li>* Polyethylene terephthalate (PET-Bottles)</li> <li>* Technical polymer blends and alloys</li> <li>* New up market plastics</li> <li>* Elastomer thermoplastics (TPE)</li> <li>* Fluor-based thermoplastics</li> </ul>
Thermosetting plastics and technical adhesives	<ul style="list-style-type: none"> <li>* Epoxy resins</li> <li>* Polyurethanes</li> <li>* Silicones</li> <li>* Phenolic resins</li> <li>* Technical adhesives</li> </ul>
Glass	<ul style="list-style-type: none"> <li>* Laminated glass</li> <li>* Low emissivity glass</li> <li>* Composite glass</li> <li>* Lightweight glass bottles</li> </ul>
Ceramics	<ul style="list-style-type: none"> <li>* Fine ceramics</li> <li>* Ceramics for catalytic converters</li> </ul>
Steel	<ul style="list-style-type: none"> <li>* Coated sheets</li> <li>* High strength steel (HSLA) sheets</li> <li>* Tin free steels</li> <li>* Magnetic sheets</li> <li>* Stainless sheets</li> <li>* Continuously hot treated sheets</li> <li>* Pretreated bars</li> </ul>
Nonferrous metals	<ul style="list-style-type: none"> <li>* Titanium and alloys</li> <li>* High strength aluminum sheets for stamping</li> <li>* Aluminum alloys for casting</li> <li>* Aluminum alloys for aeronautics</li> <li>* Aluminum-lithium alloys</li> <li>* Plated copper alloys for electrical contacts</li> <li>* Superalloys</li> </ul>
Composites	<ul style="list-style-type: none"> <li>* Consumer goods composites</li> <li>* High strength organic matrix composites</li> <li>* High strength, high thermal resistance, nonorganic matrix composites</li> <li>* Carbon-carbon composites</li> </ul>
Materials for electronics	<ul style="list-style-type: none"> <li>* Metals</li> <li>* Silicon, AsGa</li> <li>* Ceramics</li> <li>* Others</li> </ul>

Table 8. Percentage of Organic Matrix Composites by Geographic Zones

Country	General Use (%)	High Performance Composites (%)
United States	42	55
France	7	5
Japan	15	21
Great Britain	7	4
Germany	10	4
Other European	12	9
Others	7	2

Table 9. Percentage of Market for Organic Matrix Composites

Type of Material	World Market <sup>a</sup> (%)	Composite Market <sup>b</sup> (%)
General use thermoset	77	58
Thermoplastic	21	30
High performance	2	12

Table 10. Demand for Composite Structures in Europe

General Use		High Performance	
Area	%	Area	%
Transportation	26	Aerospace-military	27
Building	20	Sports & leisure	27
Electronic	17	Aerospace-civilian	18
Sports & leisure	11	Land transportation	3
Others	26	Industrial	19
		Others	6

---

From a mechanical property viewpoint, predicting performance and properties remains an issue for design engineers. In France the efforts are led by Pechiney, while several groups in Japan have pursued the squeeze casting approach, notably Toyota Central Research and Development.

**Ceramic Matrix Composites.** The development of ceramic matrix composite systems has been pioneered by the aerospace industry in France, notably SEP and Aerospatiale. A 4-year collaborative study has been undertaken by SEP in France and MAN in Germany under AFME sponsorship. The themes of the program involve cooling system weight and cost reduction; reduction of fuel consumption, noise, and pollution; and the use of multiple fuel sources. The program areas involve fiber matrix selection and compatibility (e.g., mechanical and thermal), machining, and joining.

## Applications

A brief review of materials applied to naval shipbuilding and nondestructive evaluation techniques was provided by F. Lesberre of STCAN. The production of GFRP minesweepers has been carried out by Direction des Constructions Navales (DCAN) of Lorient. Currently, a 250-ton GFRP BAMO minesweeper is being constructed as well as smaller 21-ton custom observation "vedettes." In addition, DCAN of Cherbourg has constructed external decking and bow domes for submarines. Additional composite applications include torpedo tubes by St. Tropez and aerospace radomes by CUERS near Toulons.

With regard to nondestructive approaches for composite structures, the present techniques involve liquid penetrants, radiographic inspection, and ultrasonic

approaches. The techniques being developed use infrared thermal inspection or mechanical inspection (vibrothermography). Microwave techniques are used in an active and passive mode, are sensitive to humidity and moisture effects, and provide in-depth information. The use of neutron radiography has been suggested and a mobile source is being developed under the DIANE project in the EUREKA program. Participants include SODERN (France), SENER (Spain), IABG (Germany), and LTV Aerospace (United States).

## MATERIALS DATABASES

The development of national and international materials databases was addressed by six speakers. Both France and Japan have developed a composite materials database. The issues that have to be addressed were cited by S. Nishijima of the National Research Institute for Metals in Tokyo:

- materials identification
- terminology harmonization
- data exchange
- data reporting formats
- models for data evaluation and analysis

He noted the formation of several groups in the area of database development: VAMAS TWA-10 Group on Standardization of Materials DataBanks, CODATA Task Group, CEC Group, and the ASTM E-49 Group on Computerization of Materials Databases. The individuals associated for the various Japanese databases are:

- Mr. Tadao Iwasaki, Director, Information Resources Division, Japan Information Center of Science and Technology, 2-5-2, Nagata-cho, Chiyoda-ku, Tokyo 100.

- Mr. Hideaki Takahashi, Japan Key Technology Center, ARK Mori Bldg., 1-12-32, Akasaka, Minato-ku, Tokyo 107.
- Mr. Akio Shimizu, Japan High Polymer Center, 2-9-9, Higashi-Shinbashi, Minato-ku, Tokyo 105.
- Mr. Hirofumi Makiura, New Materials Center, Foundation of Osaka Science and Technology Center, 1-8-4, Utsubo-Honmachi, Nishi-ku, Osaka 550.
- Mr. Takeshi Morikawa, New Glass Forum, Japan Association of New Glass Industries, 3-1-9, Shinbashi, Minato-ku, Tokyo 105.
- Mr. T. Kitamura, Japan Reinforced Plastics Society, Maruden Bldg., 3-15-15, Ginza, Chuo-ku, Tokyo 104.

A review of the materials data banks in France was provided by Bernard Marx. Forty databases are available from a variety of commercial (34 percent), public research centers (24 percent), and university and nonprofit laboratories (21 percent). The structural materials databases are provided in Table 11.

## SUMMARY

The France-Japan conference provided a brief view of the composite efforts in both countries. Unfortunately, the view was

partial and did not include the major new composite efforts under EC and MITI/AIST sponsorship. There are several EC composite programs under the BRITE/EURAM and EUREKA programs. Although not integrated into a formal composite effort under one umbrella, they represent a significant resource investment in European composite research. The Japanese efforts in intermetallic and ceramic matrix composites represent a dedicated effort to enter the high temperature materials regime when combined with their functional gradient materials program. These French and Japanese programs are notable for their emphasis on C/C, SiC/SiC, C/SiC, and graded composite systems for elevated temperature applications.

A notable difference was the commercial sector emphasis for both the European and Japanese efforts. This will emphasize the use of lower cost pitch and glass fiber in high speed manufacturing operations. A second feature is the development of metal matrix and organic composite materials data banks for design use. This represents a maturing technology in metal matrix composites. However, the level of design reliability in terms of a statistical distribution of properties must be determined before immediate acceptance occurs in primary structures. In addition, the reinforcement, matrix, and processing variables suggest that a standard metal matrix composite has not been recognized and several variants proliferate the materials markets.

---

**Michael J. Koczak** is a Professor of Materials Engineering in the Department of Materials Engineering at Drexel University. He received his B.S. in metallurgical engineering from the Polytechnic University in 1965 and his M.S. and Ph.D. in metallurgy and materials science from the University of Pennsylvania in 1967 and 1969, respectively. Dr. Koczak has considerable research experience in the areas of powder metallurgy and composite materials with over 100 publications. He served as Liaison Scientist for the Office of Naval Research, Tokyo in 1985 and joined the ONR-Europe Office, London for a 2-year period in June 1989. Awards include the Meritorious Civilian Service Award and the Lindback Teaching Award.

---

Table 11. French Factual Materials Data Banks

Data Bank	Contents	Field
ADEP	Thermodynamic properties and transport of gaseous, liquid, or solid bodies	Thermodynamics
ADHEMIX	Characteristics of structural adhesives available on the French market	Adhesives
ALUSELECT	Assistance in selecting the principal aluminum welding alloys	Aluminum
ARTEMISE	Chemistry of rocks and materials, geology, petrography; igneous, metamorphous, and sedimentary types	Geochemistry
CETIM DIAMANT	Assistance in the conception of mechanical parts and structures	Mechanics
CETIM FATIG	Calculation of the resistance to fatigue of, in most cases, steel mechanical parts	Mechanics
CETIM FIMAC	Mechanical and physical characteristics of polymers and composites	Polymers, composites
COMPOSITE DATA	Uses, characteristics, and applications of composite materials	Composites
FATIGUE	Results of fatigue tests on metallic materials used in aeronautics	Aeronautics
GEPROC	Mechanical characterization tests on samples of composite materials	Aeronautics
G3F	Guide to composite materials and adhesives	Composites, adhesives
INFOVISION	Assistance in searching for products and manufacturers in the bearing trade	Mechanics
PMC	Assistance in selection of materials for building and road maintenance	Civil engineering
PROCOP-M	Calculation of the loss of filled polymers and the resistivity of polymers and composites	Polymers, composites
		continued

Table 11. Continued

Data Bank	Contents	Field
REFDATA	Assistance in searching reference materials for calibration	Referral materials
SG-PROMAT	Materials, products, and spheres of activity of the Saint Gobain Group	Building, mechanics
SPAO	Technical guide to polymers in the Common Market countries	Polymers
THERMODATA	Thermodynamic properties of elements, mineral compounds, and metallic alloys	Thermodynamics
THERMOSALT	Thermodynamic properties of molten salt mixtures	Thermodynamics

---

## Appendix

### TOPICS OF THIRD FUNCTIONAL GRADIENT MATERIALS (FGM) CONFERENCE 14 SEPTEMBER 1989

- \* Co Plasma Deposition of Ni-Cr-Al-Y,  $\text{ZrO}_2$ -8 wt. %  $\text{Y}_2\text{O}_3$  for Graded Structures
- \* Low Pressure Plasma Spray with X-Y-Z and Rotational Control
- \* Model of Graded Structures, Physical Properties
- \* Development of Ti-Ni-C SHS Reactions to Produce TiC/Ni Composites
- \* Production of Graded Cu-TiB<sub>2</sub> Composites via Powder Processing and SHS Reactions
- \* Modelling of SHS Reactions in Cu-TiB<sub>2</sub> Materials
- \* Ni-ZrO<sub>2</sub> Graded Composite Structures
- \* 304 Stainless Steel/PSZ  $\text{ZrO}_2$ -3 mol % Graded Composites Analysis of Strength, Thermal Conductivity, Microstructure
- \* Development of Mechanics Analysis of Graded 304SUS, PXZ Graded Structures (SUS = Stainless Steel)
- \* Thermal Gradient Analysis and Sintering Response in PZT Structures
- \* Development of SiC/C Functional Graded Materials via CVD Process ( $\text{SiCl}_4$ - $\text{CH}_4$ )
- \* Development of SiC/C Materials by Silane Reactions Thermal Conductivity and Thermal Expansion Analysis (also CVD in 3-D Fabrics)
- \* PVD of TiC/Ti Composite Layers
- \* Analysis of CVD Deposition of  $\text{SiCl}_4$ ,  $\text{CH}_4$ , and  $\text{H}_2$  Mixtures in Terms of Reaction Products for C/C, TiC/Ti, and C/SiC Composite Structures
- \* Modulus/Stress Modelling Evaluations of 304 Stainless Steel/ $\text{Si}_3\text{N}_4$  Structures with Various Void Geometries
- \* Computer-Aided Stress Design of FGM Materials
- \* Stiffness/Compliance Analysis of Layered FGM Structures, e.g., René 41/ $\text{ZrO}_2$ , Ti-Cr-Al-4V/ $\text{ZrO}_2$
- \* Interdiffusion Analysis (Moving Boundary Problem) for V-C Phase Diagrams
- \* Computer Analysis of FGMs
- \* Thermal Conductivity/Diffusibility of Graded Structures
- \* Acoustic Response of Graded SUS 304/ $\text{Al}_2\text{O}_3$  Structures
- \* Chemical Analysis of Plasma Sprayed Ni Alloy (Ni-Cr-B-Si-Fe-C) and  $\text{Al}_2\text{O}_3$  Composites
- \* Development of CVD, PCVD SiC, at Various Thickness Ranges (Strength-Modulus Evaluations),  $\text{ZrO}_2$ - $\text{Y}_2\text{O}_3$  Strength Analysis
- \* Grade Propagation Analysis/Toughness Analysis for SiC/2025-T5,  $\text{ZrO}_2$ /Ni, and  $\text{ZrO}_2$ /SUS 304 Materials
- \* Thermal Conductivity of NiCrAlY/ $\text{ZrO}_2$  +  $\text{BY}_2\text{O}_3$  FGM
- \* Design of High Temperature Testing Facility, Stress Analysis in PSZ/NiCrAlY/Mar M200 Structures
- \* Design/Development of 6,000 °C Plasma Deposition Torch for FGM
- \* Topological Microstructural Analysis of Graded Structure
- \* Thermal Conductivity Analysis of Anisotropic Graded Structures with Ellipsoid Reinforcements
- \* Development of Highly Accurate Transducers for Displacements, Acoustic Emission, and Laser Heating Devices



---

# FIRST INTERNATIONAL CONFERENCE ON SUPERCOMPUTING IN NUCLEAR APPLICATIONS

---

David K. Kahaner

---

*The First International Conference on Supercomputing in Nuclear Applications (SNA90) was held from 12-15 March 1990 in Mito City, Japan. This paper summarizes the significant presentations and vendor exhibits associated with Japanese software and hardware.*

---

## INTRODUCTION

The First International Conference on Supercomputing in Nuclear Applications (SNA90) was organized by the Japanese Atomic Energy Research Institute (JAERI). JAERI was incorporated in 1956 with the purpose of "contributing fully to atomic energy research, development, and utilization of the nation's program." Major projects are: (1) nuclear energy production system including high temperature gas-cooled reactor and fusion reactor, (2) nuclear safety research, (3) radiation applications, and (4) nuclear ships. JAERI basic research and support involves cooperation with many outside organizations. In 1989 there were about 2,500 people employed at five sites. Most of these are within 2 hours of Tokyo. The largest and oldest site is the Tokai

Research Establishment with about 1,400 employees. The 1989 budget for JAERI was ¥105B (about \$700M). The JAERI computer center supports the central computing needs of these laboratories. Last year this amounted to the following:

Number of users .....	2,167
Number of batch jobs .....	796,965
CPU time .....	27,202 h
Number of output sheets .....	1,422 million ?
Number of time share sessions .....	660,578

About 35 percent of computer time is devoted to fusion, 20 percent to safety, and 16 percent to high temperature gas reactor research. Less than 2 percent of computing time is associated with nuclear power ship research.

The meeting participants included about 660 people broken down as follows:

<u>Country</u>	<u>Participants</u>	<u>Talks</u>	
Belgium	2	1	
Denmark	1	1	
FRG	3	4	
Finland	1	1	
France	15	7	
Italy	4	3	
Japan	608	78	
Portugal	1	1	
Spain	1	0	
Switzerland	1	0	
U.K.	6	5	
U.S.A.	18	16	

those I heard discussed afterwards, several threads emerged:

- (1) New fluid dynamics algorithms.
- (2) "Newish" algorithms, or old algorithms, made to run on new computer architectures. The largest fraction of these involved developing a program to run on one of today's supercomputers. A few papers were by researchers who were trying to use more advanced computers, such as the multiprocessing Sequent.
- (3) Software for better man-machine interfaces in the control room of a nuclear power plant, for simulation of power plants, for process control, etc.
- (4) Safety. Although there were only a few talks on this issue, it was often mentioned as being very important.

The participants were affiliated as follows:

Japanese Government.....	1
Universities .....	42
Government organizations .....	256
(JAERI 180)	
Companies.....	306
(Exhibition staff 110)	
Press .....	3

Of the American participants about one-third were from various Department of Energy (DOE) laboratories, the remainder from companies or universities. Other than some keynote speeches and a panel discussion, all the technical sessions were run via three parallel sessions. There were more than 120 technical presentations. A proceedings is being prepared. It is available for ¥15,000 (about \$100) from

Kiyoshi Asai, Conference Secretariat  
Computing Center, JAERI  
Tokai-mura, Naka-gun  
Ibaraki 319-11 Japan

Not being an expert in nuclear technology, I attended only those sessions focused on interesting computer applications (excluding robotics). Of the talks I did attend, and

## SUMMARY EVALUATION OF THE JAPANESE ACTIVITIES

The Japanese papers indicate that their researchers (in nuclear fields) are up to date in the use of vector supercomputers for modelling, behind in the use of graphics in these applications, and on par or slightly ahead of the United States in integration of advanced software and hardware, including graphics, for running nuclear plants. Research in the use of new computer architectures was not much in evidence, and what I did see was mostly outside the nuclear industry and laboratories. Within JAERI, I saw no evidence of the sort of advanced research into using new computers such as the hypercube, Connection Machine, etc. that is now occurring at Oak Ridge, Los Alamos, or Livermore.

---

Keynote speeches were presented by Eugene Wachspress (Univ. of Tennessee), who is well known for early work on numerical algorithms used in reactor simulation, and S. Kondo (U. of Tokyo), whose work I did not know but is well respected in the nuclear community. Wachspress presented a brief history of computing in nuclear applications and a request for better benchmarks on realistic problems. He emphasized the need for better software, as this has not kept pace with the rapid developments in hardware, and for testing and prototyping on workstations.

Kondo presented a thoughtful analysis of the need for research in the nuclear industry. In Japan, nuclear energy has reduced dependence on imported oil from 78 percent in 1973 to 55 percent in 1985 in spite of substantial public opposition to nuclear activities of any kind. Kondo pointed out that in spite (or because) of dim prospects for an increase in nuclear energy production in the near term, research must continue on a number of key issues. These are:

- (1) Reactor safety
- (2) Next generation reactors (light water reactors and fast breeders)
- (3) Nuclear fuel cycle
- (4) Fusion
- (5) High temperature gas-cooled reactor
- (6) Radiation applications

Kondo also pressed for "generic" research in areas such as

- (1) Advanced materials
- (2) Application of artificial intelligence (AI) and robotics
- (3) Development and application of lasers
- (4) Biological study of radiation risk

All of the last four are of particular application to the nuclear field, but generic research will be much more broadly useful. To the specific areas of this meeting, Kondo noted that advanced computation needs to play a larger role in (1) plant operation, (2) design, and (3) simulation.

Finally, he described in general terms a proposal to the Science and Technology Agency (STA) titled "ADES" (Advanced Design and Evaluation Systems for New Generation Nuclear Reactors). The goal of ADES is twofold: (1) to develop a comprehensive intelligent design support system that makes it possible for nuclear reactor designers to quickly and flexibly use the vast knowledge and experience of specialists in diverse disciplines necessary for the design, construction, and operation of a nuclear plant, and (2) to execute and interpret numerical simulations on high performance computers to validate various characteristics of the proposed design easily by the support of intelligent information processing systems.

Iain Duff (Harwell) gave an early talk about supercomputer use in Europe. His paper gave statistics by industry, by country, and by vendor. He noted that in the United Kingdom no automotive maker owns a supercomputer and wondered if this wasn't related to the state of the British automotive industry. He mentioned that the trend toward more parallelism is quite apparent in new supercomputers and the challenge is to develop algorithms to harness all of this additional hardware power.

Koichiro Tamura gave an important talk summarizing the results of the Japanese high speed computing system project at the Electrotechnical Laboratory (ETL) that began in 1981 and is now ending. Tamura's talk provided no really new information, as

---

most of the results have been published during the course of the project. Nevertheless, it was fascinating to hear an overall evaluation. He stressed several times that (1) the project was not aimed at developing a commercial supercomputer but only to evaluate key technologies to see how far they could grow if extensive research and development efforts were put into them; and (2) that one of the stated goals of the project (to produce a 10-GFLOP machine) is now considered quite modest even compared to recent commercial products, but should be appreciated in the context of (1) above, and also that the goal was set more than 10 years ago. Further, when the project goals were set it was felt that silicon device technology improvements were coming to an end, and the rapid advances in this technology were not anticipated. Tamura noted that one of the important subtasks associated with this project was the research in Josephson junction devices. This has been continued in the face of difficult technical problems. IBM, for example, quit a similar project in 1983. Tamura felt that substantial progress has been made and that two private companies recently announced some successes in this area. The project also involves developing "real" computers, including a data flow machine (Sigma-1), a four-processor local memory parallel computer (PHI), both for general purpose computation, and a special purpose satellite imaging system. The Sigma-1 machine has now been superseded by the EM-4. Tamura admitted that many of the problems associated with software have not been solved but that the project has nevertheless made several important contributions.

There were a large number of talks summarizing experiences vectorizing an existing algorithm for a Cray or NEC SX-2. In the context of solving today's engineering problems, this is work that obviously needs to be done. However, I do not think that new general insights can be derived from these, except to reaffirm that many practical people still feel that vectorization with modest parallelization is very effective and that the efforts to develop highly parallel applications remain heavily research oriented.

There were a few talks about really new computer activities. Hiroyuki Sato (Fujitsu) discussed building a molecular dynamics simulation program on CAP-256, which is a cellular array processor containing 256 identical processor elements arranged in a two-dimensional (2D) grid. CAP shares many of the same features as the PAX computer that I wrote about in a previous *Scientific Information Bulletin* article.\* One difference is that CAP can be configured to look like topologies other than a 2D array, for example, a hypercube. Another important ingredient of the CAP system is very fast video capability. Each processor has a 96-KB video RAM. In other words, a portion of the host's video screen is mapped directly from each processor. This leads to excellent imaging performance and makes such a system useful for rendering and other parallel-type image applications.

Sato's computations were performed on an early version of CAP, which used 8087 chips on each processing element. These are cheap, but very slow by today's standards, so his performance figures are rather poor. The newest version, CAP II, is not yet available for sale, but has 256 processing

---

\* D.K. Kahaner, "The PAX computer and QCDPAX. History, status, and evaluation," *Scientific Information Bulletin* 15(2), 57-65 (1990).

elements, each a 32-bit spark chip. CAP II is claimed to be about 50 times faster than its predecessor. CAP I was on display at the exhibit hall, but the exhibitors were less positive than Sato about the eventual appearance of CAP II, and this agrees with later "official" remarks by Fujitsu about waiting for user acceptance of parallel processing before supporting such products.

At the Fujitsu vendor exhibit the following paper was distributed: "Parallel Neurocomputer Architecture Towards Billion Connection Updates per Second," by H. Kato, H. Yoshizawa, H. Iciki, and K. Asakawa of Fujitsu Laboratories, Kawasaki, Japan. This paper was not presented at the conference and had no apparent relation to it. The paper describes a new architecture, an error back-propagation learning algorithm, and some planned improvements and other research plans. The authors state that a 256 processing element prototype is under development, but they were not available to discuss the project.

Y. Namito of the Nuclear Technology Division, Ship Research Institute, gave an interesting talk about joint work with researchers at the Radiation Physics Group at the Stanford Linear Accelerator Center (SLAC) titled "Viewing MORSE-CG Radiation Transport with 3-D Color Graphics." Namito and colleagues took a multipurpose neutron/photon transport code, MORSE-CG, and coupled it with color graphics software UGS77 from SLAC to allow users to have real time display of neutron/photon events in complicated geometries. Namito showed several examples. The graphical output works very well as long as there are not too many particles. This struck me as a nice collaboration, with genuinely useful output.

B. Kirk (Oak Ridge National Lab) described very good results of optimizing a code for 2D one-group diffusion equations

on a Sequent Balance 8000 with 10 processors, but this work is already known in the United States. Kirk explained that the coding effort for the Sequent was quite modest, but only after they rewrote the scalar code to run on a hypercube!

There were a significant number of papers dealing with development of sophisticated graphical interface tools and also the use of AI techniques. The display devices are typically U.S. or Japanese graphical workstations. The Japanese seem at the same level as other research teams in this area as are the Europeans. The Japanese appear to be particularly good at putting together complete solutions. I did not see any papers discussing the methodology of large scale software development for process control. Perhaps these papers would have been out of place in a "supercomputing" meeting.

The Cray vendor exhibit was visually and technically impressive. They had a Macintosh hooked to a laserdisk system with a large number of precomputed graphical demonstrations waiting to be displayed. The user interface was entirely in Japanese. One major disappointment was that I didn't see any Japanese applications, although I spent quite a bit of time there. Everything I saw was actually from a U.S. or European laboratory, university, or equivalent. Perhaps I should not have been surprised; there are few Crays in public institutions in Japan, but I expected something from the JAERI computer center or from the Ministry of International Trade and Industry (MITI) center in Tsukuba.

D. Owen (Univ. of Wales, Swansea) gave an interesting presentation on the use of a transputer system for finite element calculations. I liked this for two reasons. First, transputers seem like an attractive way of getting parallelism cheaply. Although the current performance is suffering because

of financial problems that the parent INMOS Company had a few years ago, the fact that INMOS was bought out by a French-Italian conglomerate means that the next generation of transputers will really appear and these should offer a significant performance improvement. Further, software vendors are now beginning to market good development software that releases the programmer-user from reliance on the low level OCCAM language needed in the past. For the engineer who wants to solve problems today, but faster, a better bet is to use more traditional vector computers, but transputers have high performance potential and research on them seems to be mostly overlooked in the United States. Duff put it very succinctly, "For places with more people than money." A talk by C. Bastian and S. De Jonge from the Belgium Central Bureau of Nuclear Measurements, "On-Line Analysis of Nuclear Reactions Using Arrays of Transputers," certainly could be appreciated in that same context. Second, I thought it significant that Owen could have organized his machine in any topology that worked but ultimately chose a two-dimensional grid, much like PAX and CAP. He didn't know anything about those projects nor did they know anything about his.

In the nuclear application area, one nice paper was by H. Murayama and N. Nohara (National Inst. of Radiological Science), who described the issues associated with three-dimensional (3D) positron emission tomography (PET). Currently, 2D reconstruction techniques are in widespread use in nuclear medicine, but 3D imaging will require new computing algorithms and is a very good candidate for parallel processing. The speakers described an extension of the 2D fast Fourier transform algorithm that could be applied for the 3D problem, but for a  $256^3$  data set this will require around 30 GFLOPS!

Talks at a large meeting like this are always of varying quality, but one by Kubota, Murata, and Kawai (Keio Univ.), "Automatic Distributed Systems Simulator by Nature Algorithm Using Highly Parallel Computer," was sufficiently off base that I was forced to comment during the discussion. Their idea is to do away with clever algorithms for fluid problems and instead use simple models that are easy to develop and then use the growing power of parallel processors, such as PAX. Their simulator discretizes continuous partial differential equations automatically. "But in the teraflops age it will be put to practical use and in the super teraflops age it will be the standard." Two people have been working on this project for 4 months!

A panel discussion on "Expanding Roles of Supercomputing for Future Nuclear Development and Utilization" was chaired by M. Akiyama (U. of Tokyo) and included panelists T. Asaoka (JAERI, Japan) I. Duff (Harwell, U.K.); E. Hollnagel (CRI, Denmark); A. Kavenoky (CEA, France); and E. Wachspress (U. of Tenn.). Each of the panelists gave a 10- to 15-minute opening position statement and then the floor was opened to questions. With the exception of Hollnagel, all the panelists (and members of the audience) felt, as expected, that nuclear power plants are vastly complex and there is ample need for at least two orders of magnitude improvement in the computational power needed to solve the problems of modelling, simulation, operation, maintenance, safety, etc. Hollnagel worried about supercomputer programs getting so complex that they become the master rather than the servant and felt that more effort should be expended on validating techniques, rather than on brute force. His remarks were mildly out of sync with most of the other participants, who had a

---

more engineering view of getting work done today. Duff, who has more computer science background and less nuclear expertise than the others, pointed out that hardware, software, and infrastructure all need to be developed. He felt as most others did, that a high degree of parallelism appears to be the only answer to really dramatic performance improvements, but that the software issues are very complex. Wachspress again emphasized the need for benchmarking standardized programs.

During the question-and-answer period a Fujitsu representative explained that his company was committed to improving support tools, code optimizers, and AI products and generally making computers easier to use. He summarized the hardware problems that he felt were being overcome. These include new device technology, packaging, and cooling, and all should lead to an order of magnitude improvement in computational speed even without high parallelism. He felt that teraflop computing could be achieved before the year 2000 via parallelism, but Fujitsu would only move in this direction if it was clear that users would accept and support such an approach. In other words, don't expect them to lead the way. Based on the very practical "nuts and bolts" scientists I saw at this meeting, there are many who will only reluctantly rework existing vector computer software to run on new architectures.

## **CENTURY RESEARCH COMPUTER CENTER**

As a supplement to the technical presentations, various tours were organized. I went on one to the Century Research Computer Center, in a growing high-tech suburb on the outskirts of Tokyo. This computer center is run as a service bureau

and provides computer time to the parent company and to other clients, some of whom are involved in nonscientific applications. I have been in many computer centers, but this one is noteworthy, not only for its modern and spacious appearance but particularly for the physical and data security that have been built in. From the siting of the building in a minimal earthquake prone area, far from airports or air traffic lanes, strong electric, magnetic, and microwave fields, sloped for water runoff, firm ground support, etc., to very extensive entry-exit system monitors, windows sited and automatically coverable against terrorists, to double and triple redundancy in the computer support systems, this facility is really remarkable. Normal ac electric power is backed up by three diesel generators, only one of which is actually necessary, and these are further backed up by batteries (uninterrupted power supply). The cooling systems are equally redundant; dual chilled water systems can use electricity, gas, or kerosene. The point of all this is to be able to convince corporate clients that their "data" are safe. There are presently 10 Fujitsu computers, 4 IBM mid-range units, and 1 Cray XMP, but the facility can support significant expansion. The building currently houses about 200 people. I was given a list of software packages that are supported; most of these are engineering analysis, design, or simulation packages developed outside Japan. I asked why there was no Japanese supercomputer, such as a NEC SX-2 or Hitachi 820, on the premises and received what by now is a stock answer--no software available. The center is not in the business of doing research but simply providing reliable computer cycles. The center has direct connections to New York, London, Sydney, and Bahrain. They have significant business clients in Europe but none yet in the United States. This facility is worth visiting. Contact

---

Century Research Center Corporation  
3-6-2, Nihonbashi-Honcho  
Chuo-ku, Tokyo 103  
(03) 665-9826, Fax: (03) 662-1927

The parent company, Century Research Center Corporation (CRC), is one of the oldest information service companies in Japan, founded in 1958. Last year it had sales of about \$1.2B.

## CONCLUDING REMARKS

The conference organizers and most of the participants felt that this meeting was valuable. Indeed several speakers emphasized that in the past nuclear application computations were the major motivators for high performance computing. It was certainly true that the U.S. weapons laboratories were the earliest sites of supercomputers, and that supercomputers, wherever they are located, draw talented scientists to them. The plans are to hold a second conference in about 3 years, probably in Europe.



---

# PERFORMANCE OF JAPANESE SUPERCOMPUTERS VIS-A-VIS CRAY COMPUTERS

---

Hideo Yoshihara

---

*This article is part of a final assessment report for the Office of Naval Research Far East titled "Supercomputers and Computational Fluid Dynamics in Japan."*

---

## EXPANDED SUMMARY

1. The performance of the single-CPU Fujitsu VP-400E, Hitachi S-820/80, and NEC SX-2A and the 8-CPU Cray YMP/832 was measured on an alternating direction implicit (ADI) Navier/Stokes code on a mesh approximately  $10^2 \times 10^2 \times 10^2$ .

2. Actual speeds attained were 0.395 GFLOPS for the VP-400E, 0.602 GFLOPS for the S-820/44, 0.414 GFLOPS for the SX-3A, and 1.5 GFLOPS for the YMP/832. This corresponded to actual/peak speed ratios of about 30 percent for the single-CPU Japanese computers and 56 percent for the 8-CPU Cray YMP. Because of the idealized definition of peak speed, a performance of 56 percent is outstanding but 30 percent is poor.

3. Reasons for the poor performance of Japanese computers were as follows:

- High startup (pipe fill-in) overhead in the arithmetic processor pipes due to reduction of vector length (production run) by its spread over many pipes.

- Large memory latency in the VP-400E and SX-2A primarily due to use of slow MOS chips. (Delay in retrieving numbers from memory for bussing to CPU.)

- Inadequate memory/register bandwidth for the VP-400E.

4. The performance of the autovectorizer of Japanese computers was outstanding, vectorizing 99 percent of the benchmark code without directives.

5. Reasons for outstanding performance of the Cray YMP/832 were as follows:

- Well-balanced architecture. Very low startup overhead in the processor pipes (no dilution of vector length). Low memory latency and adequate memory/register bandwidth.
- Outstanding performance of the Autotasker, which identified independent parts of the code, assigning their calculation to different CPUs with minimum idle time.

---

6. The benchmark on the recently offered Fujitsu VP-2600 (1 CPU, 4 GFLOPS) and NEC SX-3/44 (4 CPU, 22 GFLOPS) is scheduled for April and September 1990, respectively. Much-awaited results will be reported in the fall issue of the *ONRFE Scientific Information Bulletin*. Expected results of the benchmark are as follows:

- Fujitsu VP-2600: Pipe startup overhead should be similar to the VP-400E, but the number of independent paths between memory and register has been doubled, and memory latency has been essentially eliminated by overlapping fetch/store instructions. An actual speed of approximately 1 GFLOPS can be expected with an actual/peak speed ratio of 50 percent, taking the peak speed a more realistic 2 GFLOPS rather than the advertised 4.
- NEC SX-3/44: With 16 pipes per CPU, pipe startup overhead will be significantly increased. Memory/register bandwidth should be adequate for the expected reduced actual speeds with four vector fetch and two vector store paths. Memory latency has been mostly eliminated by overlapped fetch/store instructions. Assuming increased pipe startup overhead to be counterbalanced by reduction of memory latency, an actual speed of about 7 GFLOPS can be expected, still an incredible speed. Here a parallelization efficiency of the order of that for the Cray Autotasker is additionally assumed, but obtained, however, with heavier assist from compiler directives.

7. In future supercomputers, much needed increased peak speeds must be obtained by increasing the number of processor pipes

per CPU and increasing the number of CPUs. With the ADI Navier/Stokes algorithm, an increased number of pipes/CPU will decrease effective vector length, thereby increasing pipe startup overhead. Similarly, increasing the number of CPUs will decrease granularity and thus increase parallelization overhead. Both trends will decrease computer speed and hence deteriorate performance in ADI algorithms.

Other Navier/Stokes algorithms must be explored such as explicit methods with greatly increased vector length, or column relaxation methods with increased code granularity. Such benefits are accompanied by corresponding decreases of convergence rate so that a balancing of the opposing factors will be necessary.

A benchmark, not comparing different computers for a given algorithm but comparing different Navier/Stokes algorithms on a given single- or multiple-CPU computer, is thus recommended.

Finally, remember that the present computer assessment is based solely on the speed performance on a specific, albeit a mainline, CFD algorithm. Relative performance will undoubtedly change for other programs including other Navier/Stokes algorithms.

## INTRODUCTION

Japanese supercomputers were reviewed and assessed through two activities. First was a benchmark on a Navier/Stokes code, carried out together with Professor K. Fujii of the Institute of Space and Astronautical Sciences (Sagamihara) (Ref 1\*), that would exercise key components of the supercomputers in a real computational

---

\* K. Fujii and H. Yoshihara, "A Navier/Stokes benchmark for Japanese and U.S. supercomputers," *Scientific Information Bulletin* 14(2), 69-74 (1989).

fluid dynamic (CFD) environment. Computers benchmarked included all operational Japanese supercomputers and the 8-CPU Cray YMP/832. Computer company participation was enthusiastic. The benchmark provided an opportunity to meet and know key working level supervisors and senior programmers. Second was a review of the architecture of the new supercomputers, the 1-CPU Fujitsu VP-2600 and the 4-CPU NEC SX-3/44, with senior company architects. This review was made together with Dr. K. Neves of Boeing Computer Services who was provided ONR invitational orders. Results are reported in Reference 2\*.

## BENCHMARK PERFORMANCE OF SINGLE-CPU JAPANESE COMPUTERS

Japanese supercomputer companies have concentrated on single-processor computers with the determined goal of producing the fastest single-CPU computer. Aside from reducing cycle time, large peak speeds were produced using many parallel arithmetic pipes: 12 pipes for the 1.7-GFLOPS Fujitsu VP-400E, 8 pipes for the 1.3-GFLOPS NEC SX-2A, and 12 pipes for the 4-GFLOPS Hitachi S-820/80. Here the peak speed is the number of floating point operations (FLOP), as an add or multiply, that an ideal computer can perform per second assuming one clock cycle per FLOP. Peak speed in GFLOPS (billions of floating point operations per second) is thus obtained by dividing the number of independent CPU add and multiply pipes by the clock cycle time in nanoseconds (ns).

For computers with hard-chained add/multiply pipes as the VP-400E and S-820/80, each add or multiply segment of the

chained pipe was considered as independent in the determination of the brochure peak speed. When the operations are predominantly dyadic (simple add or multiply) as in the benchmark code, only one of the segments in the chained pipes can be in operation at a given time, so that it is more meaningful to count the chained pipe combination as one pipe instead of two. Accordingly a more realistic peak speed for the VP-400E for the benchmark problem is 1.14 GFLOPS rather than the advertised 1.7 GFLOPS. Similar considerations would apply to the Hitachi S-820/80, resulting in a relevant peak speed of 2 GFLOPS rather than 3. NEC computers do not have such chained combination pipes, so that the applicable peak speed would not change from the brochure value.

Hard-chaining of multiply and add pipes, as in the VP-400E and the SX-2, is intended to alleviate memory/register bandwidth constraints for combined multiply/add operations. Because of the significant impact on the peak speed, structuring a code to maximize the multiply/add operation count will clearly be cost effective on these computers.

Actual speeds measured in the benchmark were 0.395 GFLOPS for the Fujitsu VP-400E, 0.602 GFLOPS for the Hitachi S-820/80, 0.414 GFLOPS for the NEC SX-3A, and 1.50 GFLOPS for the Cray YMP/832. Actual/peak speed ratios corresponded to approximately 30 percent for the single-CPU Japanese computers and 56 percent for the 8-CPU Cray YMP/832. With such a highly idealized definition of peak speed, a performance of 56 percent is outstanding but 30 percent is poor.

Causes for the low performance of the single-CPU Japanese computers are clear.

---

\*K. Neves, "Supercomputers. The next generation," *Scientific Information Bulletin* 14(4), 77-95 (1989).

The most significant cause in the present benchmark was the high processor startup (pipe fill-in) overhead. In an arithmetic processor, a floating point (FLOP) operation is not achieved until the pipe (assembly line) has been filled. This startup time is an overhead, and it will reduce the computing speed unless it can be amortized over a sufficient vector length (production run). To characterize the pipeline performance for a given arithmetic operation (as a computing kernel), a number  $n_{1/2}$  is defined as the vector length required to achieve half the peak speed. Neves (Ref 2) suggested that a vector length three times  $n_{1/2}$  is necessary for an acceptable pipe startup overhead. In a multi-piped processor, increasing the number of pipes increases the peak computing speed, but more importantly it increases  $n_{1/2}$  since the original vector length must be partitioned over many pipes. (This is akin to splitting the production run in the case of many parallel assembly lines.) An increase of  $n_{1/2}$  leads to increased pipe fill-in overhead in the multi-piped computers and hence to a low actual/peak speed ratio.

There is a further overhead (memory latency) arising in the process of fetching numbers from memory for deposit in the vector registers. Memory latency, for example, depends on the type of memory chips used, how skillfully irregular retrievals as gather/scatter are carried out, and whether bank or line conflicts in memory are avoided. The Fujitsu VP-400E and the NEC SX-2A use slow, but inexpensive, MOS chips and have accordingly large memory access times (55 ns and 40 ns, respectively). The Hitachi S-820/80 employs fast, but expensive, bipolar chips and thus has a shorter 20 ns access time. Unquestionably large memory latency in the VP-400E and SX-2A contributed to

their reduced performance in the benchmark. It will be seen later that in the new Japanese supercomputers, the Fujitsu VP-2600 and NEC SX-3, memory latency is avoided (after the first fetch) by overlapped fetch/store instructions.

Finally, numbers must be supplied from memory to the CPU via the vector registers at a sufficient rate to prevent stoppage of the CPUs; that is, memory/register bandwidth must match the realizable speed of the CPUs, for example, by providing a sufficient number of fetch and store paths. Minimally, two fetch paths and one store path, for example, should be in place for dyadic operations.

Memory/register bandwidths for the Japanese computers are as follows: 0.70 GW/s for the Fujitsu VP-400E, 2 GW/s for the Hitachi S-820/80, and 1.38 GW/s for the NEC SX-2A. Here GW/s is billion words per second. More meaningful is the number of words that can be transmitted from memory to CPU for each floating point operation (FLOP) at half peak speed, that is, W/FLOP\*. Thus one has 1.2 W/FLOP\* for the Fujitsu VP-400E, 2 W/FLOP\* for the Hitachi S-820/80, and 2 W/FLOP\* for the NEC SX-2A. For dyadic operations memory/register bandwidth is clearly inadequate for the Fujitsu VP-400E but adequate for the Hitachi S-820/80 and NEC SX-2A.

In summary, the low performance (low actual/peak speed ratio) of the single-CPU VP-400E, S-820/80, and SX-2A in the benchmark problem was due to large processor pipe startup overhead, large memory latency (VP-400E and SX-2A), and inadequate memory/register bandwidth (VP-400E). The autovectorizers for all three computers were highly effective, attaining a vectorization ratio of 99 percent.

---

## MULTI-PROCESSOR PERFORMANCE

Multi-processor computers have a clear advantage over single-processor computers for codes having large granularity, that is, independent portions of the code containing significant numbers of operations. In these cases, independent parts of the code can be calculated concurrently on different CPUs, thereby reducing the elapsed computational time. To be effective, the autoparallelizer must not only determine which parts of the code are independent but must skillfully schedule these parts on different CPUs to avoid CPU idleness. Because of the overhead only the large granularity outer loops are parallelized. At this level it is usually a straightforward task for the programmer to implement directives to supplement the autoparallelizer if the latter fails its tasks. Inner loops, where the granularity is small, are vectorized.

In practice, most computing centers with multi-processor computing systems strongly discourage use of all CPUs by a single user to maintain high throughput, that is, many jobs per day. This is usually accomplished by charging disproportionately large occupancy charges for multiple-CPU usage and assigning a very low priority that usually leads to unacceptable turnaround. Practical outcome is that users today cannot count on the benefits of concurrent computations with multiple CPUs.

### CONTRASTING PERFORMANCE OF THE MULTI-PROCESSOR CRAY YMP/832

The approach of Cray Research to supercomputer design has been different from that of the Japanese companies. Peak

speeds have been achieved by multiple CPUs with few pipes in each CPU. The peak speed of each CPU of the YMP is 0.33 GFLOPS, with a total peak speed of 2.67 GFLOPS for the 8 CPUs. Each CPU processor has one add and one multiply pipe so that the multi-pipe dilution effect on vector length is absent. For each CPU there are two memory/register fetch paths and one store path, resulting in 4 Word/FLOP at half peak speed. With bipolar chips, memory access time is 30 ns. Unquestionably the Cray YMP/832 has a well-balanced architecture.

Performance of the YMP/832 in the benchmark was outstanding. It attained an actual/peak speed ratio of 0.56 based on the 6.41 cycle time of the benchmark YMP. CPU pipe overhead and memory latency were insignificant in the YMP for the vector lengths of the benchmark code. With two fetch paths and one fetch/store path connecting memory and register for each CPU, there was adequate bandwidth.

Since widely differing algorithms are available for the Navier/Stokes problem, the degree of parallelization possible in a given algorithm is of interest to the computational fluid dynamicist. For the benchmarked Fujii/Obayashi Navier/Stokes code, elapsed time with 1 CPU was reduced by a factor 7.22 with 8 CPUs, that is, a multiple-CPU efficiency of 90 percent. The difference of 7.22 from 8 is then a measure of the nonparallel content of the code and imperfections of the parallelization including its overhead. Of more importance to the computer manufacturer is the percentage of the "parallelizable" part of the code (Amdahl number) that was parallelized. In the present benchmark the Autotasker (Cray's automatic parallelizer) with the help of four directives achieved a parallelization ratio of 98.8 percent of the Amdahl number.

This remarkable performance of the Autotasker is the result of many years of multitasking experience starting with the XMP series.

## SUPERCOMPUTER COMPETITION IN THE NEAR TERM

Figure 1 shows existing and planned supercomputers. Near-term competition will primarily involve the Fujitsu VP-2600,

NEC SX-3/44, C<sup>3</sup> 3 (C<sup>3</sup> = Cray Computer Co.), and CRI C-90 (CRI = Cray Research Inc.). Here it is anticipated that the VP-2600 will form the basis for an expected multiple-processor computer from Fujitsu. In the following, some of the features of these computers are given together with their expected performance on the Navier/Stokes benchmark.

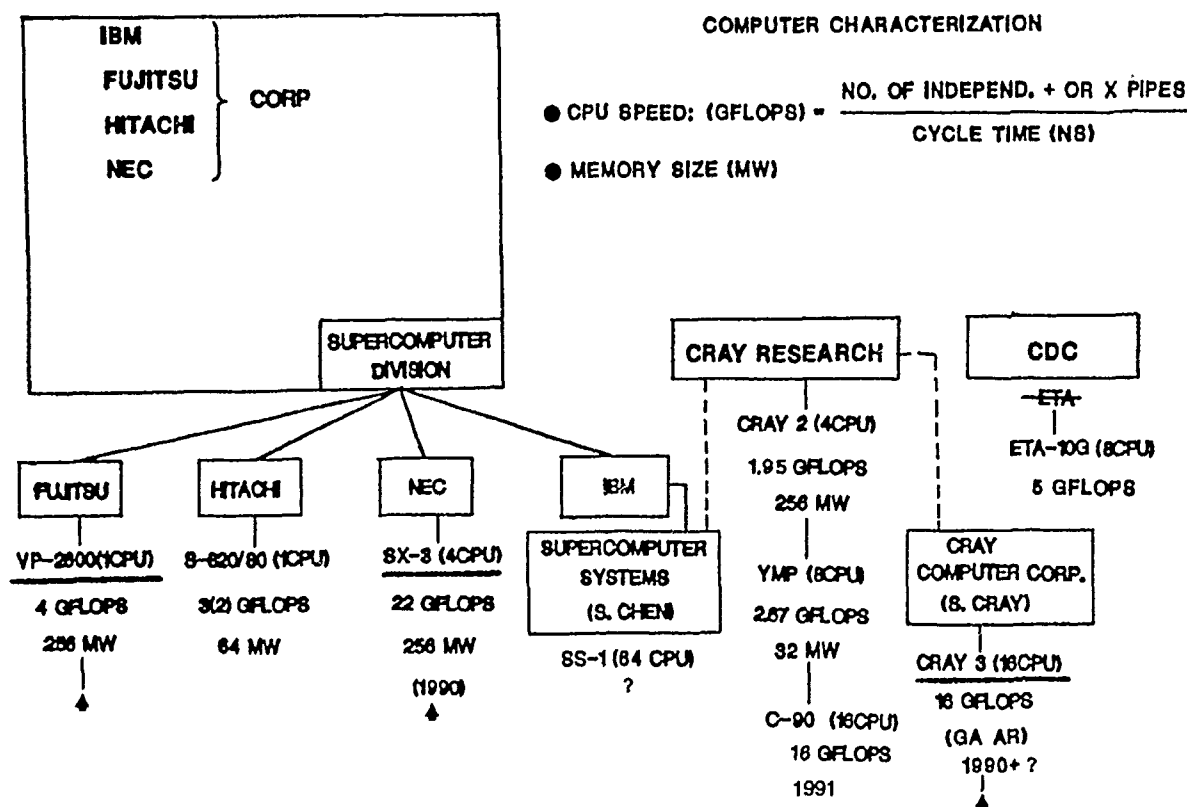
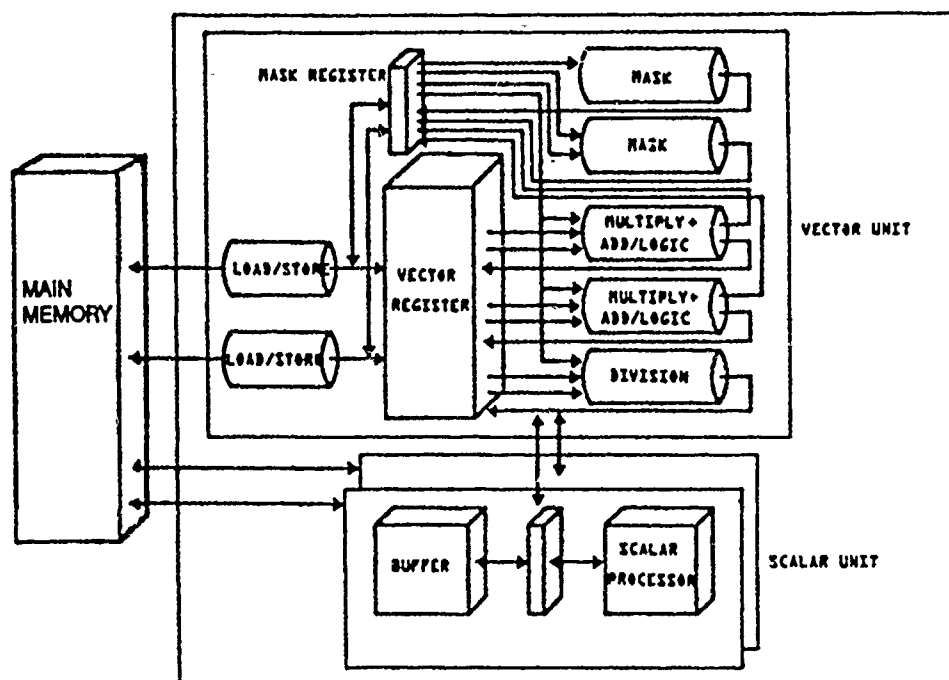


Figure 1. Existing and planned supercomputers.

## Features of the Fujitsu VP-2600 and the NEC SX-3/44

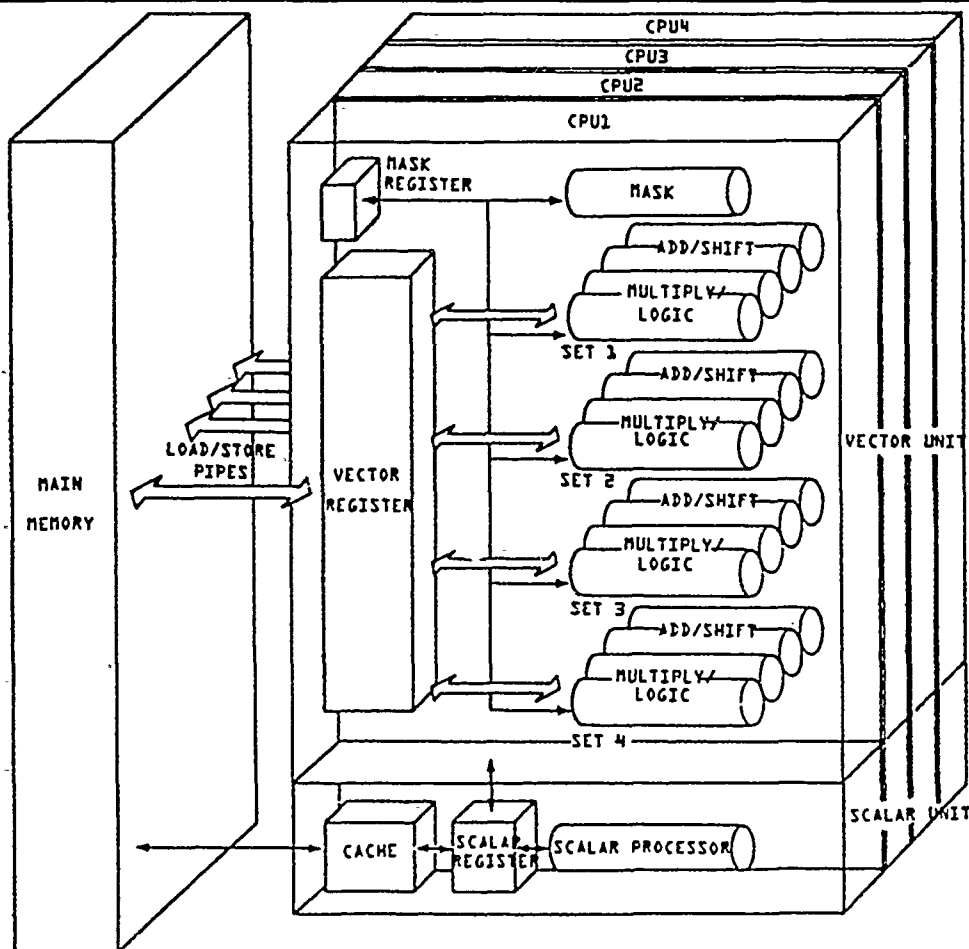
Two new Japanese computers, the single-CPU Fujitsu VP-2600 and the 4-CPU NEC SX-3/44, will be available during the summer and fall of 1990, respectively, and will be benchmarked under the same guidelines as the previous benchmark. The benchmark on the VP-2600 is scheduled for the spring of 1990, with the single-CPU measurement for the SX-3 to follow several months later. The 4-CPU SX-3/44 benchmark is scheduled for the fall of 1990. Slip-pages in the above benchmark dates may be expected due to the inevitable tuning required for the new compiler and higher priority benchmarking for potential customers. The above Navier/Stokes benchmark results and their analysis will be given in a future ONRFE *Scientific Information Bulletin* article.

System schematics for the VP-2600 and the SX-3/44 computers are shown in Figure 2. In the VP-2600 the CPU is composed of four floating point units each with two chained multiply/add pipes. Counting the total number of pipes as 16, one obtains the brochure peak speed of 4 GFLOPS with the 4-ns clock. Since the benchmark code consists predominantly of dyadic operation, the number of pipes in the VP-2600 is effectively eight, half the advertised number. This, then, results in a halving of the peak speed to 2 GFLOPS. For the SX-3/44, there are 4 sets of floating point units per CPU, each unit containing 2 add and 2 multiply pipes for a total of 16 independent pipes per CPU. With a clock of 2.9 ns, a peak speed of 5.5 GFLOPS per CPU results for a total of 22 GFLOPS with 4 CPUs. Operationally the SX-3/44 is basically two SX-2s tied in parallel.



(a) Fujitsu VP-2600. Courtesy of Fujitsu Corp.

Figure 2. System schematics.



(b) NEC SX-3/44. Courtesy of NEC Corp.

Figure 2. Continued.

### Expected Performance of the VP-2600 and SX-3/44

The actual/peak speed ratio of the VP-2600, assuming a reduced peak speed of 2 GFLOPS, should improve over that of the VP-400E. Pipe fill-in overhead should be less, memory/register bandwidth with two vector fetch paths should suffice, and the memory latency should be largely eliminated by the overlapped fetch/store instructions. An actual speed of about 1 GFLOPS might

be anticipated for the VP-2600 in the benchmark. If, however, the chained pipes can be completely unchained by the compiler, then the peak speed will be doubled to 2 GFLOPS.

For the SX-3/44 with 16 processor pipes per CPU, greatly worsened pipe overhead must be expected, resulting in a doubling of the  $n_{1/2}$ s of the SX-2A. Memory/register bandwidth of the SX-3/44 should sustain the reduced actual speeds despite the reduced cycle time of 2.9 ns, half that of the SX-2A. Overlapped fetch/store instructions will



---

greatly reduce memory latency. The NEC autoparallelizer cannot be expected to perform as effectively as the Cray Autotasker at this early stage, but with straightforward compiler directives a reasonable parallelization efficiency can be expected. Assuming the increased pipe startup overhead to be countered by the reduced memory latency, the NEC SX-3/44 should perform at the still phenomenal speed of about 7 GFLOPS.

### Performance of the C<sup>3</sup> 3 and CRI C-90

Both the C<sup>3</sup> 3 and the CRI C-90 are 16-CPU computers with peak speeds of 16 GFLOPS. C<sup>3</sup> 3 achieves 1 GFLOPS/CPU peak speed using gallium arsenide semiconductors with a cycle time of 2 ns with each CPU having one add and one multiply pipe. In the CRI C-90, however, silicon semiconductors will be retained. At the moment the cycle time and the number of processor pipes of the C-90 cannot be confirmed, but to achieve 1 GFLOPS/CPU, its hardware and architecture must be significantly different from those of the YMP/832. It would not be unreasonable to suggest a cycle time of 4 ns for the C-90 (that of the VP-2600), and the 1 GFLOPS/CPU could then be achieved by doubling the number of processor pipes of the YMP/832 to 4 pipes/CPU. It would thus not be unreasonable to suggest an actual/peak speed ratio per CPU for the C<sup>3</sup> 3 and the CRI C-90 to be the same as that of the YMP/832 for the Navier/Stokes benchmark, that is, 0.5 GFLOPS/CPU. However, doubling the number of CPUs to 16 will decrease the granularity and hence increase the parallelization overhead. Thus an actual speed somewhat under 8 GFLOPS for the C<sup>3</sup> 3 and CRI C-90 is not unreasonable for the benchmark, that is, an actual speed in the neighborhood of that of the NEC SX-3/44.

### CONCLUSIONS

There is strong contrast in the architectural approach in the supercomputer design between Japanese companies and Cray. The emphasis in Japan has been on designing a single-CPU computer with the highest peak speed, sometimes at the expense of a balanced architecture. High speeds were achieved using many parallel processor pipes. A large number of pipes decreases the effective vector length, leading to reduced computing speeds through increased pipe fill-in overhead. Adequate memory/register bandwidth can be obtained by providing a sufficient number of fetch paths, but this has been difficult for the Japanese supercomputers, which have extremely high single-CPU peak speeds.

Cray supercomputers, in strong contrast, have achieved high speeds, not only by decreasing cycle time, but by combining many CPUs with each CPU having few pipes in a well-balanced architecture. Use of 16 CPUs in both computers leads to increased parallelization overhead by the reduction of granularity.

It is clear that the ADI Navier/Stokes code of the benchmark is unsuited for the NEC SX-3/44 because the 16 pipes in each CPU dilute the already marginal vector length. It is also unsuited for the 16-CPU C<sup>3</sup> 3 and CRI C-90 because of the reduction of granularity by the large number of CPUs. In applications requiring high peak speeds of these computers, other Navier/Stokes codes with greater vector length or larger granularity must be considered. In the present benchmark problem with a mesh approximately  $10^2$  points in each coordinate direction, there will be a factor  $10^2$  increase in the vector length if the coordinate sweeps are carried out explicitly rather than implicitly,

---

Or more dramatically, if an explicit difference method, for example, using a high-order Kutta-Runge scheme, is used in place of the ADI algorithm, there will be a further  $10^2$ -fold increase in vector length. There is, however, a penalty accompanying these increases of vector length; namely, the rate of convergence of the iterative procedure is correspondingly decreased. Lowered pipe fill-in overhead must then be weighed against the increased number of iterations needed for convergence. Similarly, increased granularity is achieved by using a Jacobi column relaxation instead of the benchmark ADI procedure. Here subsequent relaxations can be initiated on successive CPUs as soon as needed updated inputs have been calculated in the prior relaxation. Again such a relaxation process will have a lowered convergence rate as compared to the ADI procedure.

A benchmark, not comparing computers but measuring the performance of different Navier/Stokes algorithms on a representative computer as the SX-3/44 or Cray 3, would therefore be of significant interest.

Finally, one is reminded that the present computer assessment was based solely on the speed performance on a specific, but a mainline, CFD algorithm, namely, an ADI Navier/Stokes code. Relative performance of the benchmarked supercomputers will undoubtedly change for other programs including other Navier/Stokes algorithms.

In the future, U.S. dominance in supercomputers is in jeopardy. Future Cray supercomputers must share performance leadership with Japanese supercomputers as the NEC SX-3/44. Creative geniuses of U.S. computer architects, as Seymour Cray, will have difficulty overcoming the corporate depth of Fujitsu Ltd., Hitachi Ltd., or NEC Corporation.

---

Hideo Yoshihara served as a liaison scientist for the Office of Naval Research Far East from April 1988 until May 1990. His assignment was to follow the progress of advanced supercomputers and to review and assess the viscous flow simulation research in the Far East. Dr. Yoshihara formerly was with the Boeing Company, where he was Engineering Manager for Applied Computational Aerodynamics. He was also an affiliate professor in the Department of Aeronautics and Astronautics of the University of Washington, an AIAA Fellow, and a former member of the Fluid Dynamics Panel of AGARD/NATO.

---

---

# REACTIVE POLYMER PROCESSING

---

J. Thomas Lindt

---

*Reactive processing of polymers concerns manufacturing methods that combine the traditionally separated steps of polymerization/polymer modification, devolatilization, blending, structuring, and shaping into a single engineering operation. This paper presents a coordinated view of the subject, highlighting Japanese work to which the author was exposed during his visit to Japan in 1989. Reactive processing is expected to play an important role in the development of new advanced composite materials in Japan and in the ongoing efforts to continuously improve the performance of existing polymers through chemical modifications.*

---

## INTRODUCTION

The commercial synthesis and chemical modifications of high polymers have been a traditional domain of chemistry and chemical reaction engineering, while finishing, structuring, and shaping operations constitute the discipline of (conventional) polymer processing. In contrast, the relatively new specialty of reactive polymer processing (RPP) offers a new perspective of the manufacturing path from the raw materials to the finished products by attempting to carry out a number of the traditionally separated chemical, thermal, and mechanical operations simultaneously in a single process. The benefits of RPP are in both rationalization of polymer manufacturing processes and in development of new materials, sometimes not accessible by any other means.

The RPP route can increase manufacturing efficiency by reducing the investment and operation costs as well as the environmental impact. The potential savings are

due to the elimination of hazardous solvents, elimination of certain reversible thermal and mechanical conversions, and possible reduction of transportation costs.

Since its inception, RPP has also been closely tied to the development of new materials for automotive and aerospace applications. In addition to the rationalized manufacture of these materials, substantial benefits have been accrued due to the weight reduction when metals and other traditional materials have been replaced by polymer-based materials.

A 100-kg weight reduction in every automobile would save about 10 billion liters of gasoline per year in the United States alone. Lightweight polyester, polyurethane, nylon, butyl rubber, and other polymer design components have been introduced into automobiles through novel RPP methods.

The main impact of the use of polymeric materials in the aerospace industry is on flight operating costs and aircraft performance. In recent years, polymer-based composites have been used in secondary structures in aircraft frames.

---

Currently, there is an extensive amount of patent literature on chemical and morphological modifications of polymers through reactive processing. Through these processes new materials with carefully engineered structures are expected to emerge. Most existing polymers have been subject to chemical and morphological modification studies in order to optimize their properties. Chemically processed blends and composites have also received much attention. Many of these new materials are targeted for automotive applications.

This article attempts to present a coordinated view of reactive processing as it has developed over the past 10 years with some highlights of the activity in this area in Japan.

## **REACTIVE PROCESSING AS A MULTIDISCIPLINARY ENDEAVOR**

From a chemical standpoint, RPP is a vehicle to carry out polymer reactions in the absence of solvents or other carrier liquids. Polymerization reactions, cross-linking, chemical modifications of the polymer backbone, grafting onto a polymer chain, inter-chain reactions, formation of interpenetrating networks, and modifications of the molecular weight distribution of polymers are amongst the commercially exploited reactions.

To the physical chemist or rheologist, RPP may represent a means to control the evolving physical structure, often in the presence of multiple, and transient, liquid and solid phases. The vapor phase participates in the formation of cellular and micro-cellular materials also produced by RPP techniques.

The engineer is faced with the task to rationally design and optimize a manufacturing operation according to the anticipated interactions between the physico-chemical system and the equipment chosen to perform a specific duty. A solution is then sought by integrating the general transport principles and the information available on the reaction kinetics and thermodynamic and transport properties of the system in question with the ultimate objective to optimize the material properties. This approach has been applied to reaction injection molding (RIM) since the mid 1970s, and it has been later formalized for the broader area of reactive processing, as a separate engineering specialty. Since then, RPP has become a standard topic of technical meetings of most professional societies active in the polymer area.

## **CHEMICAL SYSTEMS**

In RPP, fast chemical reactions are usually used. In cyclic operations, such as RIM, reactions are completed within a few minutes, sometimes in a less than one. In continuous processes, such as reactive extrusion and pultrusion, the reaction time must be less than the minimum residence time in the equipment, also of the order of minutes. The most notable exceptions are the slow curing systems, e.g., epoxies, containing continuous fibers for aerospace applications.

The reaction rate must be controllable to prevent a thermal runaway. This is a nontrivial problem since the reactions are exothermic and run in viscous media of low thermal conductivity. Moreover, the glass transition of the finished polymer must be low enough to allow for a reasonable processing temperature and complete reaction.

---

The need to control possible phase separation phenomena occurring along the reaction path may also restrict the choice of reactants.

The reactants may be gases, liquids, and solids, such as reactive fillers. While gaseous reactants, e.g., chlorine and ammonia, are used in reactive extrusion, as indicated by the patent literature, they do not play a major role in molding operations. On the other hand, the evolution of gases occurs during formation and molding (or casting) of polyurethane foams either by direct reaction between water and isocyanate or indirectly by vaporization of a physical flowing agent driven by the reaction enthalpy of polymerization.

Both chain and step polymerization reactions are of interest to reactive processing. Examples of step reactions of interest to RPP are condensation, addition, ring opening, and ester exchange. The best known, commercially important polymers produced by bulk polyaddition reactions include polyurethanes, polyureas, polyamides, polyesters, epoxies, polysiloxanes, polyethers, polyacrylates, and formaldehyde-based polymers. In the absence of low molecular weight by-products, these reactions are well suited for molding operations where the removal of gases is relatively difficult.

By far, it is the polyurethanes that have been exploited industrially most successfully. The success of polyurethanes as engineering plastics and optimized insulation materials has made them a model case for RPP applications. Only relatively recently, polyureas have emerged as a serious contender in this class of reactions. The urea reaction is faster and gives materials of improved heat resistance and durability.

While polyurethane- and polyurea-based RIM systems represent currently over 95 percent of global RIM production, certain chain polymerization reactions yielding vinyl- and diene-based polymers are of growing interest. Amongst the emerging commercially important systems are the highly reactive dicyclopentadienes, with reaction times of some 10 seconds, yielding cross-linked olefin resins.

Most chemical systems used in the cyclic reactive operations, e.g., RIM, compression molding, and autoclave molding, use cross-linking reactions to improve mechanical properties of the product. Multifunctional monomers or oligomers undergoing step polymerization reactions are typically used.

By comparison to RIM, in-situ polymerization reactions are only one of the several types of reactions used in continuous RPP, most notably in reactive extrusion (REX). Chemical modifications of existing polymers play a significant role. Cross-linking reactions are relatively unimportant in continuous RPP operations.

One of the advantages of continuous, as opposed to cyclic, processing is the ability to operate in stages, allowing a sequential, and continuous, introduction of reactants and/or removal of reaction by-products and other chemical species. Thus, not only polyaddition reactions can be used, as is the case in the aforementioned molding operations, but also polycondensation reactions can be exploited. Small molecules liberated by polycondensation reactions are removed by externally controlled diffusion processes. Amongst the commercially exploited systems of this class are polyesters, polyetherimide, and some formaldehyde-based polymers.

---

Examples of chain polymerization reactions used in continuous RPP include styrene and diene polymers.

Chemical reactions used to modify existing polymers in the molten state include side- and end-chain grafting, homopolymer chain coupling, polymer functionalization and functional group modification reactions, and reactions to modify the molecular weight distribution. The polymer modification reactions are used to improve material properties of the original polymer.

Grafting reactions yield block or graft copolymers. Polyethylene, polypropylene, ethylene-vinyl acetate copolymer (EVA), ethylene-propylene elastomers (EPDM), polystyrene, polybutadiene, and other polymers have been subject to grafting reactions. Grafts have been introduced through reactions with organic anhydrides (e.g., fumaric, maleic, and nadic anhydride); acids (e.g., acrylic acid and analogs); acrylic and methacrylic esters and amides; styrene; and other reactive species. Numerous examples of such reactions can be found in the patent literature.

Polymer functionalization and functional group modification reactions include hydrolysis, transesterification, sulfonation, imidization, and halogenation. Amongst the polymers subject to such reactions are butyl rubber, polyethylene terephthalate, EVA, various polyolefins, EPDM, and polymethylmethacrylate (PMMA).

Modifications of the average molecular weight of polymers can also be achieved by reactions in the molten state. Both thermally and chemically activated reactions have been used to reduce the width of the molecular weight distribution as well as the average molecular weight with polyesters, polyacetal/polyether copolymers, and various polyolefins, most notably polypropylene. To improve its spinnability, controlled degradation of polypropylene has been

practiced industrially for more than a decade. The current knowledge of this process includes mathematical models proposed for process design and optimization that integrate the reaction kinetics, rheology, and transport phenomena occurring during REX.

The molecular weight of some homopolymers, such as polyolefins, polyesters, polyamides, and polyols, can be increased through coupling reactions. The polymer chains can be coupled by polyfunctional species such as epoxides, in which case the coupling species becomes a part of the chain, or by monofunctional species that activate one end group on the chain that propagates the reaction. The monofunctional coupling agent does not become a part of the coupled chain. Again, examples of coupling reactions exploited industrially can be found in the patent literature.

## PROCESSES

The choice of a given manufacturing route is dictated by the shape and the chemical and physical structure of the product. RPP has been used to produce single- and multi-component materials based on glassy and crystalline polymers. Amongst the multi-component RPP systems are reactive blends, particle-filled polymers, fiber-reinforced composites, and chemically generated polymeric foams.

RPP processes can be divided into cyclic and continuous operations. Cyclic operations are used to produce three-dimensional moldings of varying degree of complexity. Continuous operations yield one- or two-dimensional shapes, such as fibers, various profiles, film, sheet, or granulate, when cut.

Continuous operations can be broken down further into internal and external processes. The former refers to processes contained within the equipment walls while

the latter refers to operations performed at the machine exit. The internal continuous RPP operations may include different types of chemical and shear-induced reactions, particle coagulation, melting, homogenization and blending of compatible and incompatible liquids, melt compounding with various solids, foaming, stripping of low molecular weight species and degassing, and various combinations thereof.

Through the external operations, shaping of the product and morphology development in the material, in the possible presence of chemical reaction, such as pultrusion, are accomplished.

In cyclic RPP operations, most notably RIM, the elementary phenomena involved are typically limited to mixing, polymerization, shaping, and structure development, a combination somewhat similar in scope to the external continuous operations. An important difference is, however, the relative ease with which the cyclic processes can accommodate nonflowing, e.g., cross-linked and highly solid loaded, polymeric systems.

The most common cyclic RPP operations include RIM, monomer and foam casting, compression molding, transfer molding, and autoclave molding.

The most important continuous RPP operations are reactive extrusion, reactive calendaring, pultrusion, and continuous monomer and foam casting. Some of these processes have been developed as the continuous counterparts of the aforementioned cyclic operations. Such pairs are the batch and continuous monomer and foam casting, compression molding and calendaring, autoclave molding and pultrusion and, in some cases, RIM and REX. It should be noted, however, that from the process design standpoint such analogies are superficial and may be misleading.

In addition, there exists a definite need to develop hybrid reactive coprocessing techniques using interfacial chemical reactions to improve interfacial and adhesion characteristics of sandwiched structures produced, or to be produced, by co-extrusion, co-injection molding, and co-blow molding.

## ENGINEERING ANALYSIS

The miscibility of polymeric liquids is, in general, governed by entropic factors. The lengths of the chains limit the amount of possible conformations of the system and thereby the entropy contribution to the free energy of mixing. With the changing molecular weight during RPP, the compatibility of the coexisting species may thus vary with time and may become dependent on the specific reaction path. Typically, the phase equilibria are complex and not much quantitative information is available. It has been recognized that many RPP operations are carried out with incompatible components or that phase separation may occur as a result of chemical changes along the reaction path; this has been observed, for example, with polyurethanes.

In the case of reactive blends, a carefully controlled phase morphology is typically a necessary condition for obtaining optimum material properties. RPP of blends may be chosen to preserve the blend morphology during shaping operations, e.g., injection molding.

Equally important is to control the crystallization phenomena that may occur simultaneously with the reaction as observed in nylon RIM, for example.

In addition to the need to understand the nature of the possible phase transitions, quantitative information is often required on the equilibrium interfacial species concentrations that drive the various diffusion processes involved in RPP.

---

Interfacial phenomena play, in general, an important role in the formation and processing of heterogeneous systems. Data on surface energy in melt-melt systems, such as reactive blends, gas-melt systems, undergoing gas-melt reactions or foaming, and in reacting melt-solid composite systems are required for morphology design and control of mechanical properties of heterogeneous systems.

The rheological, diffusion, and thermal properties are dependent on the gradually evolving structure of the reacting medium. General fundamentals governing the generalized diffusion processes are yet to be developed.

From the physico-chemical standpoint, most industrial systems are too complicated to be used for a meaningful analysis of the processing fundamentals.

There is a definite need to generate data bases for future RPP studies. New instruments will have to be developed that can handle fast reacting, often volatile, systems.

For some selected single-phase systems, the viscosity and diffusivity as functions of the molecular weight (distribution), temperature, and the rate of deformation can be predicted. Partial data sets of transport properties exist on some commercially important RPP systems, e.g., epoxies, polyesters, and polyurethanes. In such cases, process design methods rooted in continuous mechanics have been or can be applied. The history of the material during its passage through the equipment as well as the equipment requirements can be revealed through simultaneous mathematical modelling of viscous flow, reaction kinetics, diffusion, and thermal phenomena.

Both direct and indirect methods have been used to monitor the progress of chemical reaction [differential scanning calorimetry (DSC), nuclear magnetic resonance

(NMR), infrared spectroscopy techniques (IR, FT-IR), etc.]. When dealing with the "overall" reaction kinetics, indirect thermal measurements using, for example, DSC, have been used; typically these techniques have been applied to step polymerization reactions. Often the complete chemical history is, however, required to assess the origin and development of a chemical and morphological structure. In such cases, the existence of individual species has to be monitored by, e.g., FT-IR techniques. The measurements may be complicated if fast reactions are involved.

Measurements directed toward the molecular weight (distribution) and the structure of the medium are difficult. Accurate and robust on-line measurements of both the rheology and morphology are being developed.

Indirect on-line measurements are already in use in RPP of advanced composites for aerospace applications. These methods, necessitated by high costs of the molded parts, are based on empirical correlations between the molecular parameters and some selected material properties.

## TECHNOLOGICAL SIGNIFICANCE

The ultimate goal of reactive processing is to produce tailor-made chemical and morphological polymeric systems for the many uses in our technological society. Chemically modified neat polymers and reactive blends and composites are in the forefront of this trend. The interest is world wide. The following examples of industrial RPP activities in Japan highlight these worldwide trends.

Of particular interest has been RPP of advanced composites in aviation. Currently, the Japanese Government has been involved in a related area using similar materials. While the main emphasis in the United States



---

has been on compression molding of these materials, the recent disclosure by the Government Industrial Research Institute-Osaka at the 5th Annual Meeting of the Polymer Processing Society (PPS) International in Kyoto in 1989 indicates considerable involvement in RIM of epoxies with a variety of reinforcements. Interactions between the reinforcement and the polymeric matrix have been studied in Japanese industrial laboratories, e.g., Fuji Heavy Industries and Mitsui Toatsu Chemicals, for new high temperature polyimide-based composites. Mitsui has also reported efforts emphasizing the processing aspects of pultrusion and resin transfer molding.

In the United States, The Netherlands, and Japan, anionic polymerization of  $\epsilon$ -caprolactam has been used to produce RIM nylon 6. Recently, Ube Industries reported their results concerning the simultaneous polymerization and crystallization that control the material properties. Impact-modified RIM nylon has alternatively also been prepared by polycondensation reactions between aliphatic dicarboxylic acids, aliphatic amines, amino acids, and  $\omega$ -lactam at Mitsubishi Monsanto Chemical Company.

Systematic efforts to evaluate the various RIM systems are underway. A published attempt by Matsushita Electrical Company deals with urethane, epoxy, polyamide, and acrylonitrile-butadiene-styrene (ABS) RIM systems. Molding of foamed polyurethanes from both a materials and processing standpoint has been the subject of publications by Mitsui, emphasizing the effect of chemical composition and processing on the foam cell structure.

Continuous RPP, most notably reactive extrusion, is intensely studied. The initial growth started during the 1966-83 period when some 400 patents in REX were issued in the free world, approximately half of them in Japan with the rest shared between the

United States and Western Europe. In recent years this activity has intensified considerably. The research information has only started to be shared at scientific meetings.

The reactive extrusion process for toughened polyamides by Sumitomo Chemical Company is an example of this trend in Japan. Nippon Polyurethane Corporation has developed a REX process for temperature-resistant polyurethane elastomers using polyols with isocyanurate rings. In the area of radical polymerization REX, Nitto Electric Industries has developed a bulk process for acrylic polymers to control costs of solvent recovery and minimize environmental hazards. Industrial examples of the widely practiced controlled degradation of polyolefins, to reduce the breadth of the molecular weight distribution, are the work of the Nissan Chemical Company and Japan Steel Works. The latter appears to be the major source of Japanese REX equipment.

Much of the global activity in REX concerns grafting reactions of monomers or polymers onto the backbone of another polymer with or without cross-linking. Into the former category fall the grafting reactions of vinyl monomers with polypropylene to improve its impact strength, an Asahi Kasei process, and a large variety of maleic anhydride grafting reactions on different polymers, for example, ethylene-vinylacetate copolymer (Japan Steel Works), propylene-ethylene-butadiene copolymer (Nissan Motors), and polypropylene (Tokuyama Soda Company). Mitsubishi Petrochemical has successfully produced grafts of polyesters on polyphenylene. Grafting-introduced cross-linking has been used to prepare organic silane-modified polyolefins by Fujikura Cable Works and Showa Electric Wire Company and to cross-link aromatic polyesters by dicarboxylic acids and various unsaturated species by Teijin Company. Many other examples can certainly be

---

found in the Japanese language literature, but a detailed survey of the Japanese industrial activity in the RPP area is beyond the scope of this article.

While deeply involved in polymer rheology, chemistry of polymers, and polymer reaction engineering, Japanese universities have not emphasized reactive processing to the same degree as their overseas counterparts. During the 5th Annual Meeting of the PPS in Kyoto, there were no contributions by the Japanese academe to the reactive processing symposium. A year later Professor Omi of the Tokyo University of Agriculture and Technology, one of the organizers of the Kyoto symposium, presented a paper on reactive processing of polystyrene during the 6th Annual Meeting of the PPS in Nice as the single RPP academic contribution from Japan. It should be noted, however, that reactive processing, as a distinct engineering specialty, may have been recognized at Japanese universities later than in North America, and as a result much of the relevant work is being carried

out as part of the more traditional programs and is yet to be integrated into the general framework of RPP.

Future advances in RPP may play a key role in the future of the polymer industry. With a qualified reference to the steel industry in the G-7 countries, one may state that the long-term survival of the national polymer industry may ultimately depend on the added-value products derived from commodity polymers, including chemically and structurally modified materials.

According to the recent projections of the Japanese Ministry of International Trade and Industry, new materials, in general, and advanced composites with extended environmental durability, in particular, will be among those technologies dominating the early 21st century in Japan. Reactive processing of polymers, concerning molecular engineering of the polymer phase(s), morphology development, and interactions between the phases, is expected to play an important role in such developments.

---

**J.T. Lindt** is a Professor of Polymer Engineering in the Department of Materials Science and Engineering at the University of Pittsburgh. His research interests concern reactive and heterogeneous polymeric systems.

---

---

# CENTURY RESEARCH CORPORATION (CRC), TOKYO

---

David K. Kahaner

---

*This report illustrates the breadth of applications and research areas in which this "service bureau" type organization is involved.*

---

## INTRODUCTION

As part of the Supercomputing in Nuclear Applications meeting, I visited the Century Research Computer Center and reported on this in another article in this issue of the *Scientific Information Bulletin*. At that time I met Dr. Hiroyuki Kadotani, who heads the Technology Department.

Dr. Hiroyuki Kadotani  
Head, Technology Department  
Engineering Division  
Century Research Corporation  
3-6-2 Nihonbashi-Honcho  
Chuo-ku, Tokyo, JAPAN  
(03) 665-9819

Dr. Kadotani, a nuclear physicist, invited me to visit the main offices of the company to learn more about its work, and I took advantage of this invitation on 5 April.

To summarize, the Century Research Corporation (CRC) was founded in 1958 as Tokyo Electronic Computing Service Co., changed its name in 1971, and currently has slightly more than 1,200 employees. About 730 of these work directly for CRC, the remainder for the subsidiaries described below. CRC has 10 offices in Japan as well as one in Seoul, Korea, and another in Santa Clara, California. The company is privately

owned, with C. Itoh Co., Fujitsu Ltd., Nippon Express Co. Ltd., and Kawasaki Steel Corp. among the major owners. Staff and revenues have been steadily growing since the company's founding. Revenue for 1991 is projected to be about ¥25B (about \$175M U.S.). About one-third of CRC's income is from scientific, technical, and engineering services, which primarily means running problems for users in the fields of civil, aerospace, electrical, nuclear, mining, structural, and chemical engineering, etc. Another one-third comes from commercial data processing such as network and office automation services, about one-fourth from software development and sales, and the rest from consulting and facilities management.

CRC has four affiliated (subsidiary) companies:

- CRS (CRC System Corp.). Markets software, but is also engaged in sales of hardware and related equipment, and services such as communication satellite control, computer operation, and international communications. (390 employees)
- CRT (CRC Technical Corp.). Provides services related to computer hardware, such as consulting for system creation, and system maintenance. (60 employees)

- CRE (CRC Educational & Editorial Corp.). Provides education and training of company employees and overseas trainees, data processing education, translation, and industrial promotion for the State of Saarland (FRG). CRC also acts as the Japan representative of the State of Oklahoma. In this capacity CRE tries to encourage Japanese businesses to establish plants and factories as well as tries to locate markets for Oklahoma's products. Kadotani and CRC feel that they have been successful. (20 employees)
- CTCC (Century Computer Center Corp). Runs the computer center near Yokohama that I reported on earlier. (40 employees)

CRC has its employees spread in a variety of buildings in central Tokyo, as well as branch offices in various suburban locations. There is talk of moving the entire operation (sans president, of course) out to the suburbs as office space is less expensive and it would be easier to pull together staff now separated.

## SOFTWARE DEVELOPMENTS

Kadotani and I toured part of the office and laboratory facility in which he works. I was primarily interested in the kinds of software that CRC has been developing and how it compares with that in the United States. I knew already that I was not going to meet any numerical analysts or many computer scientists engaged in theoretical research. Kadotani is very well versed in engineering software development, less so in other areas (even some that are active projects at CRC). He listed the following application areas and the software packages that CRC provides to support users in these areas. Asterisks (\*) indicate programs developed directly by CRC.

### *Structural and Civil Engineering:*

* ALPS	NSC/NASTRAN
ANSYS	NISA Series
* CAISSON	* NOAMAS
DYNA2E	* SIRFRAM
DYSAS	* SLOPE3
* FANSY Series	SURFES
* FINAS	* TOMAS

### *Nuclear Engineering:*

ANISN	ORIGEN
CITATION	QAD
COMETHE III-L	RELAP5
DOT 3.5	SCALE3.1
FEMAXI-III	TRAC-PF1
HEATING	TRUMP
KENO	TWOTRAN
MORSE-CG	WIMS

### *Fluid Flow Analysis:*

FIDAP	PHONETICS
-------	-----------

### *Impact and Crash Analysis:*

AUTODYN-2D	* MANJUSRI
DYNA3D	NIKE3D
HONDO2	PISCES
MADYMO	

### *Petroleum and Chemical Engineering:*

HESTRAN	PROCESS
PIPEPHASE	

### *Plant Design and Plant Engineering:*

ALDPIPE	DYNAFLEX
DIS	

### *Mining Assessment:*

PHOENIX	SIROMINE
---------	----------

---

### *Environmental Engineering:*

\* ANDOSE                      \* NOISE Series

### *Optical Design:*

ACCOS-V                      FLASH-AV  
CODE-V

### *Electronic Engineering:*

CDRC                        \* MAGNA Series  
LOGGAP                      SPICE2

### *Graphics and CAD/CAM/CAE:*

\* ATLAS                      \* GP2E  
UNIRAS                      \* CAD/HOUSE Series  
SET                            CAPLAS/IRIS

This year CRC has introduced several new packages of its own design, including a sunshine analysis program for PCs, field analysis system for acoustics, a neural net simulator, and a CAE animation system. Interestingly, a large portion of CRC's consulting business is related to the nuclear industry, but at present CRC has no programs developed in-house.

CRC has a substantial number of business activities in the United States, including work with AB Associates, Century Dynamics, Cullinet Software, DIS/ADLPIPE, Endeco Design Automation, Engineering Design Automation, Engineering Mechanics Research, General Atomics, Marsoft, NOVA Graphics International, Optical Research Associates, Phase Three Logic, Prose, Quantative Technology, Radiation Research Associates, Science Applications International, Scientific Calculation, Seismograph Service Corp., Sierra Geophysics, Scientific Software-Intercomp, Simulation Sciences, S. Levy, Swanson

Analysis Systems, System Control Technology, Texas Instruments, MacNeal-Schwendler, Regents of the University of California, and the S.M. Stoller Corp.

The point of giving this list is to emphasize that CRC has its feet firmly planted in applications. It is not a research organization but rather sells its services. Kadotani explained that CRC sees very little future in selling computer time but intends to concentrate on selling solutions, i.e., solving specific problems for clients. (This assessment agrees very well with the information I heard at the computer center the preceding month.) As such, CRC feels that it is in its own interests to have a substantial activity in "researchy" things, such as artificial intelligence (AI), neural networks, etc. I saw several examples during my visit.

### **CD-I**

This is a joint venture between CRC and the Dutch electronics manufacturer, Phillips. The system that I saw was composed of a Phillips PC and CD player, attached to a standard TV monitor. A PC program has been prewritten onto the CD and is loaded into the PC on which it then runs. The program, written in C by CRC, has special system calls that allow it to access the CD for additional data, and the hardware includes a high speed data channel to get CD data to the TV screen and speakers. The program also keeps track of a screen cursor that it moves around in response to user inputs through a remote control device. In many ways this is very similar to interactive programs that I (and probably you) have written; a main program monitors the keyboard (in this case the digital remote control) and "XOR"s a cursor to move in response to user input. It also runs a main program and calls various subroutines

---

depending on the status of the cursor or other input selections. The key new feature here is that the CD player can hold tremendous amounts of digital data, not only standard numeric data but image and audio data as well. In the demonstration that CRC had prepared, the screen first contains a menu of selections that the user can pick from via cursor. One of them is a travelogue; selecting it brings up what looks like an ordinary "video" of Greece. While this is running the user can point to a menu along the top of the screen selecting the language of the narration. The demo disk allowed 4 choices, but the system is capable of 16. Of course, the film is accompanied by digital stereo, also from the CD. The demo disk also included a computer game, this one substantially enhanced by very high quality images and impressive sound. Also, it was very nice not to have wires attached to the TV. The scientists working on this project explained that the demo I watched took about a year to complete, but a big part of that time was spent learning about the capabilities of the system. When I commented on the use of what seemed to me to be fairly special hardware (Phillips), they explained that they were now working to build a board that will go into a Sun workstation to allow the CD and TV to be driven from that. I also asked about the relation of this work to one of the new HDTV standards and was assured that images of that quality will be incorporated, although CRC has not decided which standard to follow.

My own feeling is that the application potential for such systems is substantial in many fields including science, but exploiting it will take a good combination of understanding the hardware/software interface as well as understanding the needs of users. CRC apparently believes this, too, as it has

been developing a collection of CD based application packages for various levels of users, from those who want to build their own applications all the way to end product users. For example, for the latter CRC has a package containing 16 different engineering analysis software modules on a single CD ROM. CRC also intends to market use of the laboratory in Tokyo for those who want to develop an interactive video but do not want to purchase all the necessary equipment. In the scientific world today "visualization" is a hot topic. This essentially means graphics, and graphics needs hardware. This is especially true in the context of interactive visualization. I do not think there is any way to build really high performance applications that do not take advantage of the characteristics of the target hardware. But I am not aware of many U.S. universities or laboratories that are experimenting with this kind of equipment or that have the level of expertise that I saw demonstrated here. It is fairly expensive to obtain all the hardware required to make a CD master, although it is well within the range of computer science departments and laboratories. Of course, CRC has depended to a large extent on technical expertise collaborations with Phillips. Nevertheless, this is remarkable activity, especially considering that CRC is only of modest size by U.S. standards and is also involved in many other projects.

## TRANSPUTER SOFTWARE

Transputers are highly self-contained computer boards developed in the United Kingdom. Their main advantage is physical simplicity of installation; it is easy to build a parallel computer. Most systems use the T800 INMOS transputer. This is a micro-computer with on-chip RAM for high speed

processing, a configurable memory interface, a floating point unit, a peripheral interface, and four serial communications links for interprocessor communications. In the United States, Topologies markets a transputer board (Topology 1000 System) for Sun workstations, and CRC has been developing software for it. CRC's Sun is configured with four 20-MHz CPUs, each with 4 MB of DRAM local memory. This is the smallest configuration marketed by Topologies and is a good starting point for experimentation and software development. CRC already marketed an electromagnetic field analysis program MAGNA/FIM. (FIM refers to finite integral method, or more traditionally boundary integral method.) Now a version of this program has been developed for the Topology 1000 System that CRC claims runs 10 times faster than the original. I had no opportunity to verify that. But Kadotani and I spent some time studying his latest effort, which is to develop a parallel version of the Monte Carlo program Keno, a program heavily used in the nuclear industry. Monte Carlo is often a good candidate for parallelization because there isn't much communication between different processors. Each CPU generates particles with characteristics determined by probabilistic densities and follows them through "random" motion in the material. In the CRC implementation one CPU keeps track of summary data and one, two, or three CPUs (depending on the program configuration) track the particles. Kadotani developed his program and then tested it on three fairly common applications, a benchmark problem from Argonne National Laboratory, another from the Japanese Atomic Energy Research Institute (JAERI), and a third, classic problem, originally described in 1966 in *Nuclear Science and*

*Engineering* (NS&E). The amount of computer time for such problems depends on the number of "histories" or particles that are followed; Kadotani ran 15,000 or 30,000. This is enough to generate standard deviations of about 0.005 on the important statistics. His results are as follows:

<u>Computer</u>	<u>Amount of Computer Time (s) for Problems From--</u>		
	<u>Argonne</u>	<u>NS&amp;E</u>	<u>JAERI</u>
Sun 3	248	4203	3533
Topologies			
1 CPU	75	1134	956
2 CPU	43	594	491
3 CPU	34	416	340
IBM 3084	21	378	314

Kadotani was very proud of the results, especially those that show execution times only slightly more than an IBM 3084. On the other hand, these figures should be read with some care. I have personally observed the Sun to run poorly on some Fortran applications, but I have also seen that very dramatic improvements could be obtained by careful tuning of the program with the help of performance enhancers available on the Sun. At the same time the transputer version is new and has been carefully recoded, although Kadotani feels that he spent only a minimum of time on the programming.

In any case, I don't think that the figures are central to the point I want to make, which is that this research is being done within the confines of a very application oriented organization, definitely not a research institute devoted to numerical analysis or computer science.

---

CRC has also been marketing a neural computing package (RHINE) that runs on a system of transputers installed on an NEC PC. I did not have an opportunity to try this product, but CRC also markets hardware and software for neural networks that were developed by CAIC (Science Applications International) and that can be installed in IBM PCs. Associated with the announcement of this latter product, CRC held a "Neural Network Show" in Tokyo in November 1989 with various lectures on neural networks and an attendance of about 150.

## OTHER ACTIVITIES

CRC is involved in several other computer related activities. For example, CRC is in charge of the operation and the software development for Japan Video Cypher. This company provides audio and visual scrambling services through the first Japanese commercial communication satellite, JCSATI, launched in March 1989. CRC markets an economic database service in Japan that includes some modelling capability and built-in graphics. The 1989 annual report on the Japanese information service industry was researched and planned by CRC under a commission from the Japan Information Service Industry Association, and CRC's president is vice president of this association. CRC has developed a network for pharmaceutical and cosmetics wholesalers that can process the sales of these companies. CRC is also developing other specialized networks for gas stations and fast food stores. CRC is also involved in

economic planning studies for countries such as Saudi Arabia, Hong Kong, Zaire, Thailand, and others.

## CONCLUDING REMARKS

Traditionally, CRC has had a policy of buying the fastest computer that was available. This was the essential reason for the installation of a Cray X/MP in the computer center. It would be natural for CRC to upgrade this to a Y/MP or perhaps a NEC SX-3, but there is now a serious internal debate to decide if this is the correct way to go. Apparently many in the company feel that given the company's current business mix and the rapidly increasing power available in the workstation market, there is no need for a larger supercomputer. Kadotani says that he likes to work on Crays but cannot refute the usefulness of the workstations. My own guess is that CRC will buy a super mini, which will be very useful right now. Later, if it appears not to be big enough, CRC can still make use of it while looking for something larger.

Finally, I asked Kadotani why an American company would prefer to contract with CRC for computer applications developed in Japan instead of a nearby U.S. company. He felt that the Japanese could develop software more quickly because they have a less formal approach, although the result may be less polished internally. More philosophically, he suggested that the answer to my question was the same as why Americans buy Japanese cars instead of their own.



---

# RESEARCH ON VARIOUS ELECTRONIC THIN FILMS IN JAPAN

Robert F. Davis

---

*This article describes research on thin films at laboratories in the Department of Electronics and Electrical Engineering at Nagoya and Kyoto Universities.*

---

## NAGOYA UNIVERSITY

### Dr. Mizutani's Laboratory

This group is conducting research on thin films and their applications, ceramic devices, electrically conducting polymers, and polymeric insulators. In the thin film studies, they are using a variety of methods of deposition including plasma (rf and microwave), standard and photo-assisted chemical vapor deposition (CVD), RF sputtering, ion beam sputtering, ion beam assisted deposition, and electrochemical methods. The types of films include amorphous silicon, carbon and silicon carbide for solar cells, zinc oxide varistors and sensors, high  $T_c$  superconductors, and polymeric films including Langmuir-Blodgett.

In the area of varistors, it has been known for decades that it is the material (namely bismuth oxide and other materials in low concentrations) on the boundaries of ZnO that exerts control over transient voltages in power transmission in an electrical circuit. Mizutani's efforts are to duplicate the bulk varistor in terms of materials and capabilities, but in 100-nm-thick thin film form. Using RF sputtering of the targets of

zinc oxide and, subsequently, that of bismuth oxide, they have achieved devices that are highly nonlinear in their log current versus log voltage response in forward bias. They are not as good in reverse bias. They are now applying ion beam sputtering to the growth of these materials.

The primary electroluminescent (EL) polymer being studied is poly -p-xylenolene, which can be doped with various materials to produce new EL devices. A bright green EL polymer under development has a brightness of 20 millicandles/cm<sup>2</sup>. The primary problem is that the organics are not stable at room temperature; thus, the degradation is rapid and the lifetime is short. Other materials being considered for EL devices include zinc sulfide and zinc selenide.

### Dr. Hawakawa's Laboratory

Dr. H. Hawakawa's high  $T_c$  superconducting materials group consists of three staff and eight graduate students [see "High Temperature Superconducting Thin Films in Japan," by M. Osofsky, P.R. Broussard, and E. Callen, *Scientific Information Bulletin* 13(4), 1-23 (1988)]. Industry is collaborating by providing equipment and personnel

---

to deposit and characterize the films. Dr. Hawakawa's primary modes of deposition are RF sputtering (three machines including that used by the industry personnel) and electron beam deposition (one machine not yet operational). The chemical systems under study are Y-Ba-Cu oxide, Bi-Sr-Ca-Cu oxide, and Nd-Ce-Cu oxide. The group has achieved the usual results: a critical temperature around 80 to 95 K and critical current densities ( $J_c$ ) in the  $10^5$  amps/cm<sup>2</sup> range at zero magnetic fields. The values of  $J_c$  are highly field dependent. Dr. Hawakawa has also produced working devices of superconductor-metal-superconducting junctions and bridges, as well as three terminal devices.

### Professor Akasaki's Laboratory

Professor Akasaki has 1 associate professor, 4 research associates, and approximately 10 students under his direction. His research efforts include crystal growth of III-V and II-VI compound semiconductors and their alloys by liquid phase, vapor phase, metal organic vapor phase, and molecular beam epitaxial techniques and characterization of these films via photoluminescence, cathodoluminescence, Raman scattering, x-ray diffraction, and light beam induced current methods. Associate Professor Sawaki is conducting theoretical research regarding the fundamental physics of semiconductor materials and optoelectronic devices and high field transport and transient properties of semiconductors and superlattices. However, it was the recent work in GaN that proved to be the most interesting (for me).

Professor Akasaki and his research associate, Dr. H. Amano, have recently made some breakthroughs regarding light emission from p-n junction diodes of this material. Dr. Amano discovered that during

cathodoluminescence (electron beam irradiation) studies, doped GaN became increasingly resistive. Moreover, continued irradiation caused it to go p-type. It is his contention that the dopants (Zn, Mg, etc.) initially occupy interstitial sites in the GaN lattice. Under electron beam irradiation the Ga dislodge from their lattice sites and exchange positions with the dopant species. This leads eventually to p-type conductivity. Even more exciting is that blue light emitting diodes (LEDs) have been made from p-n junctions of this material. The success of the LEDs may depend on the deposition of an undoped GaN film on amorphous AlN, which had been previously deposited on sapphire at approximately 500 °C. This procedure could improve the microstructure of the GaN films in terms of the density of line defects. It seems significant that light emission could not be achieved when p-n diodes were fabricated in GaN material deposited directly on the sapphire. This is somewhat puzzling because the deposition temperature of the amorphous AlN is now raised to about 1,000 °C for the growth of the GaN layers. It would seem that the amorphous AlN would crystallize at this higher deposition temperature. Professor Akasaki's group has dedicated three reactors to this project: one for producing thick GaN films for substrates by the classical chloride deposition process and two for depositing the GaN films by metal organic chemical vapor deposition using triethylgallium and ammonia. They are also building a larger "manufacturing" facility at Nagoya University to produce these LEDs. It is to be commissioned in about mid-April 1990.

The brightest diode produced by the group emitted 50 millicandles/cm<sup>2</sup>. That figure is at least three times the output of silicon carbide diodes. Lasers have not been

---

attempted but are definitely on the agenda. To produce p-n junction devices, one needs a cavity. Akasaki and Amano also noted that one must increase the hole concentration AND the electron density in the n-type GaN to achieve a greater light intensity.

Toyota Research Laboratory near Nagoya has established a research program for GaN films and devices. Sharp Inc. will initiate the same in the very near future. Professor Akasaki looks forward to Japanese synergy with the new industrial laboratories.

Professor Akasaki also runs an active ZnS, ZnSe, and ZnSSe thin film program. They are putting lithium nitride and sodium nitride into ZnSe to produce p-type conduction. Blue LEDs have also been made from p-n junctions of this material, but at date they are not stable at room temperature because of the diffusion of the lithium or sodium in the lattice.

### Professor Uchiyama's Laboratory

Professor Uchiyama is best known for the development of multilayer magnetic films of, for example, Pt/Co, Gd/Co, and Pd/Co for the magneto-optical recording industry that is now flourishing in Japan. His efforts have been commercially rewarding. His new assignment is that of director of the first Ministry of International Trade and Industry (MITI) initiated university-industry collaboration program to assist technology transfer between the two entities. MITI will construct the buildings that will house the university staff (and perhaps one or more from industry, as well). But industry must supply the capital for the collaborative research projects. One such building and organization will be established on each of the primary technical universities in Japan. This will provide the much needed funds to

improve the university laboratories to meet or exceed those of the United States. The progress and success of this venture should definitely be tracked.

### Professor Hirano's Laboratory

Professor Hirano and his staff have also conducted thin film studies on ZnS. They found that ZnS can be successfully grown with a very good surface by vapor phase epitaxy on GaP if In is added to the film. Otherwise the surface is very rough. The In concentration must be  $10^{19}$  per  $\text{cm}^3$ . In goes into the Zn site. Lattice mismatch between ZnS and GaP is only 0.9 percent. The group has also shown that if amorphous BN is deposited on hot-pressed polycrystalline AlN and the assemblage heated to  $1,200^\circ\text{C}$  under 5 GPa of pressure, the a-BN transforms to cBN. One must be careful to avoid any oxide on the AlN because the conversion to cBN will not occur if it is present. He has also taken small crystals of cBN from the AlN-catalyzed transformation process and used them as seeds in a compact of a-BN. Heating this compact at high pressure caused the entire mass to transform to cBN at pressures considerably less than that needed to convert hexagonal BN to cubic BN. He also advocates the use of borazine ( $\text{B}_3\text{N}_3\text{H}_6$ ) and  $\text{NH}_3$  to produce cBN from the gas phase. (He noted that Ichinose of Nagasaki University uses  $\text{BCl}_3$  and  $\text{NH}_3$  to produce cBN.)

## KYOTO UNIVERSITY

### Professor Matsunami's Laboratory

Professor Matsunami's group is using a modified gas source molecular beam epitaxy approach in the atomic layer epitaxy

(ALE) of silicon carbide. They use 99.999 percent pure  $\text{Si}_2\text{H}_6$  or  $\text{SiH}_4$  and 99.9999 percent pure  $\text{C}_2\text{H}_2$ , the latter of which has a maximum pressure of 1.4 atm to ensure safety in handling. (In the United States,  $\text{C}_2\text{H}_2$  is usually mixed with acetone to produce a safer (and much dirtier) material.) The use of  $\text{Si}_2\text{H}_6$  combined with  $\text{C}_2\text{H}_2$  produces a higher growth rate than  $\text{SiH}_4$ . Propane ( $\text{C}_3\text{H}_8$ ) does not carbonize at the desired growth temperature of 900 °C and ethane ( $\text{C}_2\text{H}_6$ ) is not suitable for vacuum systems, as the chamber pressure goes very high when the gas is introduced into the growth system. By contrast, an ethylene ( $\text{C}_2\text{H}_4$ ) mixture of 10 percent in  $\text{H}_2$  shows almost the same results as  $\text{C}_2\text{H}_2$ .

At present they are growing their ALE SiC layers at 1,000 °C (or higher) on the beta-SiC(100) films produced on Si(100) by conventional CVD processes using  $\text{C}_3\text{H}_8$ ,  $\text{SiH}_4$ , and the carrier gas of  $\text{H}_2$ . They have also experimented with carbonizing the Si(100) surface with  $\text{C}_2\text{H}_2$  in the ALE system at 900 °C then growing the SiC films directly on this converted surface.

The above "homoeptitaxy" of SiC on SiC by either method cannot be obtained by the simultaneous introduction of  $\text{Si}_2\text{H}_6$  and  $\text{C}_2\text{H}_2$ , as islands of free Si appear (at least on the CVD SiC grown on the converted Si(100) surface) at 1,100 °C. If the working pressure is equal to or less than  $10^{-4}$  Torr, SiC growth does not occur when the  $\text{Si}_2\text{H}_6$  is insufficient using a simultaneous supply. If pressure is approximately  $10^{-4}$  Torr, Si islands may appear. As of this writing they had not yet found the correct pressure range for the simultaneous supply of  $\text{Si}_2\text{H}_6$  and  $\text{C}_2\text{H}_2$  up to 1,100 °C. They need a higher substrate temperature, but their maximum temperature capability is 1,200 °C at this time.

If a sequential supply of each reactant gas is used, a 1,000 °C substrate temperature is best. The lower temperatures still allow a single crystal film to occur, but the film contains stacking faults, probably carried over from the underlying SiC substrate layer. At 800 °C, the growth of Si nuclei again appears to regulate growth. These nuclei will be carbonized at this temperature. It may be necessary to reduce the flow of  $\text{Si}_2\text{H}_6$  and increase  $\text{C}_2\text{H}_2$ , but this has not been tried yet. In most cases the flow rates for both gases are between 0.4 and 1.0 standard cubic centimeters per minute (sccm). The major problems to date have been caused by the use of high temperature substrates and inadequate shielding of important parts such as manipulators, insulators, and fasteners.

Mass spectrometry analysis studies have indicated that  $\text{C}_2\text{H}_2$  is not decomposed even at 1,100 °C! Matsunami believes that  $\text{C}_2\text{H}_2$  reacts with Si, which is deposited first on the substrate. In fact, Si must be present on the SiC substrate surface before  $\text{C}_2\text{H}_2$  will decompose. Several experiments have shown that  $\text{Si}_2\text{H}_6$  decomposes via the formation of  $\text{SiH}_3 + \text{SiH}_3$ . Each of these products decomposes to  $\text{SiH}_2 + \text{H}$ .  $\text{SiH}_2$  is the precursor that physisorbs on the SiC (or Si) surface and decomposes via chemisorption to  $\text{Si} + 2\text{H}$ . These reactions begin around 400 °C and are prominent at 970 °C. Green at the University of Illinois has shown that  $\text{Si}_2\text{H}_6$  can be thermally decomposed by using an excimer laser. He has accomplished atomic layer epitaxy of Si using this approach. The bottom line is that if one is to use  $\text{Si}_2\text{H}_6$  and  $\text{C}_2\text{H}_2$  SIMULTANEOUSLY to grow SiC, one must precrack the  $\text{C}_2\text{H}_2$  in the same manner as one does with  $\text{AsH}_3$  and  $\text{PH}_3$  to grow GaAs and GaP. It probably should be cracked in ALE as well. Nitrogen has been

---

introduced by the decomposition of  $\text{NH}_3$  using low pressure Hg lamps [see C.H. Wu, *J. Phys. Chem.* 91, 5054 (1987)]. This element is a donor dopant in SiC.

In certain close-packed structures such as SiC, there exists a special one-dimensional type of polymorphism called polytypism. Polytypes are alike in the two dimensions of the close-packed planes but differ in the stacking sequence in the dimension perpendicular to these planes. In SiC, the stacking sequence of the close-packed planes can be described by an ABC notation. If the pure ABC stacking is repetitive, one obtains the zinc blende structure. This is the only cubic SiC polytype and is referred to as 3C or beta-SiC, where the 3 refers to the number of planes in the periodic sequence. The hexagonal (...ABAB...) sequence is also found in SiC. Furthermore, both can also occur in more complex, intermixed forms, yielding a wider range of ordered, larger period, stacked hexagonal or rhombohedral structures of which 6H, 4H, and 15R are the most common. All of these noncubic structures are known collectively as alpha-SiC. Dr. Woo, a research associate in Matsunami's laboratory, is conducting research on the high temperature bulk growth of different polytypes of SiC. He has achieved colorless, transparent, single phase 4H of the C face of 6H under Ar at 1 atm pressure and 2,100 to

2,200 °C to a thickness of 1 cm. At lower temperatures, he obtains the 6H polytype. He has also grown colorless, single phase 15R on the C or Si face of 6H under 1 atm of argon at 2,050 to 2,075 °C to a thickness of 1 cm. The source material for the 6H and 4H polytypes was a green, Acheson-grade SiC; for 15R it was an Al-doped beta-SiC (N was not detected by inductively coupled plasma spectroscopy) from Tokyo Steel Corp. Below 2,150 °C, he obtains 3C-SiC on 3C, but he gets a mixture of 3C and 6H (the 01bar14 plane is the growth plane for the 6H) at 2,150 °C and above. Dr. Woo also has developed computer-generated RHEED patterns to determine his polytypes and has correlated these results with those of Raman spectroscopy, which has become the most common method for determining SiC polytypes.

In common with other groups, Matsunami is conducting research on step (ledge)-controlled epitaxy, which consists of cutting or polishing the substrate surface 2° to 4° off-axis from a low index plane to achieve a much larger density of ledges. The depositing film will much more likely nucleate on the ledge planes than on the planar terraces. Since the ledge planes will be unique, structures characteristic of the ledge planes will be produced, thus enabling one to control which SiC polytype is produced.

---

**Robert F. Davis** is a professor of materials science and engineering at North Carolina State University. He received a B.S. degree in 1964 from North Carolina State University, an M.S. degree in 1966 from Pennsylvania State University, and a Ph.D. degree in 1970 from the University of California, Berkeley, all in ceramic engineering. From 1970-72 he was a research scientist with Corning Glass Works in New York. He joined North Carolina State University in 1972. Dr. Davis is a member of the Materials Research Society and is a Fellow of the American Ceramic Society.

---

# THE SIXTH INTERNATIONAL SYMPOSIUM ON PASSIVITY

---

Clive R. Clayton

---

*At the Sixth International Symposium on Passivity and its satellite meeting at Tohoku University, passivation of both metals and semiconductors was covered. This article highlights some impressions gained from the sessions on metals.*

---

## INTRODUCTION

The Sixth International Symposium on Passivity was held at the Green Hotel, Sapporo, Japan, from 24-28 September 1989. It was organized by the Japan Society of Corrosion Engineering. Professor Norio Sato, Hokkaido University, was the chairman.

The symposium was attended by 211 delegates from 16 countries and attracted 190 papers. It covered passivation of both metals and semiconductors with parallel sessions to cover each area. This article will highlight some impressions gained from the sessions on metals (see LIST OF PAPERS PRESENTED for paper titles and affiliation of authors).

## PASSIVE FILM CHARACTERISTICS

Professor Sato provided an overview on metal passivity. In discussing typical passive film characteristics, Sato included the following:

- Thin surface oxide layers grow in thickness at a rate of 1 to 3 nmV<sup>-1</sup>.
- Layers are amorphous during the early growth stage, then become partially crystalline.

- Outer film layers incorporate anions from the electrolyte, producing a cation selective layer.
- The inner film is dehydrated, metal excessive, and anion selective. Such a bipolar film shows cation egress and prevents anion ingress.
- Most passive films are n-type semiconductors, e.g., films on Fe and Nb. Fewer are p-type, e.g., films on Ni and Cr. Some are insulating, e.g., films on Al and Hf.

## INFLUENCE OF THE ELECTRIC FIELD

The effects of electric fields are as follows:

- External polarization causes band bending upwards if the applied potential is anodic, downwards if cathodic, thus causing a potential drop.
- At modest polarization overvoltages the Helmholtz layer potential remains constant.

- At higher values the energy levels become degenerate or metallic at the film/electrolyte interface; consequently, the Helmholtz potential begins to shift with applied voltage.
- The anodic dissolution of the anodic oxide film is only independent of electrode potential as long as the Helmholtz layer potential remains constant.

## PASSIVE FILM BREAKDOWN

Passive film breakdown is associated with the following:

- Aggressive anions compete with hydroxyl species.
- Local film dissolution may be accelerated due to (1) locally high concentrations of chloride as a salt or complex; (2) introduction of cation vacancies, which may cluster at the metal/oxide interface; or (3) electrostrictive stresses caused by adsorbed Cl species, causing mechanical failure of the film.
- Local metal dissolution may result in either pit formation or repassivation.
- Stable pits are formed above the critical pitting potential and this value becomes more negative with size of the precursor.

The general dependence of passive film thickness on applied anodic potential need hardly be echoed. Nevertheless, it is satisfying to reflect that such dependence was confirmed by both ex-situ vacuum techniques such as x-ray photoelectron spectroscopy (XPS) and in-situ methods such as ellipsometry, quartz crystal microbalance, etc. A notable study was reported by

H.H. Strehblow, who used XPS with an attached cell. His work showed the evolution of film thickness with time, starting with millisecond passivation. This demonstrated the effectiveness of careful ex-situ analysis.

Perhaps the most notable passive film structural information was obtained by in-situ x-ray absorption fine structure (XAFS) measurements--especially those reported by M. Froment on Ni and NiMo alloys. His work, which relied on first neighbor calculations on O around Ni, provided definitive evidence of a high free volume lattice. This was contrasted with ex-situ RHEED analysis of NiO.

The role of cation selective anions adsorbed in outer deposit layers of anodic oxide films was emphasized in H. Bohni's presentation on the role of  $\text{PO}_4^{3-}$  species in the outer layer of P-bearing amorphous alloys. In several papers the carrier type and density of semiconducting passive films were discussed. A particularly notable paper was presented by T.D. Burleigh. He discussed the photochemistry of the passive films formed on a range of metals. Of particular importance was the observation that the passive film was n-type and photoresponsive. Active dissolution was found to occur through an oxide film in which electrical conductivity was high because of a degenerate band (Fermi level in conduction or valence band).

A major activity in the study of pitting corrosion concerned stochastic studies of the birth and death of pits. The lead paper in this section was given by T. Shibata, the author of this model. B. Baroux described a multistep development of this model that considered a combination of stochastic behavior, pit initiation kinetics, and the point defect model. T. Okada presented a different two-step model that considered the first stage to depend on a local perturbation in

ionic concentration and electric field in the solution to cause local accelerated film dissolution and accumulation of chloride species. The second stage is the modification of the oxide film to a chloride in a small hemispherical zone, which grows inwardly.

D.D. Macdonald presented a model in which individual properties of breakdown sites are statistically distributed. In particular, the passive film breakdown of Ni and dilute binary alloys of Ni in borate and phosphate buffers containing chloride ions was considered from the point defect model viewpoint.

R.C. Newman discussed the influence of alloy and environmental composition on localized corrosion. The main thesis was the influence of alloy addition on the dissolution and passivation kinetics of micro-crevices or cavities at the complete exclusion of passive film structure and composition.

## NEW ADVANCES IN PASSIVE FILM RESEARCH

In a keynote address M. Keddam reported on a physical basis for interpreting impedance data by simultaneous measurement of the frequency response of such physical quantities as mass, measured by a quartz microbalance electrode (QMBE), and the amount of charge stored in the surface layer.

A paper by Sato's group reported on the use of a piezoelectric element attached to an electrode for studies of anion (adsorption) induced surface stress. This technique was used to demonstrate that  $\text{SO}_4^{2-}$  adsorption played no role in the reduction of passive films formed on Fe and Cu and was used to determine the potential of zero charge of the bare metal surfaces in borate buffer solution. While channeling and nuclear reaction analysis are well-known ion beam

tools, a novel application to the characterization of passive films on (100) single crystals of Fe-Cr-Ni and Fe-Cr-Ni-Mo was reported by P. Marcus. The technique enabled ex-situ probing of the passive film composition and that of the underlying alloy.

D.D. Macdonald reported on the enhanced sensitivity and quantitative characteristics of a new sputter depth profiling method known as SALI or surface analysis by laser ionization. The technique, however, offers no direct chemical state information.

While the scanning tunneling microscope (STM) has become a ubiquitous laboratory instrument, its in-situ use in monitoring of corrosion-induced surface morphology is problematical. A paper on this technique was to be given by A. Miyasaka of Nippon Steel Corporation, but a surrogate speaker failed to convince this listener that the interpretation is unambiguous.

A. Davenport described recent work using glancing angle x-ray studies of passive films on Al. Her study utilized the fluorescent yield at the x-ray adsorption edge of a specific species, e.g., Cr K $\alpha$ , and to stimulate fluorescence from the very near surface region by reducing the angle of x-ray incidence so as to cause external reflection.

Photochemical studies of passivation, while not new methodology, have come into vogue. The upsurge in such studies prompted the organization to invite Professor H. Gerischer of the Fritz-Haber Institute to provide a keynote on this topic.

## SATELLITE MEETING AT TOHOKU UNIVERSITY

The satellite meeting at Tohoku University, Sendai, was chaired by Professor Koji Hashimoto. A dozen foreign invited speakers and at least an equal number of



Japanese speakers discussed (mostly) amorphous alloys and their properties; a good deal of the work included surface studies.

Following a general review by A. Inoue (coauthored by the director of the Institute for Materials Research at Tohoku University, Professor T. Masumoto) of the properties and opportunities for further development of amorphous alloys, Professor K. Suzuki presented an excellent paper on the structure of amorphous alloys as determined by neutron scattering. Unfortunately no discussion on structural influence on properties was offered as has been discussed, for example, by Lashmore (National Institute of Standards and Technology) and Watson (Brookhaven National Laboratory). Nevertheless, the influence of various polymorphs on corrosion and passivity is a study waiting to happen.

K.E. Heusler presented a paper concerning the kinetics of dissolution of crystalline and amorphous alloys. He discussed the rate-controlling processes involved in bare metal dissolution, transfer through the passive film, and dissolution of the passive film. This general model included surface binding energy variations relating to specific surface structures in crystalline and amorphous systems.

M. Janik-Czachor discussed the passivation behavior of an  $\text{Fe}_{.40}\text{Ni}_{.40}\text{B}_{.20-x}\text{P}_x$  alloy. Of the many tools at our disposal in obtaining chemical state information about passive films, in Janik-Czachor's report only Auger electron spectroscopy was used. The speaker deferred to Heusler's previous comments regarding the relationship between the surface composition of the alloy and the dissolution and the relative dissolution rate constants for the components in the alloy.

The present writer then delivered a paper on the passivation behavior of Ni<sub>20</sub>P and Ni(3-10)Cr<sub>20</sub>P. The role of P in the

passivation of these systems was discussed in terms of anodic surface segregation of P, which controls both anodic kinetics and prevent entirely the formation of an oxide-based passive film in favor of hypophosphite and phosphate based films. The electrochemical behavior of black P, a metallic allotrope, was compared with that of Ni<sub>20</sub>P, and specifically in the low potential regions of Ni-Cr<sub>20</sub>P alloys. Finally, the cation selective influence of surface phosphate groups was discussed.

Several papers explored the electrocatalytic and heterogeneous catalytic behavior of amorphous alloys. This work benefited from an excellent overview by D.L. Cocke that provided some important guidelines to material selection. Clearly, this is an area with considerable scope for further enquiry. The reviewer was particularly struck by the number of examples of intermetallic phase formation below the oxide film in the amorphous alloys discussed, though surprising little attention was given to this behavior. This would certainly suggest that there is a "shot-gun" approach to many of the amorphous alloy systems studied and little attempt to engineer an interesting fundamental enquiry.

## CONCLUDING REMARKS

Perhaps most notable at these meetings was a renewed excitement towards the challenge of the complex problems faced in attempting to understand passivity and its breakdown. I was particularly impressed with the dangers of attempting to provide universal models. For example, pure metals and alloys may well differ by virtue of the fact that a pure metal may only develop an oxide film whereas an alloy may develop an alloy surface phase such as an intermetallic, a sulphide, nitride, etc., as well as an oxide

film. XAFS did not seem to have generated as much in-situ data as one might have expected since the fifth symposium in Bordeaux. This is probably due to the inherent difficulty of analyzing the fine structure of such complex systems. Perhaps it is my bias that leads me to conclude that there continues to be too little communication between the electrochemists and surface analysts, and without this communication the field will move forward more slowly and less steadily. The pair of symposia were stimulating and provide an impetus to many of us to improve our communication over the coming years. The support of Dr. A.J. Sedriks, Materials Division, Office of Naval Research, for my attendance at these meetings is greatly appreciated.

## LIST OF PAPERS PRESENTED

### Sixth International Symposium on Passivity

Baroux, B. (Ugine Res. Center, France), "A Multistep Birth and Death Model for Local Breakdown of Passivity"; Okada, T. (Ind. Products Res. Inst., Japan), "Two-Step Initiation Hypothesis of Pitting Corrosion in Passive Metals"

Bohni, H. (ETH-Honggerberg, Switzerland), "Passivity and Breakdown of Metallic Glasses"

Burleigh, T.D. (Alcoa, U.S.), "Photocurrents on Passive and Active-Passive Metals"

Cohen, C., and D. Schmaus (Univ. of Paris VII, France), A. Elbiache and P. Marcus (Ecole Natl. Sup. Chem. Paris, France), "Channeling and Nuclear Reactions Analysis Study of Passive Films Formed on FeCrNi and FeCrNiMo (100) Single Crystals"

Cortes, R. (Univ. of Paris, Sud, France), M. Froment, A. Hugot-Le Goff, and S. Joiret (Univ. of Paris VI, France), "Characterization of Passive Films on Ni and Ni Alloys by RefLEXAFS and Raman Spectroscopy"

Davenport, A., and H. Isaacs (Brookhaven Natl. Lab., U.S.), "Glancing Angle X-Ray Studies of Oxide Films"

Gerischer, H. (Fritz-Haber Inst., Max-Planck, FRG), "What Can We Learn on Passivity From Photoelectrochemical Experiments?"

Hoppe, H.W., and H.H. Strehblow (Univ. of Dusseldorf, FRG), "XPS and UPS Examinations of Passive Layers on Ni and Fe/Ni Alloys"

Jiang, X.-C., M. Seo, and N. Sato (Hokkaido Univ., Japan), "Piezo-Electric Response to Surface Stress Change of Iron and Copper Electrodes Covered with Oxide Films"

Keddam, M., C. Gabrielli, and H. Takenouti (Univ. P. and M. Curie, France), "New Advances in the Investigation of Passivation Mechanisms and Passivity by Combination of ac Relaxation Techniques--Impedance, Quartz Electrogravimetry and RRDE"

Macdonald, D.D., and M. Urquidí-Macdonald (SRI International, U.S.), "Deterministic Models for Passivity Breakdown"

Macdonald, D.D., M. Ben-Haim, and J. Pallix (SRI International, U.S.), "SALI Analysis of Passive Films on Nickel Alloys"

Miyasaka, A., and H. Ogawa (Nippon Steel, Japan), "In Situ Observation of Stainless Steel Surface in Aqueous Solution Using Scanning Tunneling Microscope"

---

Newman, R.C. (UMIST, U.K.), "The Effects of Alloy and Environment Composition on Passivity and Localized Corrosion"

Sato, N. (Hokkaido Univ., Japan), "Passivity of Metals"

Shibata, T. (Osaka Univ., Japan), "Stochastic Study of Passivity Breakdown"

### Satellite Meeting

Clayton, C.R., and M.A. Helfand (State Univ. of NY at Stony Brook, U.S.), N.R. Sorensen (Sandia Natl. Labs, U.S.), "An XPS and Electrochemical Study of Black P and Its Relationship to the Passivity of Ni-20P and Ni<sub>x</sub>Cr-20P Amorphous Alloys"

Cocke, D.L. (Texas A&M Univ., U.S.), "Amorphous Alloy Catalysts"

Heusler, K.E. (Tech. Univ. of Clausthal, FRG), "Dissolution Kinetics of Active and Passive Alloys Including Metallic Glasses"

Inoue, A., and T. Masumoto (Inst. for Materials Res., Tohoku Univ.), "Recent Progress of Amorphous Alloys"

Janik-Czachor, M. (Polish Academy of Sciences, Poland), "Passivity of Fe-Ni Base Glasses"

Suzuki, K. (Inst. for Materials Res., Tohoku Univ.), "Structure of Amorphous Alloys"

---

**Clive R. Clayton** is a professor in materials science and engineering at the State University of New York at Stony Brook, where he joined the faculty in 1977. He is a graduate of the University of Surrey in the United Kingdom, where he obtained his Ph.D. under the supervision of Professor J.E. Castle. A major theme of Professor Clayton's research seeks an understanding of the surface chemical processes involved in the corrosion and passivity of crystalline and amorphous alloys and thin film intermetallics, using electrochemical and spectroscopic methods. Professor Clayton is the author or co-author of more than 60 papers and 2 chapters in books, and is the co-editor of three conference proceedings on surface modification. He currently serves as Consulting Editor to the English edition of *Boshoku Gijutsu*.

---

---

# MOLECULAR RECOGNITION IN JAPAN

---

Cynthia J. Burrows

---

*The following summary is based on visits to various universities and attendance at conferences during a 7-month period in Japan, August 1989 to February 1990.*

---

## INTRODUCTION

The field of molecular recognition attempts to understand weak, noncovalent interactions occurring between specific molecules or ions and molecules. Examples of such phenomena are plentiful in biological systems: the specific binding of a substrate (or inhibitor) to an enzyme, the recognition and transport of metal ions ( $\text{Na}^+$ ,  $\text{K}^+$ ,  $\text{Ca}^{2+}$ ) through membranes and the interruption of this process by certain ion channel-binding toxins, and the sequence-specific or topology-specific binding of proteins or drugs to DNA. Modern techniques of nuclear magnetic resonance (NMR), polypeptide and polynucleotide synthesis, chemical modification of biopolymers, and cloning and mutagenesis techniques now allow biochemists to obtain molecular level information about these interactions. From the chemical viewpoint, advances in synthesis and characterization of complex molecules, especially NMR spectroscopy and computer modelling, allow chemists to design, synthesize, and evaluate synthetic molecular receptors and catalysts for both fundamental and applied goals. On the fundamental side, researchers hope to define those specific forces, such as hydrogen bonding, ion-dipole, van der Waal's interactions, or solvent effects, responsible for specific binding between molecules. The practical applications include

the development of new chemical sensors or biosensors, catalysts for the synthesis of useful materials or degradation of harmful ones, solid aggregates with important electronic or optical properties, and chemical tools for the analysis of biopolymers, such as the sequencing of the human genome.

## DEVELOPMENT OF MOLECULAR RECOGNITION CHEMISTRY IN JAPAN

Molecular recognition is a strong area of research interest in both universities and government institutes in Japan. The following summary gives a few highlights of organic and inorganic chemical aspects of this area in Japan.

Some of the earliest work in molecular recognition chemistry developed from the syntheses of large cyclophanes, cyclic hydrocarbons with an interior cavity large enough for a small guest molecule to slip in. Two pioneers of cyclophane chemistry, Prof. Kenji Koga (Univ. of Tokyo) and the late Prof. Iwao Tabushi (Kyoto Univ.), were instrumental in introducing water-soluble cyclophanes as hosts for hydrophobic guests. The cyclophanes typically contain four aromatic rings (ultimately forming the walls of a square cavity) connected by short flexible chains, usually containing ammonium groups for water solubility. Koga's group has made

major contributions in cyclophane chemistry, principally in developing hosts for aromatic hydrocarbons (Ref 1). His research group has also studied crown ethers as enzyme models. A significant advance in this field was the mimicry of peptide synthesis via a thiol-functionalized crown ether (Ref 2); this is described in more detail below. Also in the area of cyclophane chemistry, Prof. Yukito Murakami's group at Kyushu University has prepared a large number of octopus-like cyclophanes in which the cyclophane macrocycle is functionalized with four to eight long hydrocarbon chains. This provides a very large, although ill-defined, hydrophobic cavity. They have demonstrated binding of a vitamin B<sub>12</sub> derivative (Ref 3) and claim turnover catalysis of conversion of  $\beta$ -methylaspartate into glutamate.

Although the Tabushi group was one of the earliest in cyclophane chemistry, perhaps their most significant contributions have been in cyclodextrin and porphyrin chemistry; both of these areas have an unusually large number of researchers in Japan compared to the United States. One of Tabushi's major advances in cyclodextrin chemistry was the development of synthetic methods for selective derivatization of the various glucose units.

## RECENT ADVANCES IN MOLECULAR RECOGNITION

The area of signal transduction and sensors has been addressed by a number of research groups in Japan. Prof. Seiji Shinkai (Kyushu Univ.) reported a series of examples of photo-active crown ether complexes. In these cases, photo-isomerization of an alkene or azo group gives rise to conformational changes affecting ion binding. Similar

effects can be obtained through redox-switched binding using thiol-containing ion binding sites (Ref 4).

Coupling of the molecular recognition phenomenon to potentiometric sensors has been accomplished by a collaborative effort between Prof. Yoshio Umezawa (Hokkaido Univ.) and Prof. Eiichi Kimura (Hiroshima Univ.). This research program is an excellent example of the type of collaborative effort that is actively encouraged and well supported by the Japanese Government. The Kimura group has studied a number of polyammonium macrocycles capable of binding phosphates (such as ATP) and catecholates (such as dopamine) (Ref 5). A typical example is shown in Figure 1. Compound 1 is a 16-membered cyclic pentamine. In aqueous solution, it is readily protonated, taking up three to four protons depending upon the pH. The polycationic macrocycle then has a high affinity for anionic guest molecules, such as ATP<sup>4-</sup> or dicarboxylates. Alternatively, a cyclic oligosaccharide,  $\beta$ -cyclodextrin, with amine groups attached may act as the anion receptor. The macrocyclic receptor may be functionalized with a long chain hydrocarbon. When these receptors are incorporated into a Langmuir-Blodgett (LB) film by the Hokkaido group, the ion permeability of the LB film is responsive to guest anions which may be detected as an electrical signal (Ref 6). This phenomenon is shown in Figure 2. For example, electrolyte anions may readily permeate the LB film, reaching the electrode surface in the absence of complexing anions. If a guest anion is bound to the LB surface, the layer is much less permeable to other anions, resulting in a change in the electrical signal. This approach may be used to determine concentrations of guest anions in the millimolar range.

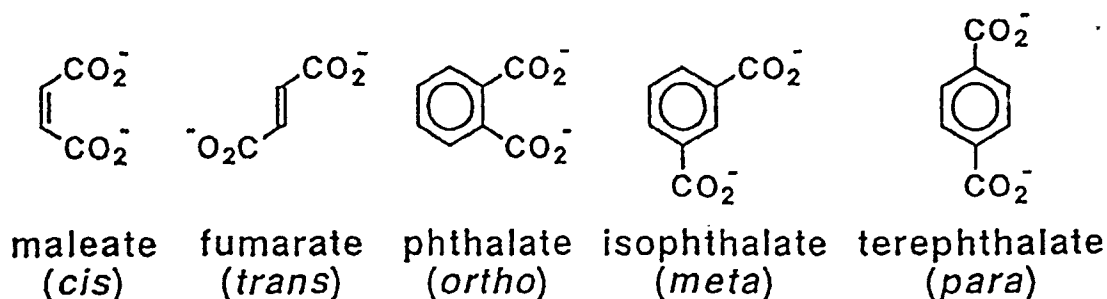
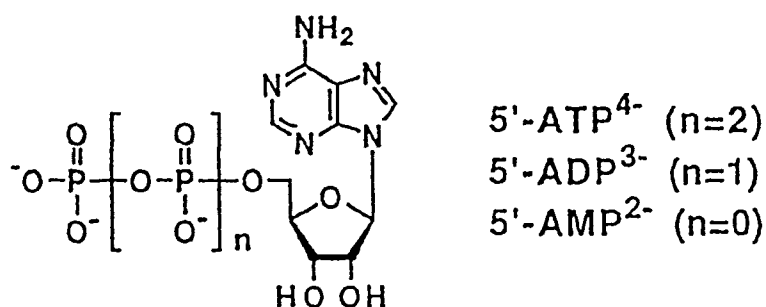
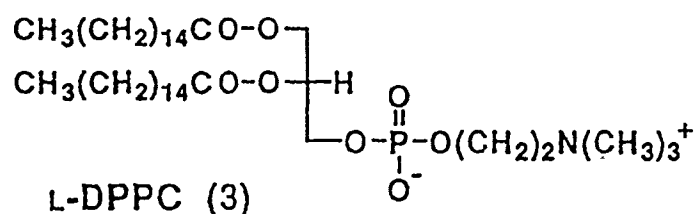
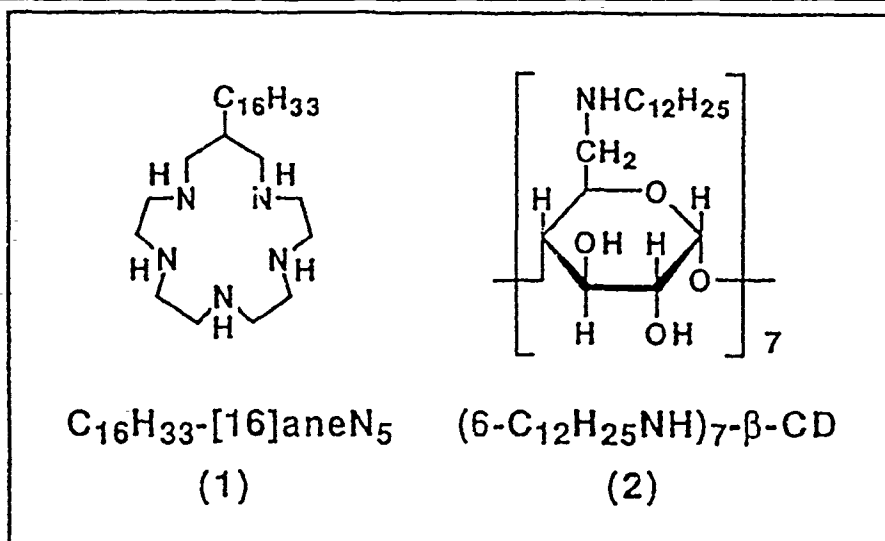


Figure 1. General structure of a macrocyclic pentamine receptor used for recognition and complexation of anions. Reprinted with permission from S. Nagase et al., "Anion Responsive Biomimetic Ion-Channel Sensors Based on Langmuir-Blodgett Membrane Assemblies Containing Synthetic Anion Receptors," to be published in *Analytical Chemistry*. Copyright American Chemical Society.

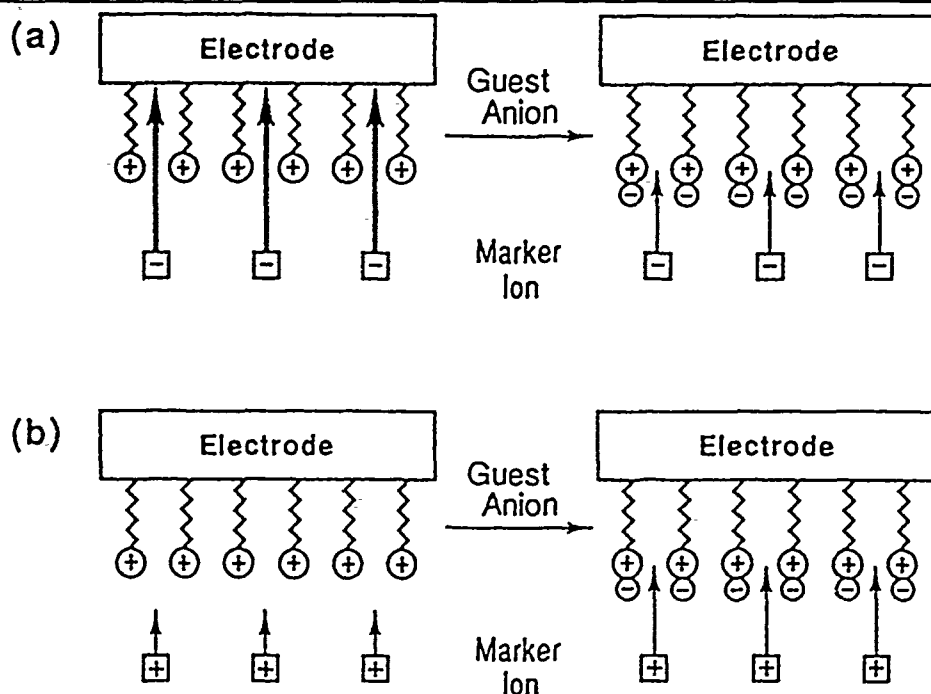


Figure 2. Electrode surfaces coated with Langmuir-Blodgett films doped with synthetic anion receptors yield potentiometric responses to marker anions or cations which are modulated by the presence of complexed anions. Reprinted with permission from S. Nagase et al., "Anion Responsive Biomimetic Ion-Channel Sensors Based on Langmuir-Blodgett Membrane Assemblies Containing Synthetic Anion Receptors," to be published in *Analytical Chemistry*. Copyright American Chemical Society.

Industrial research laboratories are also interested in molecular recognition chemistry for the specific detection of metal ions. While crown ethers have long been investigated as complexing agents for  $K^+$  and  $Na^+$ , discovery of a selective agent for  $Li^+$  recognition has proven to be quite difficult. Dr. Kazuhisa Hiratani, head of the Chemistry Department of the Ministry of International Trade and Industry sponsored Industrial Products Research Institute in Tsukuba, leads a research team investigating  $Li^+$  synthetic receptors. They have discovered that ligand L (see Figure 3) displays the highest  $Li^+/Na^+$  discrimination obtained so far. In studies of competitive ion transport through synthetic membranes, they

found that L was sufficiently lipophilic to dissolve in nonpolar solvents or membranes and possesses the appropriate "bite" angle to preferentially coordinate  $Li^+$ . The selectivity was found to be 110 for  $Li^+$  compared to  $Na^+$  and 400 for  $Li^+$  compared to  $K^+$  (Ref 7).

Another application of crown ether chemistry is demonstrated by complexation of organic amines, as ammonium ions, to 18-crown-6 macrocyclic polyethers. This particular ring size and arrangement of ether oxygens is appropriate for formation of three hydrogen bonds to a tripodal  $RNH_3^+$  group. Using functionalized crown ethers, Prof. Kenji Koga's group at Tokyo University has demonstrated the first example of peptide synthesis

using an artificial enzyme (Ref 2). This is shown in Figures 4 and 5, where Figure 4 displays the actual structure of the thiol-substituted crown ether, the "artificial enzyme" (1), which binds the ammonium substrate (2) to give an enzyme-substrate complex (3). Nucleophilic attack of the thiol at the ester carbonyl produces the intramolecular complex (4). This part of the sequence represents a mimic of a thiol protease enzyme. Use of a slightly different crown ether bearing an N-protected amino acid derivative on one thiol leads to a mimic of peptide synthesis as shown in Figure 5. A second amino acid is bound (6) and activated by thiolysis (7), and the amino group is sufficiently close to react with the adjacent thiol ester (8). This process may now be repeated to continue the peptide chain. Of the many attempts to use crown ether derivatives as enzyme mimics, this example is certainly among the most interesting.

## CONCLUSIONS

In 1987, Hiroshima University hosted the International Symposium on Macrocyclic Chemistry with Prof. Eiichi Kimura as the

principal organizer of the conference. There were over 90 oral and poster presentations by Japanese participants plus those of the foreign attendees (Ref 8). In addition to the areas described above, Japanese research activity in macrocyclic chemistry has been especially productive in the area of inorganic coordination chemistry. The Kimura group in Hiroshima has pioneered the use of polynitrogen-containing macrocycles as ligands for modulating the redox activity of Ni and Cu and the Lewis acidity of Pt, Cu, and Zn.

Overall, molecular recognition chemistry in Japan is an extremely active area of research among organic and inorganic chemists. There is no obvious effort, however, to develop communication between the chemistry and molecular biology aspects of the field. Indeed, the very noncompetitive funding system in Japan does not provide an impetus for researchers to justify their research efforts to a broad scientific community. Still, it seems likely that interest in and support of molecular recognition and catalysis in Japan will continue at a high level.

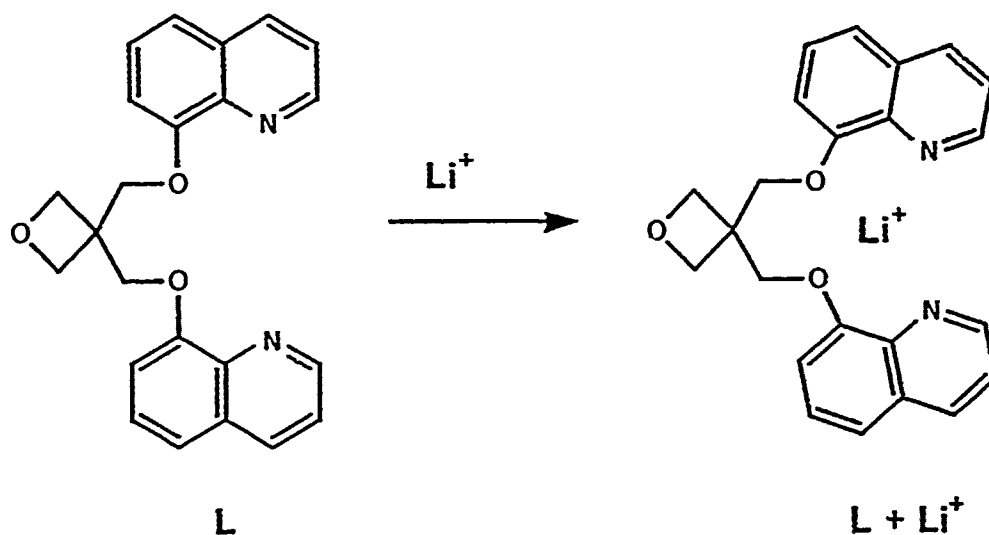


Figure 3. Structure of a quinoline-based ionophore for Li<sup>+</sup> complexation.



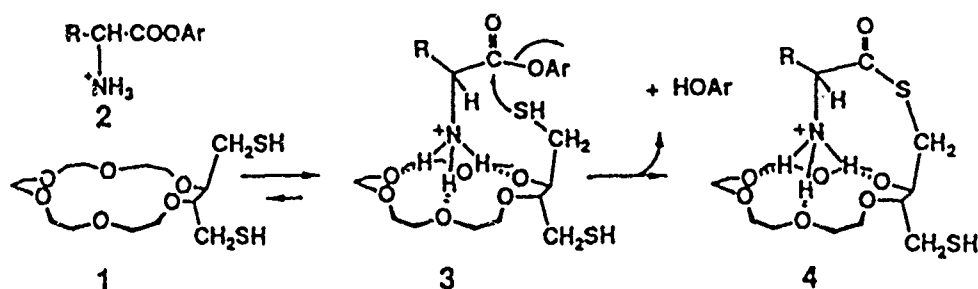
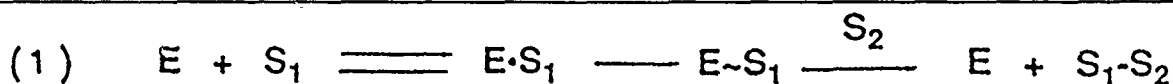


Figure 4. Thiol protease model. Reprinted with permission from S. Sasaki and K. Koga, "Multi-Functionalized Chiral Crown Ethers as Enzyme Models for the Synthesis of Peptides and Multiple Chiral Recognition in the Enzyme Model," *Journal of Inclusion Phenomena and Molecular Recognition in Chemistry* 7, 267-276 (1989). Reprinted by permission of Kluwer Academic Publishers.

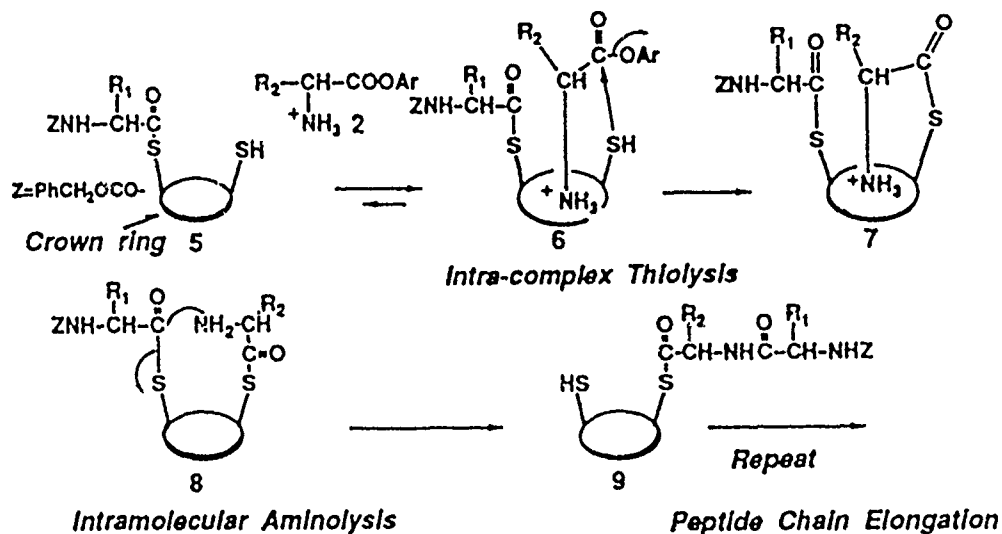


Figure 5. Enzyme model for peptide synthesis. Reprinted with permission from S. Sasaki and K. Koga, "Multi-Functionalized Chiral Crown Ethers as Enzyme Models for the Synthesis of Peptides and Multiple Chiral Recognition in the Enzyme Model," *Journal of Inclusion Phenomena and Molecular Recognition in Chemistry* 7, 267-276 (1989). Reprinted by permission of Kluwer Academic Publishers.

---

## REFERENCES

1. K. Odashima, A. Itai, Y. Iitaka, and K. Koga, *J. Org. Chem.* 50, 4478 (1985).
2. S. Sasaki and K. Koga, *J. Inclusion Phenom.* 7, 267 (1989).
3. Y. Murakami, Y. Hisaeda, and T. Ohno, *Bull. Chem. Soc. Jpn.* 57, 2091 (1984).
4. S. Shinkai, K. Inuzuka, O. Miyazaki, and O. Manabe, *J. Am. Chem. Soc.* 107, 3950 (1985).
5. E. Kimura, Y. Kuramoto, T. Koike, H. Fujioka, and M. Kodama, *J. Org. Chem.* 55, 42 (1990).
6. M. Kataoka, R. Naganawa, K. Odashima, Y. Umezawa, E. Kimura, and T. Koike, *Anal. Lett.* 22, 1089 (1989).
7. K. Hiratani, K. Taguchi, H. Sugihara, and T. Okada, *Chem. Lett.*, 197-200 (1986).
8. E. Kimura, editor, *Current Topics in Macrocyclic Chemistry in Japan* (Hiroshima Univ. School of Medicine, 1987).

---

**Cynthia Burrows** received a Ph.D. degree in physical organic chemistry at Cornell University in 1982. From 1981-1983 she was a NSF-CNRS Postdoctoral Fellow in Professor J.M. Lehn's laboratory in Strasbourg, France. Since 1983, she has been a faculty member at the State University of New York at Stony Brook, where she is currently Associate Professor of Chemistry. From August 1989 to February 1990 she was a visiting scientist at the Institute for Molecular Science, Okazaki, Japan as a Japan Society for the Promotion of Science Research Fellow. Her research interests include the study of Ni, Cu, and Pd coordination compounds as catalysts for organic reactions and the design of new molecular receptors and catalysts based on highly functionalized steroids.

---

---

# ADVANCED SCIENTIFIC COMPUTING IN JAPAN

---

Edward F. Hayes

---

*This article focuses on the current status of advanced scientific and engineering computing in Japan. The high performance computing centers that support significant amounts of basic research are briefly reviewed, computer networking is described, and U.S. and Japanese scientific and engineering research activities that use high performance computers as a tool are compared.*

---

## INTRODUCTION

The focus of this report\* is on the current status of advanced scientific and engineering applications in Japan. The study of this important topic has been a stimulating undertaking for me because of my long-term interest in high performance computing and networking in the United States.\*\*

Since the job of assessing high performance computing research in all fields of science and engineering is clearly beyond what one person can hope to accomplish in a 6-month period, I decided early on to try to focus on those areas that were in one way or another related to the "Grand Challenges" identified in the Office of Science and Technology Policy (OSTP) report on the Federal High Performance Computing Program (Ref 1). Significant progress in each of these research areas is likely to require all the computing resources and good ideas that the world community can generate. So it is important to try to understand what role the

Japanese computational science and engineering community is likely to play over the next 5 to 10 years.

Figure 1, which is taken from the OSTP report, lists some of the grand challenges and their projected computational requirements. To make progress towards the solution of these grand challenges we are going to need significant improvements in high performance computing hardware and software. Moreover, brilliant new and innovative computational approaches will be needed as well.

On the hardware side, it may be informative to compare the current capability of the three Japanese supercomputers to the U.S. supercomputers (see Table 1). If we accept the projections for the next generation of Cray and Japanese supercomputers, it seems clear that Japanese scientists and engineers who have access to these machines will be strategically positioned to make significant contributions to the solutions of one or more of these grand challenges.

---

\* This document represents an excerpt from a draft of a report titled *Advanced Computing in Japan, 1989 Study*. As a draft, it remains subject to revision. It was sponsored by the National Science Foundation (NSF) and the Department of Energy of the United States Government, under NSF Grant ECS-8902528, awarded to the Japanese Technology Evaluation Center at Loyola College in Maryland. The views expressed in the article are solely those of the author.

\*\* The author was chair of the NSF Task Force that was charged with the design and implementation of the present supercomputing centers and networking activities.

---

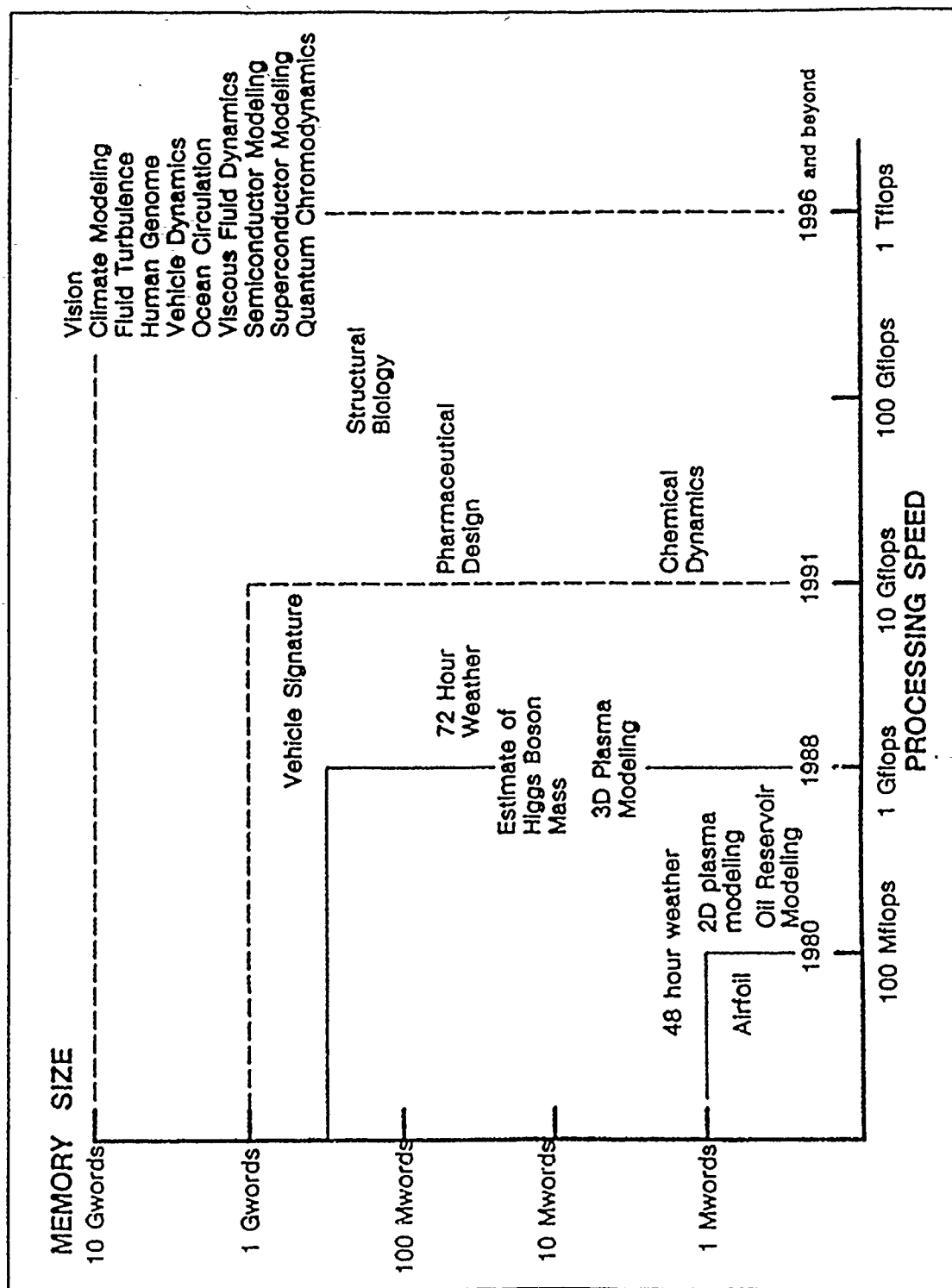


Figure 1. Some grand challenges and their projected computational requirements.

Table 1. Supercomputer Parameters

Supercomputer	Peak Performance (GFLOPS)	Memory Capacity (MW)	No. of Processors
Hitachi S-820/80	3.0	300	1
NEC SX-2	1.3	128	1
NEC SX-3 <sup>a</sup>	22	256	4
Fujitsu VP-400E	1.7	32	1
Fujitsu VP-2600/20 <sup>a</sup>	4	256	1
Cray XMP	0.84	64	4
Cray YMP	2.7	128	8
Cray-2	2	128	4
Cray-3 <sup>a</sup>	16	1024	16
Cray C-90	16	256	16

<sup>a</sup>These are projected parameter values.

On the human resource side of high performance computing, if we look at the situation at the Department of Energy (DOE) national laboratories, the National Science Foundation (NSF) supercomputer centers and the National Center for Atmospheric Research (NCAR), and at the National Aeronautics and Space Administration (NASA) centers, the number of high quality researchers and the number of significant research results are very impressive (see Ref 2-7). In the United States, the unique combination of significant amounts of time on state-of-the-art high performance computers, quality software and documentation, expert training and consulting, and convenient networking access has contributed significantly to this strength.

In Japan, the number of computational researchers and the amount of fundamental basic research activity are much smaller than in the United States. This appears to be true in all fields of computational science and engineering. In the past the differences in the level of activity have been so large in some fields that U.S.

researchers did not pay very much attention to what their Japanese counterparts were doing.

The situation in Japan is improving, however. In several computational research areas the Japanese have made significant recent progress, and the Japanese computational research work is reaching the quality, if not the quantity, of current work here in the U.S. Increasing numbers of Japanese computational scientists and engineers are gaining access to significant amounts of state-of-the-art supercomputer time, and the software environment in Japan is improving as well.

Thus, over the next 5 years it is reasonable to expect challenges to the current U.S. preeminence in most areas of computational science and engineering. You can get some measure of the current Japanese investment in supercomputers from Table 2. As of August 1989, there were 125 supercomputers installed in Japan. About 30 of these supercomputers were installed at academic centers.

Table 2. Installed Supercomputers  
in Japan as of  
August 1989

Manufacturer	No.	Percentage
Cray	17	13.6
ETA	2	1.6
Fujitsu	57	45.6
Hitachi	28	22.4
NEC	21	16.8
Total	125	100.0

The organization plan for this report is as follows. The first section contains a brief overview of the high performance computing centers in Japan that support significant amounts of basic research. The second section is a brief status report on computer networking in Japan, followed by more detailed discussions of a few of these academic centers. The final section contains some qualitative comparisons between U.S. and Japanese scientific and engineering research activities that use high performance computers as a tool.

## OVERVIEW OF ACADEMIC SUPERCOMPUTER CENTERS

Since the focus of this report is on basic research applications using supercomputers, no attempt was made to cover high performance computing centers in industry. As noted above, only 30 of the 125 supercomputers in Japan as of August 1989 are in academic research environments.

There are four categories of supercomputer centers that allocate a significant amount of their time to fundamental basic research:

- National university centers
- National Center for Science Information System (NACSIS)
- Interuniversity institutes
- Special centers

Each of these categories of centers plays a unique and important role in Japanese high performance computing research.

The national universities have supercomputer centers that are basically service bureaus for academic researchers. These centers currently provide computing services to over 20,000 researchers. Charges are set to recover a small amount of the total cost of providing the computer time. These centers have no direct research support. The Ministry of Education provides direct operational support, but researchers must obtain their own research support for workstations and for computer charges. The seven national university centers are located at the following sites:

- Hokkaido University
- Tohoku University
- Tokyo University
- Nagoya University
- Kyoto University
- Osaka University
- Kyushu University

Table 3 indicates the kinds of supercomputers at each of these sites. There are two NEC, two Hitachi, and four Fujitsu supercomputers at these seven centers. The Tokyo University center will be discussed in more detail below.

Table 3. Status of Japanese Computing Facilities

University	Location	Mainframe	Supercomputer		Staff		Related Educational Organizations	No. of Users (approx.)	Director
			Model	GFLOPS	Permanent	Scientists			
Hokkaido	Sapporo	HITAC M-682H	Hitachi S-820/80	2	28	5	53	1600	Prof. Tagawa Ryoaburo
Tohoku	Sendai	ACOS 2020	NEC SX-2N	1.1	37	11	45	1800	Prof. Noguchi Shoichi
Tokyo	Tokyo	HITAC M-680H M-682Hx2	Hitachi S-820/80	2	69	10	274	7000	Prof. Goto Eiichi
Nagoya	Nagoya	FACOM M-780/20	Fujitsu VP-200	0.5	31	9	66	1700	Prof. Shimazu Yasuo
Kyoto	Kyoto	FACOM M-780/30	Fujitsu VP-400E VP-200	1.7 0.5	48	7	57	4200	Prof. Nagao Makoto
Osaka	Osaka	ACOS 2020	NEC SX-2N	1.1	30	6	132	1600	Prof. Yamada Tomoharu
Kyushu	Fukuoka	FACOM M-780/20	Fujitsu VP-200	0.5	30	8	93	2100	Prof. Sagara Setsuo
NACSIS <sup>a</sup>	Tokyo	HITAC M-682H M-684H ACOS 1000/10 <sup>b</sup>	Hitachi NEC		76	16			Prof. Inose Hiroshi

<sup>a</sup>NACSIS: National Center for Science Information System.<sup>b</sup>Used for electronic mail.

---

The National Center for Science Information System (NACSIS) is the second kind of center. NACSIS was inaugurated in 1986 as the center for accessing scientific data bases (e.g., Science Citation Index). While it does not have a supercomputer, this center is a significant resource for Japanese researchers and it is beginning to play an important role in computer networking both within Japan and networking to the United States.

The centers at the four interuniversity institutes constitute a third kind of academic supercomputer center. The orientation of each of these centers is apparent from their titles:

- Institute for Molecular Sciences (Okazaki)
- Institute for High Energy Physics (Tsukuba)
- Institute for Space and Astronautical Science (Tokyo)
- Nuclear Fusion Institute (Nagoya)

These institutes all have significant research supercomputing centers. They do not charge users for computer time. They tend to have smaller numbers of users (hundreds rather than thousands) and researchers are able to undertake projects that require significant allocations of computer time (i.e., thousands of hours). The research support for these centers has also included necessary funds for workstations needed for advanced graphics and visualization. Activities at the Institute for Molecular Sciences will be discussed in more detail below.

The final set of supercomputer centers includes four special centers that I thought might be of particular interest to U.S. computational scientists and engineers:

- Protein Engineering Research Institute (Osaka)
- Institute for Laser Fusion (Osaka)
- Institute of Computational Fluid Dynamics (Tokyo)
- Institute for Supercomputing Research (Tokyo)

Each of these centers has a special research mission. The Protein Engineering Research Institute and the Institute of Computational Fluid Dynamics will be discussed in more detail later.

## NETWORKING IN JAPAN

There are five basic elements to the networking environment in Japan that are important for high performance computing:

- Science Information Network (768 Kbps)
- Satellite Link to National Science Foundation (9.6 Kbps)
- MFENet Connections (9.6 Kbps)
- WIDE Project (2-3 64 Kbps)
- PACCOM Network - Science Internet

Since 1987 all of the national university supercomputer centers and NACSIS have been connected to each other by the Science Information Network (see Figure 2). The Institute for Molecular Sciences was connected to the network in July 1989. The backbone of the Science Information Network is a 768-Kbps packet line. The network uses the N-1 protocol and provides



---

time sharing and batch processing services. While the network does provide convenient access to the NACSIS data bases, the network does not appear to be used heavily for remote access to supercomputers. According to Professor Eiichi Goto, director of the Tokyo University Supercomputer Center, the strategy in Japan has been to put money into additional supercomputers rather than into building better computer networks like we have in the United States.\* This works out reasonably well for access within Japan, since Japan is a small country from a geographic perspective. The Science Information Network has been connected via satellite to NSF since the beginning of 1989.

The connection to the Department of Energy supported MFENet is shown in Figure 3. Currently this connection is only at 9.6 Kbps. According to Dr. Tetsuo Kamimura, director of the National Institute for Fusion Research at Nagoya, the MFENet-IPPJNet link has greatly facilitated collaboration between U.S. and Japanese fusion researchers.\*\* The existing link, which of course could be better than 9.6 Kbps, facilitates joint work on code development and usage, and data analysis, while minimizing the necessity for long exchange visits or frequent foreign travel by collaborating scientists. David Baldwin, director of the Texas

Institute for Fusion Studies, also echoed the importance of the network link to the overall success of the U.S.-Japanese program in plasma physics. Both Baldwin and his colleague Wendell Horton\*\*\*, who manages the U.S.-Japan technical exchange program, indicated that the Japanese program in plasma physics has developed strength in the innovation of advanced computer simulation techniques, especially the pioneering particle simulation work of Kamimura (Ref 8). Thus they were interested in the extent to which the network link will improve joint code development and, importantly, lead to needed improvement in the documentation of the Japanese codes. From this perspective there seems to be a good case for upgrading this network connection in the near future.

The WIDE project (Widely Integrated Distributed Environment) (Ref 9) was initiated in April 1988 by Professor Jun Murai (University of Tokyo). Its aim is to create a backbone network for all academic networks in Japan, as well as a research testbed for ISDN (voice and data transmission) and OSI (operating systems) studies. The backbone for the WIDE network is two to three 64-Kbps lines. The number of users is quite small (about 2,000).

---

\* Professor Eiichi Goto's view that in Japan networking is not as important as in the United States was also supported in a letter from Professor Makoto Nagao, who is the director of the supercomputer center at Kyoto University. Even if the lack of this infrastructure is not a problem for researchers within Japan, it may limit U.S.-Japanese collaborative research efforts in computational science and engineering.

\*\* Dr. Tetsuo Kamimura's comments on the importance of the MFENet-IPPJNet link were supported by Wendell Horton, manager of the U.S.-Japanese technical exchange program in plasma physics, and by Dr. David Baldwin, director of the Texas Institute for Fusion Studies.

\*\*\* Dr. Wendell Horton's report to DOE, titled "Basic and Applied Plasma Physics in Japan," provides an excellent overview of these cooperative research activities.

# SCIENCE INFORMATION NETWORK

(as of June 1989)

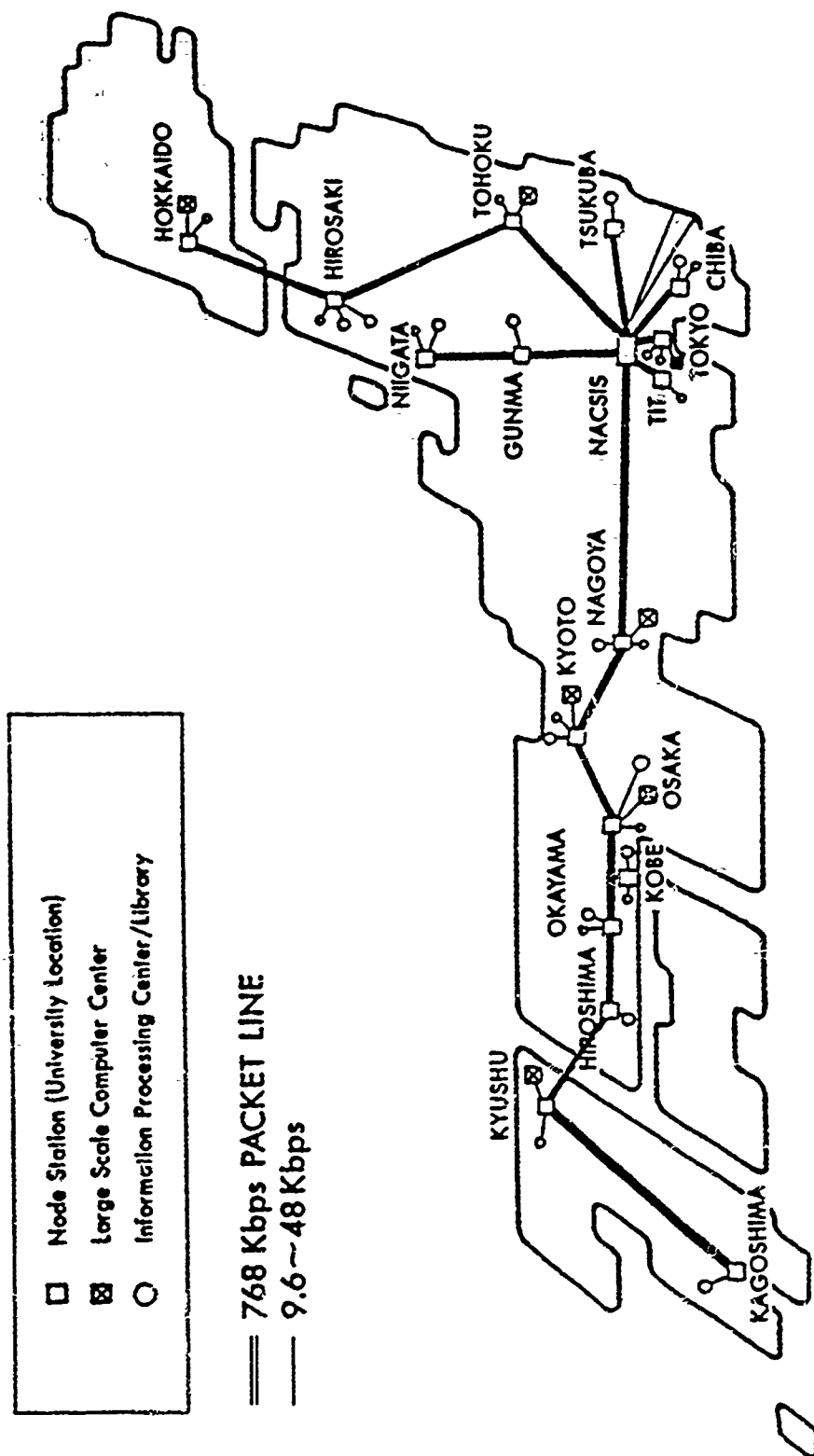


Figure 2. Science Information Network.

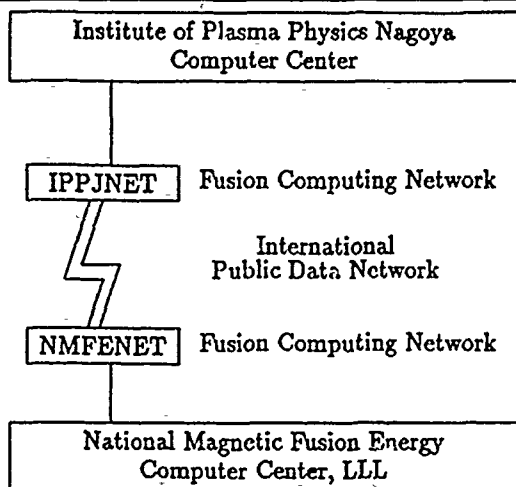


Figure 3. U.S.-Japan data linkage.

Networking in Japan is in its early stages of development. A number of the centers (e.g., the Protein Engineering Institute) are not currently connected to either the WIDE network or the Science Information Network. According to Bill Gale, visiting researcher at the Institute for Supercomputing Research, "... the rate of network growth in Japan appears slowed by lack of intra-agency government cooperation and by government regulations, absent in America since the deregulation of the telephone industry" (Ref 9).

The PACCOM project, funded by NSF and NASA in 1988, aims to construct a network infrastructure in the Pacific region. The primary focus of PACCOM in Japan is the WIDE network. A number of the Japanese researchers expressed interest in improved networking within Japan and to the U.S. Science Internet. Such developments have the potential to enhance U.S.-Japanese collaborative projects in many research areas.

## INSTITUTE FOR MOLECULAR SCIENCES

According to Will Lepkowski (Ref 10), "The Institute for Molecular Sciences (IMS) in Okazaki is a prime example of Japan's institutional future. If Japan really plans to internationalize its basic research by attracting more foreign scientists to the country, IMS is probably the model of such an effort."

IMS has 20 research laboratories, each staffed by a full professor, an associate professor, two research associates, and a few technical associates. Three of these laboratories have foreign visiting professors. The 20 laboratories are organized into five departments and one facility for coordination chemistry.

- Department of Theoretical Studies
- Department of Molecular Structure
- Department of Electronic Structure
- Department of Molecular Assemblies
- Department of Applied Molecular Science
- Coordination Chemistry Laboratories

IMS has six specialized research facilities:

- Computer Center
- Low-Temperature Center
- Instrument Center
- Chemical Material Center
- Equipment Development Center
- Ultraviolet Synchrotron Orbital Radiation Center

IMS has no undergraduate students. Since the faculty members have no undergraduate teaching duties, they are able to maintain very high levels of research activity.

Professor Keiji Morokuma, an internationally known quantum chemist, is the director of the IMS Computing Center. His research in molecular electronic structure theory is well known in the United States and around the world. His recent "Ab initio MO Study of the Full Catalytic Cycle of Olefin Hydrogenation by the Wilkinson Catalyst  $\text{RhCl}(\text{PR}_3)_3$ " (Ref 11) has succeeded in clarifying the potential energy profile for the full catalytic cycle of ethylene hydrogenation.

The IMS Computing Center has a Hitachi S-820/80 supercomputer with 256 MB of memory. The 4-GB of extended memory allows the input/output (IO) of intermediate data at a speed of about 2 GB/s. This capability has had a major impact on their code designs for molecular integrals. Since the number of integrals that must be manipulated in a linear combination of atomic orbitals (LCAO) molecular orbital calculation scales as the number of atomic orbitals (AOs) to the fourth power, the amount of IO required for a 100 AO calculation is considerable. On a Cray the IO associated with the manipulation of the molecular integrals can become the rate controlling step in a self-consistent field (SCF) calculation--this has led some researchers in the United States to attempt to circumvent the IO problem by recalculating the integrals for each SCF iteration (Ref 12). Morokuma reports that with the extended memory IO is not a bottleneck for large SCF calculations.

The IMS Computing Center has an extensive program library that includes the following:

- IMS Molecular Packages--about 200 investigator-supplied programs.

- Quantum Chemistry Program Exchange Programs--all (500) QCPE Programs have been purchased and are available.\*
- NUMPAC Library--extensive numerical calculation program library (about 1,000 subroutines) obtained from Nagoya University.

Unlike the situation at the national university computing centers, the IMS center has extensive graphics and visualization capabilities. The color video that Professor Iwao Ohmine made of his molecular dynamics calculations of water may be the most extensive anywhere in the world (Ref 13). Some of this work was carried out in collaboration with Peter Wolynes of the University of Illinois. Wolynes spent about 7 months at IMS while on sabbatical leave from the University of Illinois. Wolynes is one of the top U.S. theoretical chemists.

One of the features of the IMS Computing Center that is attractive to international visitors such as Wolynes is that it is possible to undertake significant computational problems (i.e., the combination of the raw computing power and the modest number of users facilitates the highest quality computational studies). Currently Wolynes is back at Illinois, but Fred Mies of the National Institute for Standards and Technology (previously the National Bureau of Standards) is at IMS collaborating with Professor Hiroki Nakamura, an internationally known atomic and molecular scattering theorist.

The initiative of such U.S. researchers to go to IMS is an indication of the quality of the research program there.

---

\* The Quantum Chemistry Program Exchange, the University of Indiana, Bloomington, Indiana, is a source for the programs.

Unlike the U.S. supercomputer centers, the IMS center does not have any computer operators or systems staff. The computers run completely unattended. The Hitachi software package provided to IMS has been designed to facilitate this mode of operation. When system fixes are necessary Hitachi is called in to do the job. This environment makes running a supercomputer center relatively easy, according to Morokuma. The operations overhead is low and they can allocate their time and efforts to computational research problems. The IMS Computing Center has a total staff of six (one associate professor, one research associate, and four technical staff members). With this size staff the IMS center is not able to mount major software development projects like those at the NSF supercomputer centers.

## UNIVERSITY OF TOKYO COMPUTING CENTER

This center is the largest of the seven national university centers. All computer equipment at the center is rented, not purchased. The annual rental is about \$10M. The rental approach enables the center's computing capacity to be expanded or upgraded as needed. The history of the center's upgrades is as follows:

- 1966 - Hitachi 5020E (256 KB)
- 1973 - Hitachi 880/8700 (3 MB)
- 1980 - Hitachi M-200H (16 MB)  
VAX11/780 (4 MB)
- 1981 - Hitachi M-200H x 4 (64 MB)  
VAX11/780 (4 MB)
- 1982 - Hitachi M-280H x 2 (64 MB)  
VAX11/780 (4 MB)

- 1983 - Hitachi M-280H x 3 (96 MB)  
S-810/20 (128 MB)  
VAX11/780 (4 MB)
- 1989 - Hitachi M-682H x 2 (384 MB)  
M-680H (128 MB)  
S-820/80 (512 MB)  
VAX8600 (20 MB)

The center has maintained state-of-the-art supercomputers for over a decade.

Professor Eiichi Goto, the director, is a distinguished, internationally known developer of computers (Ref 14). While he is an effective director for the center, his real professional love seems to be his quantum magnetic flux (QMF) ERATO Project, which is aimed at building the fastest single-processor computer (Ref 15).

The center currently has a Hitachi S-820/80 supercomputer with a 512-MB memory. In addition, it has three Hitachi M68xH high speed mainframe computers, each with an attached Integrated Array Processor, not shown in the 1989 equipment list above.

At present about 7,000 researchers use the center. It has about 50 permanent staff of which 10 are classified as research scientists--somewhat smaller than at the NSF supercomputer centers.

According to Professor Goto, the center receives no support for research projects. This is one of the reasons that the center does not have the complement of advanced graphics and visualization facilities found at most supercomputer centers in the United States. The center currently provides only limited support for graphics; they have a small number of Suns and Vaxes.

Of the 16,611 CPU hours used in FY 1988, about 40 percent was for science research projects and 52 percent for engineering projects.

---

The center seems to be run very efficiently, but the resources available to any single user are limited. This apparently leads to many small projects and a few large projects. Some users claim that buying their own advanced workstation may be a better investment of limited funds. If supermini-computers become available to current users in large numbers, this could result in significant changes in the user mix.

My impression based on published research results in several fields is that although this center supports many researchers, the integrated quality of the research is lower than that at the NSF supercomputer centers or at the other types of supercomputer centers in Japan. Charging for time and trying to serve too many researchers tends to drive out excellent major projects--the ones that supercomputers are needed to solve. However, the center meets an important need for high performance computing cycles for academic research.

## PROTEIN ENGINEERING RESEARCH INSTITUTE

The Protein Engineering Research Institute (PERI) was founded in April 1986. The organizational structure of PERI is as follows:

- Structural Analysis of Proteins
- Structure-Function Correlation and Design of New Proteins
- Protein Synthesis
- Isolation, Purification, and Characterization of Proteins
- Data Base and Computer Analysis

While all of the divisions use the computing facilities in their research, most of the high performance computing and software work is being carried out by the fifth division, the Data Base and Computer Analysis Division.

The PERI Computing Center has a Fujitsu VP-400E supercomputer with a 256-MB main memory. It is used primarily for molecular mechanics, molecular dynamics, and molecular orbital studies of protein structure and function. Figure 4 shows how the supercomputer is attached to other computing equipment (i.e., VAX 8800 and various workstations). According to Mr. Toru Yao, director of the Data Base and Computer Analysis Division, there are about 50 users of this computing facility.

Peter Kollman, University of California at San Francisco, and Andy McCammon, University of Houston, both know key people at PERI including Haraki Nakamura, who Kollman believes is doing some very important work on long range electrostatic interactions similar to the work of Barry Honig at Columbia University. Both McCammon and Kollman indicated that Professor Nobuhiro Go is probably the top person in Japan in the simulation of protein dynamics and structure. His recent work with Akinori Kidera (Ref 16) at PERI using the normal mode space for Monte Carlo simulation of x-ray diffraction data looks very promising based on their recent human lysozyme test.

In preparing this section, I consulted with Professor George Phillips, Rice University, and Professor Florante Quiocho, Baylor College of Medicine. They are experts in protein structure and dynamics and know about the research activities at PERI. They indicated that PERI is probably the top laboratory in Japan for protein engineering research.

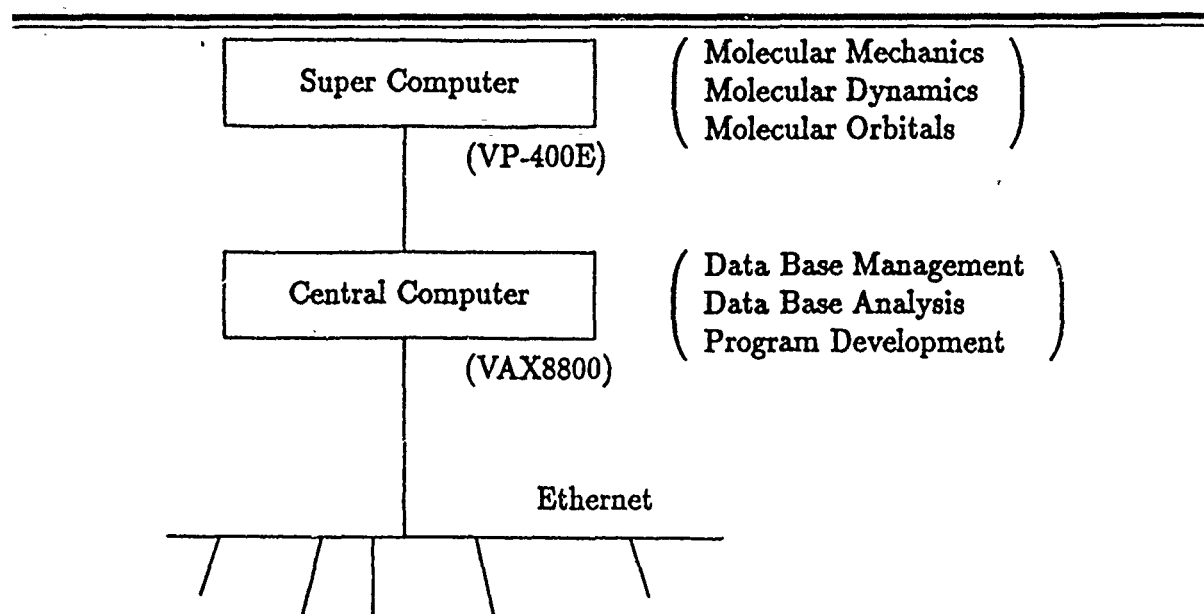


Figure 4. The PERI Computing Center.

The program software available at the PERI Computing Center includes the most advanced program software in the field. The main codes in their program library are as follows:

- Molecular Calculation Codes: AMBER, CHARMM, DISCOVER, FEDER, PRESTO, Gaussian86, JAMOL4
- Data Base Analysis Codes: BION, IDEAS, DSSP, Original Programs
- Codes for Prediction of Structure: HOMOLO, PRDSEC, N14PRDG, NJM
- Codes for Determination of Structure: PROTEIN, FRODO, PROLSQ, GROMOS, DISGEO, DADAS

Much of this software has been ported from outside Japan, particularly the United States. For example, FRODO is a code for displaying protein structures that was developed by

Professor Florante Quioco from the Baylor College of Medicine. The Japanese-developed software includes PRESTO, which is a PERI-developed program; the JAMOL program from IMS; and DISGEO, developed by Professor Nobuhiro Go for nuclear magnetic resonance (NMR) analysis.

While the researchers are making extensive use of imported software for determination of protein structures there did not appear to be significant efforts to develop new, innovative methods for determining structures. PROTEIN is a suite of crystallography programs developed by Huber in Germany, and FRODO and PROLSQ are both from the United States. The only major program that they do not seem to have is Professor Alex Brunger's program EXPLOR.

The software development projects directed at data base analysis have resulted in several original program codes. This seems to be the main focus of their software development activity.

The laboratory is very well funded by the Ministry of International Trade and Industry (MITI) (70 percent) and by 14 private companies (30 percent). They have state-of-the-art x-ray and NMR facilities. They also have excellent graphics and visualization capability. Their video movie of protein dynamics (human lysozyme) is comparable to protein dynamics videos generated by researchers in the United States.

## INSTITUTE OF COMPUTATIONAL FLUID DYNAMICS

The Institute of Computational Fluid Dynamics (iCFD) is a private company that is owned and operated by Professor Kunio Kuwahara. Kuwahara is an associate professor in the Research Division for Space Systems Engineering of the Institute for Space and Astronautical Science. iCFD currently operates four supercomputers (see Table 4).

Table 4. Power of iCFD Computers

Computer	CPU Speed (GFLOPS)	Memory (MB)
Fujitsu VP-200	0.533	256
Fujitsu VP-400E	1.7	512
Hitachi S-820/80	3.0	512
NEC SX-2	1.3	256
Total	6.5	1536

With the total peak speed and memory of the 8-CPU Cray YMP/832 being 2.5 GFLOPS and 256 MB, it follows that the iCFD computers are approximately equivalent to 2.6 YMPs on the basis of CPU speed and to 6 YMPs in terms of memory size.

According to Dr. Hideo Yoshihara, formerly with the Office of Naval Research, Liaison Office Far East, the total computing power represented by these computers exceeds, for example, that of the National Aerodynamic Simulator at the NASA Ames Research Center (Ref 17).

Kuwahara indicated that he established iCFD to obtain access to the large amounts of supercomputer time necessary to carry out fundamental fluid flow studies. Support for this company comes mainly from Japanese automotive manufacturers. iCFD research is centered on the calculation of complex unsteady incompressible turbulent flows over bluff bodies such as automobile configurations.

According to Professor Steve Orszag of Princeton University, Kuwahara's research is having a major impact on the very much smaller computational fluid dynamics research community in Japan. While his earlier work was not up to the standards of the leading researchers in the United States, his current simulations are approaching those standards in terms of mesh size and time scale segmentation.

Kuwahara has sponsored three computational fluid dynamics meetings in Japan (1985, 1987, 1989). These meetings brought together (by invitation only) some of the top U.S. and Japanese researchers in the field. As a result, many of the top U.S. researchers in computational fluid dynamics are familiar with Kuwahara's research.

Kuwahara has assembled an impressive array of graphics workstations including the Ardent Titan and Stellar workstations. His color video tapes of complex flows are impressive. iCFD has developed a scientific visualization system for production of high resolution video movies. Their color videos showing particle path lines, streamlines, and pressure levels are probably among the best in the world.



---

Currently, the iCFD staff can rapidly generate simulated wind tunnel results for sections of cars and airplanes. For instance, a single Navier-Stokes simulation of side-wall effects of two-dimensional transonic wind tunnel using 1.5 million grid points (necessary for good three-dimensional detail) took about 25 hours on the VP-200.

## COMPARISONS BETWEEN THE UNITED STATES AND JAPAN

The number of Japanese researchers in most areas of computational science and engineering is smaller than in the United States by a considerable margin. However, the numbers are growing in each of the fields surveyed as part of this study. These fields are:

- Chemistry
- Fluid Dynamics
- Protein Engineering
- Plasma Physics
- Laser Fusion

The quality of the Japanese efforts in the first three fields has been described in the previous sections. A discussion of the Japanese plasma physics and laser fusion efforts has not been included here. These fields are already a strong component in the current U.S.-Japan bilateral research program, and reports already exist on these activities that are available within DOE. My investigation of these two areas is consistent with the findings in these reports.

It seems likely that for the next 5 years the United States will continue to have the larger numbers of computational researchers in each of the fields listed above. In the past, these larger numbers of researchers have stimulated more creative computational approaches to solving significant research problems. Thus, if we assume that U.S.

researchers will continue to have access to adequate amounts of state-of-the-art supercomputers, it seems likely that the leadership the United States has provided in developing new approaches, algorithms, and software will continue.

In terms of access to significant amounts of needed resources (e.g., megaflops, fast IO, graphics and visualization workstations), the situation over the next few years may actually favor Japanese researchers. Before visiting Japan, I talked with a number of people about the benchmarks that have been made of the U.S. and Japanese supercomputers (Ann Hayes at Los Alamos National Laboratory, Bob Borchers at Lawrence Livermore Laboratory, and Dave Kuck at the University of Illinois). A common theme in these conversations was that, while there has been a great deal of interest in benchmarking, the information available from benchmarking studies only gives semi-quantitative predictions on the relative performance of various supercomputers. Benchmarking is fraught with challenges and problems (see, e.g., Ref 18 and 19).

Nevertheless, it may be informative to report the benchmark results obtained recently by K. Fujii and H. Yoshihara for an unsteady Reynolds-averaged Navier/Stokes code (Ref 20). This code is nearly 100 percent vectorizable. The benchmark results for the Japanese and U.S. supercomputers are given in Table 5 (from Ref 20). Comparison of the actual speeds achieved for single processors shows that the actual GFLOPS achieved by the Hitachi S-820/80 is ahead of all the others. However, if one looks at the elapsed time comparisons in Table 6, it is clear that the eight-processor capability of the Cray YMP/832 wins out in terms of the shortest processing time.

In Table 6, there are three cases of interest:

Table 5. Benchmark Results - Fujii/Obayashi Navier/Stokes Code

Computer	Peak GFLOPS	Actual GFLOPS	Actual/ Peak
Cray YMP/832	0.334	0.175	0.524
Fujitsu VP-400E	1.7	0.395	0.232
Hitachi S-820/80	3.0	0.602	0.201
NEC SX-2A	1.3	0.414	0.319

Table 6. Benchmark Results - Elapsed Time

Computer	CPU (min)	Elapsed (min)	CPU/ Elapsed
Cray YMP/832			
1: (200 iter./1 CPU)	57.57	57.58	1.00
(200 iter./8 CPU)	66.42	46.37 <sup>a</sup>	1.43
2: (200 iter./8 CPU)	52.22	7.97	6.93
3: (200 iter./8 CPU)	55.07	8.15	6.76
(2,000 iter./8 CPU)	550.40	77.92	7.06
Fujitsu VP-400E <sup>b</sup>			
1: (200 iter.)	25.51	28.17	0.91
(2,000 iter.)	254.60	258.41	0.99
Hitachi S-820/80			
1: (200 iter.)	16.75	17.80	0.94
3: (200 iter.)	16.32	18.43	0.89
(2,000 iter.)	161.98	163.63	0.99
NEC SX-2A			
1: (200 iter.)	24.33	24.79	0.98
3: (200 iter.)	20.12	20.52	0.98
(2,000 iter.)	200.80	201.20	1.00

<sup>a</sup>This autotasker anomaly was circumvented by directives in Case 2.

<sup>b</sup>No changes were found to be necessary in Cases 2 and 3.

- 
- Case 1 Calculations with the code as furnished using standard compilers.
- Case 2 Code as furnished, but permitting additional Fortran-compatible compiler tuning including use of compiler directives.
- Case 3 Same as Case 2, but modifications of the algorithms and changes in the programming permitted.

While such benchmarks are not representative of the full range of supercomputer applications, most knowledgeable investigators recognize that the Hitachi S-820/80 is, for most applications, the fastest single-processor supercomputer. However, the multi-processor capabilities of the Cray YMP can provide better overall throughput and achieve better parallel computing speed for some applications (Ref 21).

From an applications researcher's perspective, benchmarks are interesting, but what really matters is what research results can be obtained and published in the literature. So the important question is what difference in supercomputer speed actually gives a researcher a significant advantage in solving a real research problem (i.e., what percentage difference in speed is important?)? Based on the quality of the results being published in the literature during the past year, it does not appear that any of the Japanese or U.S. supercomputers has a decisive lead. Any relative speed advantages in the current generation of supercomputers do not appear to be conferring particular advantages on researchers that cannot be overcome by better applications codes, greater allocations of time, creativity of the investigator in changing the basic approach, or better system and mathematical software.

In the future the situation may shift. The SX-3 is projected to have a maximum speed of 22 GFLOPS, while the Cray 3 and the C-90 are projected at about 16 GFLOPS. Thus, as we look ahead to the next releases of supercomputers and their projected capabilities, there is a possibility the Japanese machines will make somewhat greater strides relative to the projected U.S. machines, but for scientific and engineering applications the most important issues are likely to continue to be ease of use and the amount of resources that can be allocated to a significant problem.

During my visits to the Japanese supercomputer centers, I attempted to develop a perspective on the software, programming environments, and programming tools available on Japanese supercomputers. Since I was not in Japan long enough to use any of the Japanese supercomputers myself, I had to rely on information from researchers who had. This can be a risky situation, but with that as background what follows appears to be true.

- The software products available on the Japanese supercomputers are as good or better than those available from Cray Research.
- The monitoring tools provided by the Japanese vendors that are available to the scientific applications programmers appear to be as good or better than those available from Cray Research.
- Applications software being developed by Japanese researchers may be better vectorized as a result of the better tools and vendor-supplied software.

- Japanese supercomputer centers seem to be having little if any difficulty obtaining access to the best U.S.-developed applications software.

The final comparison that I want to make deals with the quality of the computational research results. I need to preface these remarks with the obvious, namely, that it would be presumptuous to suggest that I am able to do this reliably for fields outside my own specialty of computational chemistry. However, I have read a good deal about what is going on at the U.S. supercomputer centers and at least have attempted to gain a perspective. So here are my general observations:

- The United States appears to be preeminent in all basic research areas of computational science and engineering.
- The Japanese are making significant strides as the current generation of researchers matures in their use of supercomputers and a younger generation is trained in computational science and engineering.

## REFERENCES

1. *The Federal High Performance Computing Program*, Executive Office of the President, Office of Science and Technology Policy (September 1989).
2. Annual Report to the National Science Foundation from the National Center for Supercomputing Applications (1987).
3. National Center for Atmospheric Research Annual Report (1988).
4. *New Dimensions of Insight - Science at the San Diego Supercomputer Center* (1988).
5. *Projects in Scientific Computing*, Pittsburgh Supercomputing Center (1988-89).
6. *Science at the John von Neumann National Supercomputer Center*, Annual Research Report (1988).
7. *Supercomputing Review* (October 1989).
8. D.C. Barnes, T. Kamimura, J.N. Leboeuf, and T. Tajima, "Implicit particle simulation of magnetized plasmas," *J. Comput. Phys.* 52, 480-502 (1983).
9. B. Gale, "The 3rd ISR supercomputing workshop," *Vector Register* 3, 11-15 (1989).
10. W. Lepkowski, "Japan's science and technology aim toward globalization," *C&EN*, 7-14 (May 8, 1989).
11. C. Daniel, K. Koga, J. Han, X.Y. Fu, and K. Morokuma, "Ab initio MO study of the full catalytic cycle of olefin hydrogenation by the Wilkinson catalyst  $\text{RhCl}(\text{PR}_3)_3$ ," *J. Am. Chem. Soc.* 110, 3773-3787 (1988).
12. M. Haser and R. Alrichs, "Improvements on the direct SCF method," *J. Comput. Chem.* 10, 104-111 (1989). See other references in this paper.
13. I. Ohmine, H. Tanaka, and P.G. Wolynes, "Large local energy fluctuations in water; II cooperative motions and fluctuations," *J. Chem. Phys.* 89, 5852-5860 (1988).
14. K.F. Loe and E. Goto, *DC Flux Parametron - A New Approach to Josephson Junction Logic*, volume 6 of *Series in Computer Science* (World Scientific Pub. Co., Philadelphia, PA, 1986).
15. E. Goto, T. Soma, and L. Fock, "Fluxoid Josephson computer technology," in *Proceedings of the 3rd, 4th, and 5th Riken - Erato* (World Scientific Pub. Co., Philadelphia, PA, 1988).
16. A. Kidera and N. Go, "Normal mode Debye-Waller factor in protein x-ray crystallographic refinement," in *Proceedings of the Second International Conference, Protein Engineering '89*, International Conference Center, Kobe, Japan, 20-25 August 1989.

---

17. H. Yoshihara, "Professor Kunio Kuwahara's unique Institute of Computational Fluid Dynamics," *Scientific Information Bulletin* 14(3), 115-119 (1989).

18. O.M. Lubeck, "Supercomputer performance: The theory, practice, and results," in *Advances in Computers* 27, 309-362 (Academic Press, 1988).

19. M. Berry, D. Chen, P. Koss, D. Kuck, S. Lo, Y. Pang, L. Pointer, R. Roloff, A. Sameh, E. Clementi, S. Chin, D. Schneider, G. Fox, P. Messina, D. Walker, C. Hsuing, J. Schwarzmeier, K. Lue, S. Orszag, F. Seidl, O. Johnson, R. Goodrum, and J. Martin, "The perfect club benchmarks: Effective performance evaluation of supercomputers," *Int. J. Supercomp. Applications* 3, 5-40 (1989).

20. K. Fujii and H. Yoshihara, "A Navier/Stokes benchmark for Japanese and U.S. supercomputers," *Scientific Information Bulletin* 14(2), 69-74 (1989).

21. I. Ninomiya et al., "Performance of NUMPAC mathematical library package on super computers," in *Proc. Symp. Super Computing*, Grant-in-aid for Cooperative Research (A), "Research on effective use of super computers," pages 23-31, Tokyo, January 1990. The Ministry of Education, Science, and Culture. In Japanese.

---

**Edward F. Hayes** is Vice President for Graduate Studies, Research and Information Systems at Rice University. Prior to returning to Rice in 1987, he was at the National Science Foundation as head of the Physical Chemistry and Dynamics Section (1976-80), head of the Chemistry Division (1982-83, 1985-87), and controller (1983-85). Dr. Hayes was on special detail to the Office of Management and Budget, Executive Office of the President, during 1980-82. He received a B.S. degree from the University of Rochester and M.A. and Ph.D. degrees from The Johns Hopkins University. Dr. Hayes received the Mentorious Executive Award in the Senior Executive Service of the United States Government in 1986 and the Distinguished Service Award from the National Science Foundation in 1985. He is a Fellow of the American Association for the Advancement of Science and the American Physical Society. Dr. Hayes has over 70 publications on quantum theory of molecular structure, application of electronic computers in quantum chemistry, intermolecular interactions, and scattering theory.

---

---

# CHEMICAL RESEARCH INSTITUTES IN TAIWAN

---

Cynthia J. Burrows

---

*With the recent boom in the Taiwanese economy, the Government of the Republic of China is investing more money in scientific research and technology. The top research universities and institutes have facilities now nearing the level of those in the United States. They still lack personnel (graduate and postdoctoral level students), since most of the top students go to the United States for advanced training. Now, however, the situation for those students to return to Taiwan is becoming much more attractive. We should expect to see an increase in both productivity and quality of basic research in Taiwan in the next few years.*

---

## INTRODUCTION

The following is a summary of my impressions of chemical research in Taiwan based on a visit from 6-10 February 1990. My host was Prof. Chin-Kang Sha, Professor of Chemistry at National Tsing Hua University and now also Director of Natural Sciences at the National Science Council in Taipei. During my short stay, I visited National Tsing Hua University, National Taiwan University, and Academia Sinica in addition to the National Science Council. My visit was funded by a grant from the National Science Council of Taiwan.

## GENERAL IMPRESSIONS

Taiwan is in the midst of rapid development. The success of the electronics and PC industry has led to a booming economy but concurrently to a high cost of living. Prices of housing and food in Taipei now rival those of Tokyo. The general appearance of Taipei is not as modern as Tokyo; rather, it is a mixture of new, high-rise concrete and steel office buildings built in the

past 5 years and shorter, more decrepit apartment buildings built between 15 and 30 years ago. There is no rapid transit system as in Japan, so automobile travel is quite congested.

The educational system in Taiwan is similar to that of Japan with a bit more western influence. Children study more hours than in the United States and some attend evening schools or have tutors to help them study for college entrance exams. The students' goal is to obtain entrance to one of the best universities, National Tsing Hua or National Taiwan University, in order to be assured of a good job afterward. Most students attend school for a half-day on Saturday morning, although many schools are not in session on Wednesday afternoon. Similarly, the traditional work week is 5-1/2 days. Recently, many technical businesses or professionals have switched to a regular 5-day week, although the lunch break is shortened so that the 44-hour work week is maintained.

Professors in Taiwan did not complain of a drastic decline in science students compared to that experienced in the United

---

States and Japan. The job market appears to be excellent for all science and engineering professions. After a B.S. degree, students have several options. Many continue for an M.S. degree, which is a prerequisite for the Ph.D. degree. Of the graduate students in chemistry at National Tsing Hua University, my impression was that more than half would leave with an M.S. degree. Almost all of the top students would then go to the United States for a Ph.D. degree and a few to Japan. Of those going to the United States, only some stay for postdoctoral work. There is no postdoctoral program in Taiwan, but good students may return immediately to a job after receiving a Ph.D. For many years, a large fraction of the Taiwanese graduate students in the United States remained there for permanent employment. With the recent improvement in research facilities in Taiwan, many more students are now returning. Virtually all of the professors I met who were under 45 obtained graduate education in the United States. As a result, they spoke excellent English and seemed much more "westernized" than their Japanese contemporaries.

At the State University of New York (SUNY) at Stony Brook, we have about five graduate students coming each year from Taiwan. Most of them have already obtained a Masters degree, meaning that they have had both advanced coursework and worked on a thesis research project. Alternatively, students may do a research internship at Academia Sinica in lieu of an M.S. before coming to the United States. A few students are able to be accepted directly after their undergraduate studies. In addition, some wealthy Taiwanese families apparently send their children for undergraduate degrees in the United States to insure their acceptance to an American graduate program, and some even attend high school there.

---

## NATIONAL TSING HUA UNIVERSITY, HSINCHU

Hsinchu is a city of about 350,000 people located about 1 hour southwest of Taipei. It is said that 50 percent of Taiwan's Ph.D.s live in this city. It is the site of National Tsing Hua University, founded in about 1955, the Science-Based Industrial Park built in the past few years, and another industrial park north of the city. In order to qualify as a national university, the campus must have a certain minimum land area. The campus of National Tsing Hua University is quite spacious and looks very much like major universities in the United States with a combination of modern buildings and park areas. Some of the original buildings from the late 1950s and 1960s remain, but slowly they are being replaced by modern facilities. For example, the Physics Department recently moved into a new, architecturally interesting building, and the Chemistry Department will move in 2 years to an impressive new building now under construction. Recently, the decision was made to build a synchrotron light source. This will be the first in Taiwan, and its site on the edge of the Tsing Hua campus has already been selected. It is anticipated that physicists and physical chemists from the university as well as researchers in the nearby semiconductor industry will make use of this facility.

Because of my research interests, I interacted primarily with the organic and inorganic chemists at National Tsing Hua University. The organic chemists are mostly involved in natural products synthesis and synthetic methods. These were very popular areas of research in the United States over the past 15 years, although U.S. funding in these areas has rapidly dropped off. There is essentially no work being done in the area of molecular recognition in Taiwan;

perhaps because it has developed only recently in the United States, those major research groups have not trained many Taiwanese students. Similarly, the area of bioorganic chemistry does not seem to be well developed in Taiwan. Biochemistry departments are typically separate from chemistry departments, so I had no interaction with them.

Some typical research projects at Tsing Hua University are as follows. Prof. C.K. Sha is investigating the use of pericyclic reactions, especially cycloadditions involving heteroatoms, for the preparation of heterocyclic compounds. Prof. Liao's group works primarily on reactions of quinones, especially photochemical di- $\pi$ -methane rearrangements as a way to prepare new organic compounds. Prof. C.H. Cheng is an organometallic chemist studying Ni(O) chemistry. He has discovered the conversion of  $\text{NO} + \text{CO}$  to  $\text{N}_2\text{O} + \text{CO}_2$  catalyzed by Ni powder. Prof. C.P. Cheng is investigating the ability of dicobalt complexes to bind and activate  $\text{O}_2$ . Prof. B.J. Uang is focussing on natural products research using carbohydrates as a source of asymmetry and making use of Diels-Alder cycloaddition reactions.

The Science-Based Industrial Park is located adjacent to the National Tsing Hua campus. This is the "Silicon Valley" of Taiwan. Many of the PC and electronics companies are located here in quite new facilities. The land is owned by the Government and leased to industries with the stipulation that they must do both research and manufacturing. Some of the very large electronics companies are located elsewhere in less expensive areas of Taiwan where they can have a large manufacturing component.

Other industrial parks in the area are located along the major highway connecting Hsinchu and Taipei. These have no

requirement to carry out basic research. A few pharmaceutical companies that employ organic chemists are located there also. However, there is little basic research in the pharmaceutical industry in Taiwan, and they rely primarily on developments in their parent companies in Japan and the United States.

## NATIONAL TAIWAN UNIVERSITY, TAIPEI

National Taiwan University was one of the Imperial Universities established by the Japanese early in the 20th century. As such, it has maintained high standards for its students and faculty and is regarded as the top institution in Taiwan (or perhaps that position is shared with Tsing Hua University). The campus is quite large considering the now crowded conditions of Taipei, but there has been less renovation than is evident at National Tsing Hua University. The Chemistry Department is very similar to that of National Tsing Hua University in terms of its physical facilities, size (about 35 faculty members), and composition. Both departments occupy older buildings similar to many of the facilities seen in Japanese universities. Now that National Tsing Hua University will have such an impressive new building in 2 years, the Chemistry Department at National Taiwan University hopes for a similar improvement within 5 years. Both universities have quite impressive instrumentation. For example, each Chemistry Department has a few superconducting nuclear magnetic resonance (NMR) spectrometers including 400- or 500-MHz instruments. Mass spectrometry and x-ray crystallography facilities were also modern. Most laboratories were equipped with fairly modern spectroscopic and chromatographic equipment, usually purchased from whichever U.S. company has the best service record



---

in Taiwan. Unfortunately, I did not have a good opportunity to discuss research projects during my visit there.

## ACADEMIA SINICA, TAIPEI

Academia Sinica occupies a small campus nestled against the hills at the north-eastern edge of Taipei. Most of the institutes there are quite new; the biomedical research facilities just opened recently. The Chemistry Institute is set up something like a national laboratory in the United States; that is, there is a permanent professional and technical staff but no students. This means that research groups are very small, two to four people, whereas groups in universities might have four to eight students, typically. Research groups operate more on an American model in Taiwan; that is, each Ph.D. researcher or professor is head of a group carrying out independent research. There is no "kosa" system as in Japan. At Academia Sinica, some of the professional staff also hold faculty positions at National Taiwan University. In that way, they may have graduate students in their laboratories once they have completed coursework. They also have a research internship program. After obtaining a B.S. degree, a student may have a 1- to 2-year research position in a laboratory at Academia Sinica. After that, they might move to a U.S. graduate program. (One student in my own research group at SUNY, Stony Brook did exactly that, for example.)

The research facilities in the Chemistry Institute of Academia Sinica are excellent. For example, they have a laser facility, a mass spectrometry facility with a 1- to 2-day turnaround time for high resolution or FAB-MS, an x-ray crystallography laboratory with a technician who performs the

analysis, and several NMR spectrometers including a 500-MHz instrument. Researchers there felt that they, too, needed more laboratory space and a new building, although the facilities did not seem nearly as cramped as in Japan. Again, their major problem is lack of graduate students to carry out research. This is due both to their lack of a graduate program and the number of students going abroad for study. Organic and inorganic chemistry are strong areas of research; they also have four groups involved in food research. Physical chemistry did not seem to be a strong area, although I met one theoretical chemist involved in computer modeling and computational chemistry. Interestingly, they seem to have a higher percentage of women faculty members than in the United States (and, of course, Japan). This Chemistry Institute has four women as group leaders, for example, and overall I met many more professional women during a 5-day visit to Taiwan than I had met in 7 months in Japan.

## NATIONAL SCIENCE COUNCIL, TAIPEI

The National Science Council is a branch of the Ministry of Education that determines funding for research and development in basic and applied science. My host, Prof. Sha, served as the head of the Chemistry Division a year ago and moved into the position of Director of Natural Sciences last summer when the position was vacated. It was apparently unusual to have such a young scientist in that position (he is only 39 or 40). Overall, however, I found that the young and middle-aged professors were the most active in departmental affairs and administration in the universities and at Academia Sinica.

---

Funding levels for individual research grants, joint projects, instrumentation, and new buildings and facilities seem to be at an all-time high in Taiwan. For individual research grants, there is a 95 percent funding rate! Thus, virtually every professor has some level of research funding. Those who are very actively participating in high quality research receive larger sums than others. In this funding climate, one would think that there is little incentive to carry out high quality research. In addition, faculty members in Taiwan are hired as associate professors. There is no tenure decision but simply a review after 5 to 7 years to determine when (not if) the candidate should be promoted to full professor. Despite these conditions, my impression was that the chemistry faculty members at the institutions I visited were very much devoted to carrying out competitive research. It was obvious to me that their training in the United States as graduate or postdoctoral students combined with their diligent studies as young students in Taiwan made them highly motivated. Most professors in Taiwan are granted funding for about one overseas trip per year to attend a scientific meeting, although most do not take the opportunity to travel that often. Surprisingly, few Taiwanese chemists have

attained an international reputation leading to conference invitations to the United States. Probably this will change in the next few years, reflecting increased funding and consequently increased research activity. Taiwanese institutions have hosted virtually no international conferences. The reason given for this is that they do not allow Mainland Chinese, Russian, or Eastern European scholars to visit Taiwan. Some professors offered the opinion that this situation will change in the near future, however.

## CONCLUSIONS

Chemistry in Taiwan is definitely on an upswing. The top institutions now have facilities that rival good universities in the United States. Although graduate students will continue to seek training abroad, principally in the United States, during the next few years more of them will be returning to good positions at home. Both the government funding of science and the high educational standards of the students will contribute strongly to rapid progress in basic research. Barring unforeseen economic or political problems, we should look for an increase in research activity and international prominence of Taiwanese chemistry.

---

# MARINE BIOLOGY IN OKINAWA

---

Aharon Gibor

---

*This article describes the marine biological research being conducted at three Okinawan research facilities: the University of the Ryukyus and its Sesoko Marine Science Station, the Japan Marine Science and Technology Center Corals Research Station, and the Okinawa Prefectural Fisheries Experimental Station.*

---

## INTRODUCTION

There is an increased awareness of the role of hydrosphere-atmosphere interactions in influencing global conditions. The warm tropical oceans play an important part in these relationships; there is, therefore, a worldwide increased interest in the ecology of the tropical regions in general, i.e., rain forests, and also in tropical marine biology, especially coral reefs. Okinawa, being the Japanese tropical island, is naturally the site where this increased interest is taking place. The following is an account of my visit to Okinawa in the early spring of 1990. I visited the following institutions: the University of the Ryukyus and its Sesoko Marine Science Station, the Japan Marine Science and Technology Center (JAMSTEC) Corals Research Station, and the Okinawa Prefectural Fisheries Experimental Station.

## UNIVERSITY OF THE RYUKYUS

The campus of the university is located on spacious, open land. The buildings, new cement multistory structures, are of a rather standard type of architecture. My hosts at the university were Professors Tatsuo Higa and Kiyoshi Yamazato. Higa, a professor in the Department of Marine Science, College of Science, is an organic chemist. He received his Ph.D. from Ohio State University, where he worked on secondary metabolites of plants.

Higa is famous for his work on bioactive substances from various marine organisms. He is the author of a review article on this subject that was published in *Studies on Natural Products Chemistry*, Atta-Ur Rahman, editor. His present research is supported by Seapharm Inc., Harbor Branch, Florida, and Pharmamer Inc., a subsidiary of Zeltia Co. of Madrid, Spain. The dominating theme of Higa's laboratory is marine pharmacology, and like a number of other Japanese laboratories, he is engaged in an active search for new and novel drugs from marine organisms.

In Higa's laboratory, students were busy extracting and separating substances from corals and sponges. The laboratory was full of standard research instruments. Major pieces of equipment such as ultracentrifuges, sophisticated spectrophotometers, and electron microscopes are shared by several laboratories. In cooperation with outside laboratories they prepare bioassays of anticancer substances. Antifungal and antibacterial substances are tested by standard procedures. At present they are not attempting to cultivate desirable organisms but rather to identify them. There is also no specific interest in studying the metabolism of the secondary products they isolate. Okadaic acid that is extracted from sponges is one of the important natural products being tested as a possible antitumor agent.

---

Higa also explained the problems they encounter when they want to use radioactive isotopes in their studies. As elsewhere in Japan, the use of radioactive isotopes is restricted to a special facility in a separate building. Students must be trained and supervised by authorized personnel of the radioactive laboratory, and the experiments must be conducted in this special facility.

Yamazato is a biologist whose specialty is invertebrate zoology. He is considered to be a leading expert on the biology and ecology of coral reefs. He is a professor in the Biology Department and is the director of the Sesoko Marine Science Center.

## PREFECTURAL FISHERIES EXPERIMENTAL STATION

Higa accompanied me to the Okinawa Prefectural Sea Farming Center at Motobu. This turned out to be a most interesting facility. The primary concern here is to promote the growth of harvestable species of fish, invertebrates, and sea weeds. Research activities are determined by the immediate economic interests of the fishing industries. One of the unique organisms they are propagating is the giant clam *Tridacna*. This organism has promise since its flesh is valued as a food and the shell is also used. *Tridacna* is also interesting for basic biological studies because it harbors many endosymbiotic algae. Having reliable cultivation procedures should permit studies on the uptake of these symbionts by animals and their physiological contribution to the growing animals. It might be possible to affect the quality of the produced *Tridacna* by inoculating the young animals with desired symbiotic species. Other invertebrates such as the swimming crab *Portunus*, prawns, snails, and sea urchins are also being propagated. The young animals are planted in the sea in cooperation with the fisheries cooperatives.

There is also an attempt to replenish the fish populations; rabbit fish and flat fish are being propagated. An important novel contribution is the introduction into culture of an edible brown alga, *Cladosiphon okamuranus*, common name Mozuku. This is a species that is found only in Okinawa and southern Kyushu. In the past, wild stands were collected and they were highly valued. The propagation procedures that were developed were simple, and the fast-growing tropical plants yielded several harvests during the year. At present they are cultivating the native plants; no attempts have been made at genetic selection or improvements of the plants. At present more than 2,000 tons of cultured Mozuku are produced annually. Cultivation is done by the local fisheries cooperatives. Mr. Takeshi Tohma is the person responsible for the domestication of this plant. He expressed great interest in the vegetative propagation procedures that we developed and he hopes to arrange for a visit to the United States to learn these procedures.

An important aspect of their work is the cultivation of essential food organisms necessary for rearing the young larvae of the economically important animals. I saw several large, open, green ponds with what they call "marine *Chlorella*," but it is probably a mixture of marine phytoplankton. They also cultivate rotifers. The rotifers and algae are crucial for the cultivation of the larval forms of their invertebrates. They also use commercial bakers yeast and imported *Artemia* eggs in their attempts to culture various larval forms. Many of the procedures they are using were published in a book, in Japanese, titled *Aquaculture in Tropical Areas*, Midori Shobo Publications, Tokyo (1988). An English translation of this book is due to appear this year.

Another of their success stories is the establishment of productive shrimp farms.

We visited one of these that is being operated by a fisheries cooperative. The total surface area of this farm is 60,000 m<sup>2</sup>. The harvest is about 1 kg/m<sup>2</sup>/yr. There are now about 20 such farms on Okinawa. It takes about nine workers to maintain a growing farm; they employ additional workers to harvest and package the products. The shrimp are harvested by trapping the large animals; these are chilled and shipped alive packed in moist sawdust. The animals can remain alive under these conditions for up to 2 days.

The Prefectural Fisheries Experimental Station is also engaged in ecological data collection on the coral reefs and in creation of artificial fishing reefs. These studies are done in conjunction with the Aquamarine project of the Japan Marine Science and Technology Center (JAMSTEC).

## JAMSTEC'S AQUAMARINE PROJECT

The major objective of this project is to acquire the knowledge and technology to restore the growth of damaged coral reefs and to colonize new grounds, thus creating new reefs at desired locations. In the past

decade considerable damage has been done to the coral reefs by the star fish *Acanthaster planci*. The harmful effects of soil erosion, or red clay erosion, which is associated with the increased pace of urbanization along the coast, are also being noted.

This JAMSTEC project is centered in a small room filled with electronic monitoring equipment as well as diving gear and construction tools. This room overlooks a small coastal bay, which is the study area charted by JAMSTEC from the local fisheries cooperative.

They are attempting to transplant corals onto artificial surfaces. The chemical and physical characteristics of the substratum are some of the important variables that are being investigated. How to attach the original coral segment to the substratum is still under investigation. Steel wires and various adhesives are being compared. They are using a submerged structure for these studies. It is a pyramid made of iron bars that are coated by a thin layer of dilute cement. Small pieces of coral are tied to this frame with iron wire, and the growth and expansion of the coral are regularly assessed by inspection (see Figure 1).



Figure 1. Cultivation of corals on a submerged structure in Okinawa. Courtesy of Japan Marine Science and Technology Center.

---

A postdoctoral investigator from Belgium, Dr. Michel Claereboudt, is at present living on Okinawa and is studying the properties of the substratum that favor the attachment of coral. The rest of the activities here consist of measuring temperature, nutrients, and water flow. Automatic recording of these data is done by appropriate probes and sensors attached at various locations on the reefs. Data are transmitted to receivers in the laboratory.

JAMSTEC has an ambitious plan for investigating all aspects of coral reef growth. Their objectives include the construction of artificial reefs to protect coastal installations and contribute to the attractiveness of the coastline, thus promoting the tourist industry.

In my opinion, most of the work is descriptive. There are no laboratory facilities, and no controlled experiments are being conducted. The ecological data and field observations are valuable contributions to the understanding of the biology of the coral reefs, but I doubt whether generalizations on procedures for controlled cultivation of corals will result from such studies.

## SESOKO MARINE SCIENCE CENTER

Basic biological studies on the different organisms of the coral reef are being conducted at the Sesoko Marine Science Center of the University of the Ryukyus. This facility is located about 80 km north of the main university campus. The facilities include a main building with classrooms and research laboratories. The laboratories are supplied with running seawater and freshwater; constant temperature and light-controlled chambers are available. Physiological and biochemical devices are available for basic studies. Supplies and equipment for scuba diving are available. The

center owns three boats of different sizes and equipment to launch them. Several laboratory classes are regularly held at the center, mainly during the summer. Marine Biology, Marine Ecology Laboratory, Algology Laboratory, Invertebrate Zoology, and Developmental Biology are offered by the Biology Department. General Oceanography Laboratory and Marine Research Techniques are offered by the Marine Science Department. In addition, a special class in marine biology is conducted for biology students from the national universities. This class is designed to introduce these students to coral reef biology.

The research activities conducted by the staff and students are concerned with the coral reef communities as well as mangrove communities. The Marine Science Center publishes their research results in a periodical titled *Galaxea*. Several recent *Galaxea* publications from Prof. Yamazato's laboratory include the following:

"Studies on the Detachment of the Discs of the Mushroom Coral *Fungia* Fungites with Special Reference to Hard Structural Changes," 6, 163-175 (1987)

"General Description of Developmental Stages in a Soft Coral *Lobophytum Crassum* Marenzeller," 6, 185-193 (1987)

"Nematocysts Characteristic of the Sweeper Tentacle of the Coral *Galaxea Fascicularis* (Linnaeus)," 6, 195-207 (1987)

"Sexual Reproduction of Corals in Okinawa," 6, 331-343 (1987)

These papers describe basic physiological and morphological phases in the life of these organisms. Most important are the observations on the release of gametes, fertilization, and early phases in the development of the

---

animals. These papers are, of course, in-house publications, without peer review.

Two older *Galaxea* publications from Yamazato's laboratory are of interest. In 1984 they published "The Distribution of Carbonic Anhydrase in a Staghorn Coral, *Acropora Hebes* (Dana)" [3, 25-36 (1984)]. This subject is taking now new significance in consideration of marine organisms as sinks for the deposition of carbon from the atmosphere. Coral reef probably plays a significant role in this carbonate deposition.

Another paper, titled "Effect of Light on Budding of Isolated Polyps of Scleractinian Coral *Galaxea Fascicularis*" [1, 65-75 (1982)], is interesting since it suggests the role of the endosymbiotic zooxanthellae in affecting the morphological developments of the animal.

Vol. 8, No. 1 of *Galaxea* (1989) is a publication of the proceedings of the Asian and Pacific regional workshop and international symposium on the conservation and management of coral reef and mangrove ecosystems. The meeting was held in Okinawa between 25 September and 3 October 1987. The meeting was sponsored by UNESCO and the Japanese Ministry of Education. An example is the interesting article by S. Kamura (p. 217), in which the effect of grazing by sea urchins on the algal biomass and composition was studied by excluding the animals from a caged area. The exclusion of the urchins led, in several weeks, to a noticeable increase in the total algal biomass and a large increase in the number of algal species growing on the reef.

A good indicator of the increased importance and interest in marine biology is the appointment of two new staff members to the Marine Science Institute. On 1 April

1990 Prof. K. Takano joined the staff. His field of study is reproductive physiology of fish. Dr. A. Takemura was appointed to be an instructor; his area of study is also reproductive physiology of fish.

Another indicator is the list of foreign visitors. This year the list includes:

- R.T. Tsuda, Univ. of Guam
- P.W. Glynn, Univ. of Miami
- M.J. Grygier, Smithsonian Inst. of Tropical Science
- Titlyanov, Marine Biology Acad. Science, Vladivostok

## SUMMARY

Okinawa, being the tropical island of Japan, is the center of studies on tropical marine biology. An intensive search for new biologically active substances is going on. Mariculture studies include the cultivation of tropical species of plants and many tropical species of animals including the giant clam *Tridacna*. Active studies are being conducted on the biology of the coral community including attempts at transplantation and propagation of reefs.

Because of the increased interest in global environmental problems, especially the relationship between the atmosphere and the ocean surface, I foresee a resurgence and increased interest in coral reef biology. The basic studies being conducted at the University of the Ryukyus will undoubtedly be of importance to future studies in this area of science.

---

# THE STABILIZATION STEP IN THE FABRICATION OF PITCH-BASED CARBON FIBER

---

Sin-Shong Lin

---

*Stabilization is the most time consuming step in the production of pitch-based carbon fiber. Stabilization consists of oxidization of the melt-spun fiber to ensure dimensional and structural stability during carbonization required to produce the as-spun mesophase to finished carbon fiber. The chemical and structural changes associated with stabilization are reviewed and the parameters affecting this process are examined. Finally, the prospect for better or lower cost carbon fiber through improved stabilization processing is considered.*

---

## INTRODUCTION

In the fabrication of pitch-based carbon fiber (Ref 1 and 2), the stabilization process, occasionally called the infusibilization or thermosetting step, is essential to ensure that the as-spun fibers do not change in shape or structural configuration during subsequent carbonization. Our focus here is on the pitch-based fiber that is melt spun (Ref 1) from mesophase pitch (Ref 3), which is then treated by stabilization and carbonization processes to produce fibers with favorable properties of strength and modulus. The spinning process consists of pressing mesophase pitch through the capillaries of a spinneret pack to form continuous filaments that are quenched by air cooling. The spinning variables, such as winding speed, extrusion temperature, melt viscosity, flow pattern, and cooling rate, influence the fiber properties (Ref 4). The solidified filaments then pass through the stabilization step where

the fiber is mildly oxidized to become infusible for the subsequent heat treatments that are required to produce the finished carbon fiber. A schematic diagram for the fabrication of carbon fiber from mesophase pitch is shown in Figure 1.

The stabilization step can have a significant impact on the microstructure as well as the mechanical strength of the finished fiber (Ref 5 and 6). The oxygen absorbed by the fiber forms cross-linked aromatic structures that preserve the axial preferred orientation of the fiber during carbonization and reduce the solubility of the fiber constituents. In subsequent heating, these oxidized molecules react to produce larger aromatic networks by condensation, further cross-linking, and the evolution of oxygen bearing gases (Ref 7). The aggregation of the aromatic networks while their layer orientation is maintained parallel to the fiber axis produces a fiber that can be carbonized to very high modulus.



## Mesophase Pitch

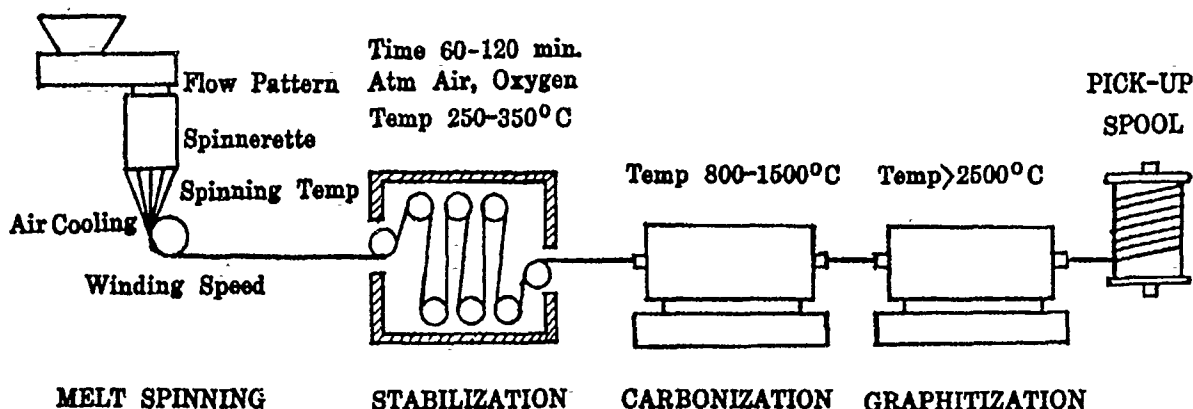


Figure 1. The fabrication of pitch-based carbon fiber. Fiber from melt spinning passes through the stabilization step followed by high temperature heat treatment for carbonization and graphitization. Stabilization is the most time consuming step in fabrication.

The orientation of crystallites in the finished fiber is initially introduced by the alignment of mesophase during melt spinning. The extent of the orientation and alignment of mesophase molecules is not significantly affected by the mild oxidation during stabilization. However, the orientation of carbon crystallites formed after carbonization is strongly dependent on abundances and distribution of the oxygen uptake during stabilization.

The chemical and structural mechanisms involved in oxidation during the stabilization are very complex. The fiber morphology is largely dependent on the extent of oxygen uptake (Ref 5), the nature of the mesophase precursor (Ref 3), and the spinning conditions (Ref 4 and 6). The distribution of oxygen in depth along the fiber radius diameter is also important (Ref 8) to the final physical characteristics of the carbonized fiber. Although some theoretical approaches (Ref 9 and 10) to predict oxygen distributions have been undertaken, a complete description of fiber behavior as a function of processing parameters is still not available

owing to the many parameters that affect and interact to determine the microstructure of the fiber.

In recent years, there have been considerable advances in carbon fiber technology around the world, but active research and development stimulated and motivated by necessity is found in the Japanese carbon community. This article summarizes the progress and findings of recent research on carbon fiber processing techniques.

## STABILIZATION CONDITIONS

The oxidative stabilization of as-spun fiber is usually performed at a temperature a few tens of degrees below the softening point of the mesophase (Ref 5). Since there is a wide variety of mesophase pitches with different softening points, the stabilization temperature varies accordingly. The conventional temperature range is 250 to 350°C (Ref 11).

The temperature may be programmed to increase stepwise with time or may be held constant. The oxidation atmosphere

may be ambient air, ozone, oxygen, or pressurized oxygen (Ref 12), with or without additives intended to enhance oxidation. In a proprietary process (Ref 13), the powder of solid lubricants is used to coat the fiber to substitute gaseous oxidation. Experimentally,  $\text{NH}_3$  gas is known to accelerate stabilization, but oxygen must be present (Ref 14).

The reaction time required to achieve stabilization varies widely depending on precursor, temperature, fiber geometry, and oxidative medium. Reaction times ranging from 60 to 120 minutes are used in industrial production. In some experiments, exposure times up to a few days have been explored to obtain gradual and homogeneous oxidation. Large-diameter fibers are difficult to stabilize due to slow oxygen diffusion. A fiber diameter of more than  $10\text{ }\mu\text{m}$  is rarely produced in a production scale. The shortest possible times are sought in manufacturing. Thus, in the production of low cost fiber, an optimum oxidation level is not necessarily sought. Adding sulfur to isotropic pitch to shorten the stabilization time during the production of low strength fibers has been reported (Ref 15).

## CHEMICAL REACTIONS

Two types of chemical reactions take place simultaneously during stabilization. One is oxygen uptake into the mesophase constituents, and the other is the evolution of volatile organic vapors and oxygen bearing gases. The weight gain is rapid (Ref 16) in the early stages of oxidation but decreases with prolonged exposure (Figure 2). The oxygen concentration desired to ensure stabilization is usually around 6 to 7 at. % (Ref 5,6,11). However, for pitches containing a large fraction of heterocyclic rings, oxygen concentrations greater than 10 percent can easily be attained. The oxygen uptake reactions (Ref 7) occur first on aliphatic side

chain branches to produce carbonyl, hydroxyl, carboxyl, and quinone groups by oxygen insertion and dehydrogenation. Oxidation increases the softening point of mesophase pitch and reduces the solubility of the mesophase in solvents such as pyridine and quinoline. Some further aromatization and cross-linking may also take place. The formation of ether/ester groups between large aromatic molecules and cross-linking leading to larger mesophase molecules by oxygen insertion and dehydrogenation could occur in the second stage of stabilization. Various oxygen containing functional groups that promote the subsequent carbonization reaction are formed in the latter stages of oxidation. Gaseous species, such as  $\text{H}_2$ ,  $\text{CO}$ ,  $\text{CO}_2$ ,  $\text{H}_2\text{O}$ , and  $\text{CH}_4$  (Ref 17), have been observed during oxidation.

The mechanisms involved in the oxidation of as-spun fibers have been studied extensively by infrared absorption (IR) (Ref 7), x-ray photoelectron spectroscopy (XPS) (Ref 18), nuclear magnetic resonance (NMR) (Ref 19), and differential scanning calorimetry (DSC) (Ref 20). The major oxidation products are carbonyl, carboxyl, hydroxyl functional groups on aliphatic or methyl side chains of large aromatic rings, aryl-ether/ester, and quinone. IR spectra of pitch obtained after the hydrogenation process (Ref 7 and 21) clearly indicate the transformations that had taken place during stabilization (Figure 3). The aliphatic C-H stretching ( $2,970$  to  $2,700\text{ cm}^{-1}$  wave number) and methylene and naphthalene stretchings ( $1,450\text{ cm}^{-1}$ ) decrease with increasing stabilization times, while the stretchings of aromatic C-H ( $3,050\text{ cm}^{-1}$ ), carbonyl C=O ( $1,690\text{ cm}^{-1}$ ), aromatic C=C ( $1,620\text{ cm}^{-1}$ ), methyl- $\text{CH}_3$  ( $1,375\text{ cm}^{-1}$ ), and phenoxyl-C=O ( $1,284\text{ cm}^{-1}$ ) are all found to increase. The formation of these oxygen addition compounds leads to the increased softening point of the mesophase. Consequently, the fiber

maintains configurational stability during the carbonization process, which follows immediately after the stabilization step. The time required for the oxidation during the step varies depending on pitch precursors. Since stabilization is the most time consuming step in the entire fabrication procedure, many attempts have been made to reduce the oxidation time and thus to increase fiber production.

During stabilization, the solubility characteristics (Ref 21 and 22) of the fiber change: the proportions of quinoline insoluble (QI) and pyridine insoluble (PI) constituents increase while those of benzene soluble (BS) constituents decrease (Figure 4). This implies that the size of the mesophase molecules increases with increasing oxygen uptake.

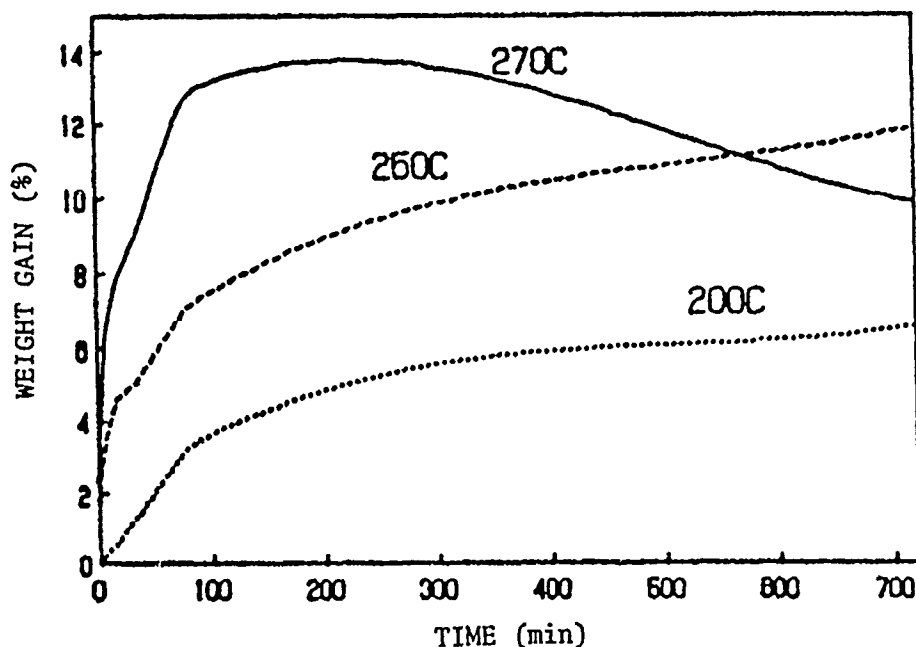


Figure 2. Weight changes during the stabilization step. The weight of as-spun fibers generally increases rapidly during the initial period of oxidation and then gradually decreases until a steady state of weight change is reached. The weight changes are caused by oxygen uptake and the evolution of gaseous species. The behavior is strongly dependent on temperature and oxidizing atmosphere of the stabilization condition. Courtesy of Ref 16.

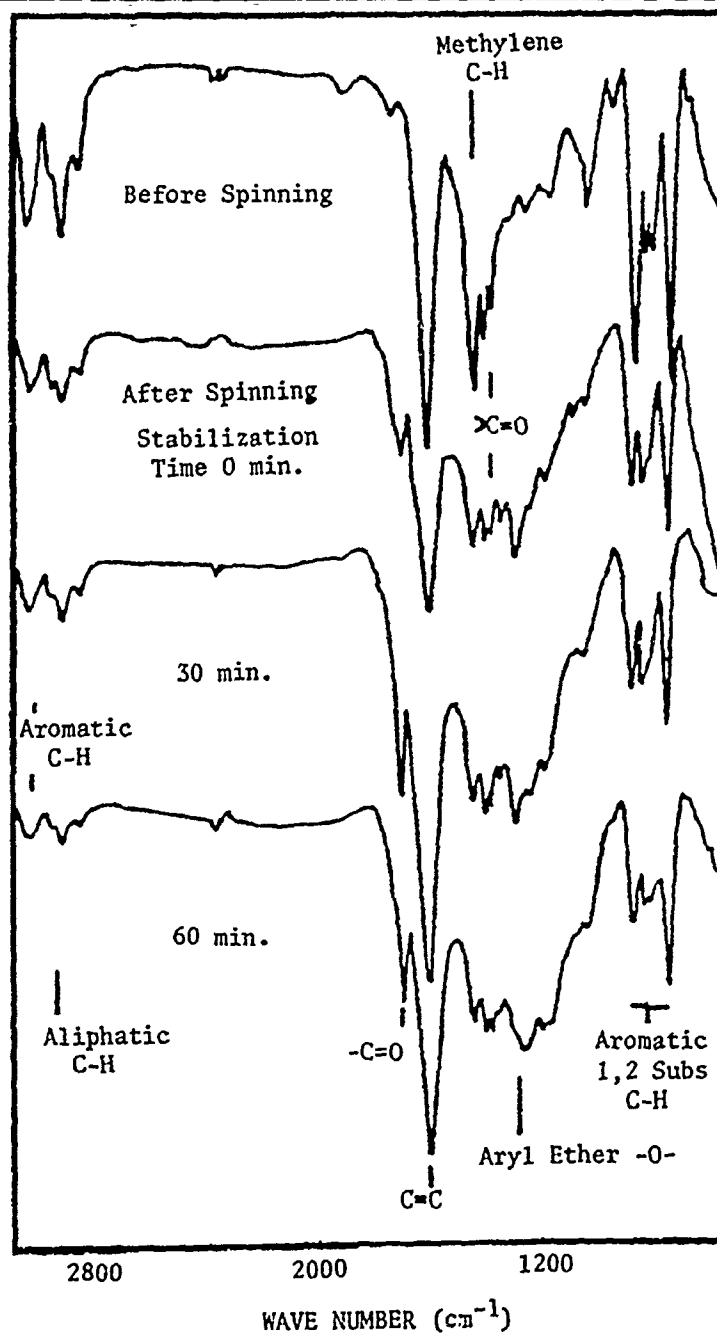


Figure 3. Infrared (IR) absorption spectra of the stabilization step. IR spectra indicate the chemical transformations that occur during stabilization as a function of increasing reaction times. The C-H stretchings of aliphatic components decrease while those of aromatic components increase. The stretchings of C=C, >C=O, and -O- also increase. The formations of larger aromatic ring compounds with C-O functional groups and aryl-ether/esters are the major mechanisms involved in stabilization. Courtesy of Ref 7.

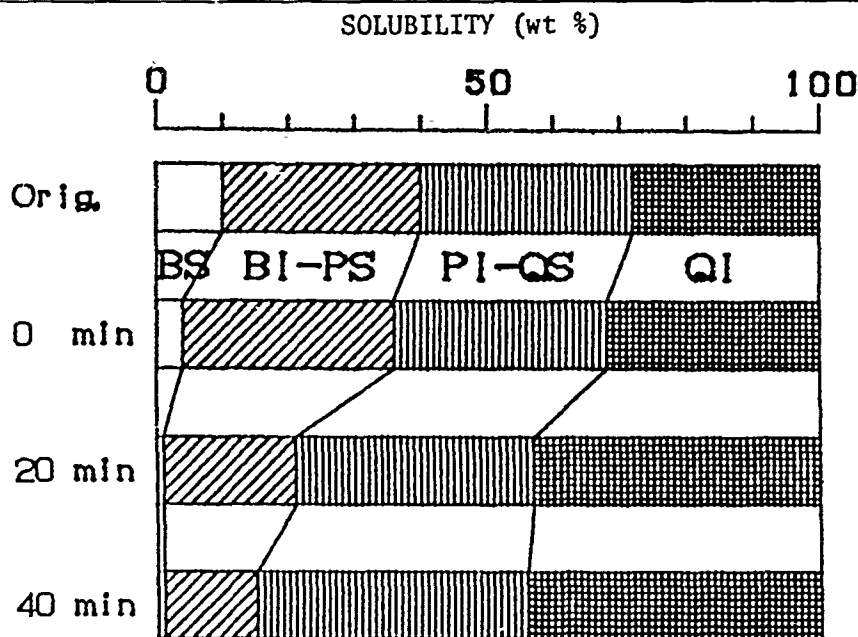


Figure 4. Solubility fractions of pitch and stabilization time. The solubility fractions of coal tar based pitch fiber change gradually with oxidation time. The quinoline insoluble (QI) and pyridine insoluble (PI) fractions increase while the benzene soluble (BS) fraction decreases, indicating the formation of large aromatic molecules. The softening point of pitch also increases. Courtesy of Ref 22.

Oxidation occurs by the diffusion of oxygen from the fiber surfaces to interiors. Presumably, complete and homogeneous stabilizations cannot be accomplished within the short time period permitted by economic considerations. In cases where only the surface is adequately oxidized, the filament after carbonization displays a cross section consisting of a skin/sheath that encircles a central region that appears to have softened during carbonization (Ref 23 and 24) (Figure 5). This tends to weaken the fiber due to loss of alignment in the central region. However, in at least one proprietary process, high modulus fiber was obtained by maintaining the original orientation of mesophases at the core (Ref 25). The process includes the formation of infusible filament skins by rapid oxidation followed by gradual carbonization to preserve the

orientation at the central region. A very high modulus fiber was obtained at a temperature 500° lower than that used in conventional graphitization at 3,000 °C. There are more QI and PI components near the fiber surface, forming the so-called skin-core or sheath-core configuration (Ref 23). The skin width increases with longer stabilization times. The thickness of the skin/sheath is found to vary with the square root of the reaction time (Ref 24), indicating that the diffusion is the controlling process. The core structure consists of lamella well oriented both longitudinally as well as across the fiber diameter. If the core softens during carbonization, some movements can occur (Ref 24), which result in the formation of elongated voids and pores. Thus, the oxygen concentration profile across the fiber diameter should exceed the minimum

required amount of oxygen and is found to have a beneficial effect (Ref 8) on the final strength of the fiber.

Since the oxidation rate varies with the constituents of mesophase pitches, different reaction kinetics and diffusion times are required for various pitch precursors. Pitches derived from coal tar contain more highly aromatic molecules and QI/PI components than pitches derived from petroleum (Ref 26). Thus, the reaction rates are slower for coal tar precursors. In order to compensate for the longer reaction times required for stabilization, polymeric compounds, such as polyvinyl chloride (PVC) pitch (Ref 27 to 29), hydrogen donor solvent

(thio-anthracene) (Ref 30), and thermoresistive polymers (polyethylene naphthalate, polyethylene terephthalate-hydroxyl benzoate) (Ref 31), can be added to accelerate stabilization. Up to 10 percent PVC pitch has been added and tested (Ref 5). The high reactivities of naphthalene and aliphatic components in the PVC pitch could promote and accelerate condensation reactions of the mesophase constituents. Indeed, the spinnability and the productivity of fiber can be enhanced substantially at lower viscosity. Moreover, a shorter reaction time and lower spinning temperature are desirable for large scale production.

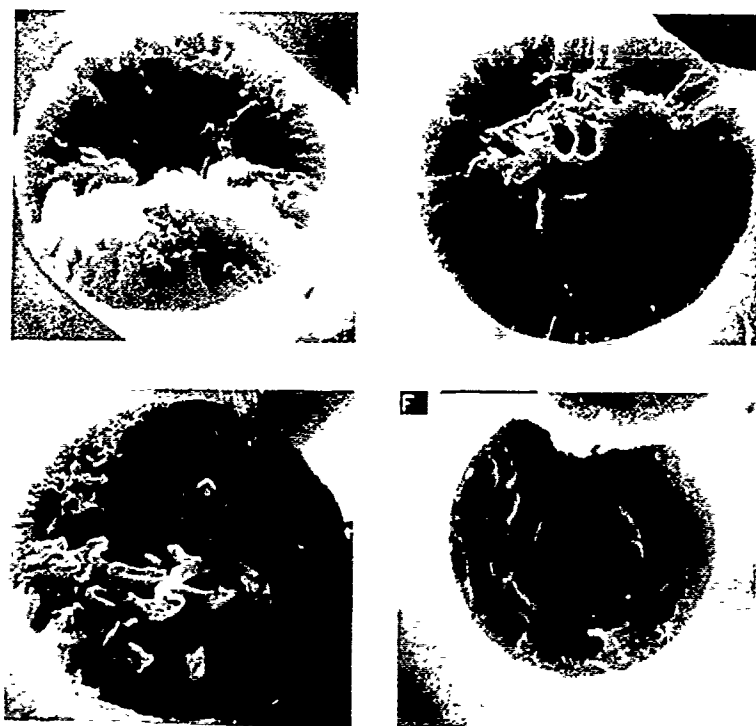


Figure 5. Skin-core configurations in pitch-based carbon fibers. Four fractured fiber cross sections reveal various skin-core configurations. The width is determined by the amount of oxygen absorbed during stabilization. The core regions exhibit various structures of remelted mesophase. The fibers, manufactured by Osaka Gas Co., Japan, are designated as F180 and F500 and are derived from coal tar sources. The photo-micrographs were taken at the author's laboratory, MTL.

During carbonization under inert atmosphere, the oxygen acquired during stabilization reacts to produce gaseous species (Ref 32 and 33), such as  $H_2O$ ,  $CO_2$ , and  $CO$ , while to a lesser extent  $H_2$  and  $CH_4$  also evolve. These reactions promote aromatization and cross-linking of mesophase molecules, leading to the formation of small turbostratic carbon or graphitic crystallites. The cross-linkings between the large aromatic layers presumably depend on the locations of oxygen atoms in the mesophase molecules; such cross-linking may determine the ultimate strength characteristics. Due to a wide variety of chemical structures and constituents in the mesophase, the reactions leading to the formation of interconnecting crystallites, which are essential to fiber strength, are still not clear.

## OXYGEN CONCENTRATION

The oxygen taken up during stabilization preserves the fiber orientation, the crystallite axial alignment, and the fiber morphology. The oxygen concentration profile across the fiber, as well as the positions of oxygen atoms in the large mesophase molecules, strongly affect the type of microstructure. Various fiber morphologies, such as skin-core, onion skin, radial, random mosaic, and cracked radial, can be produced by various oxygen concentration distributions in the fiber before carbonization.

The amount of oxygen absorbed during the stabilization step is a dominant factor in preserving the preferred orientation of carbon layers. In the case of homogeneous oxygen uptake across the filament diameter, the preferred orientation, which tends to vary with the tensile strength of the carbonized fiber, increases linearly with increasing amounts of oxygen until a concentration of 7 to 8 at. % is reached. Beyond

this oxygen content, the degree of orientation gradually decreases. The highest orientation, corresponding to the optimum oxygen concentration, is located on a broad maximum that varies with the pitch precursor. Thus, the oxygen uptake is set somewhere near this maximum in the production. The oxygen can be introduced by changing the reaction temperature and the oxidation time during stabilization. Moreover, the reaction at lower temperatures is found to be more effective than that at higher temperatures owing to the surface diffusion barrier produced by a rapid initial high temperature oxidation (Ref 34).

The skin-core type configurations are produced by a steep oxygen gradient (Ref 35) across the fiber diameter, while mosaic, radial, and onion skin cross sections (Figure 6) are obtained from more uniform distributions of oxygen. The differences among the latter three cross sections are derivable from the nature of the mesophase pitch, the spinning condition (Ref 6,36,37) including pitch viscosity, temperature, flow pattern, and the oxygen uptake at the stabilization step. Since oxygen has an indispensable role in the formation of fiber structures, the pattern of the oxygen distribution might be correlated with these three cross sections.

Although a low oxygen content at the core, resulting from insufficient oxidation time, tends to produce fiber of inferior quality, an oxygen density gradient at the core sufficient for the stabilization could lead to an interesting fiber property. The flexibility of the fiber, measured in the knot/loop strengths, is found to improve substantially. This phenomenon is probably caused by the fact that lower oxygen at the core produces many pores and voids without degrading the orientation of carbon crystallites in the skin. Since the fiber strength depends primarily on the circumferential carbon, where the highest orientation exists, these elongated

voids and pores resulting from lower oxygen content at the core provide more sliding spaces. Thus, fiber structures with a greater flexibility or plasticity could be produced. The fibers are excellent for use in weaving three-dimensional tight knit fabrics.

## OXYGEN DIFFUSION MODELING

In stabilization, oxygen uptake occurs from surfaces to interiors. The amount of oxygen uptake is found to be roughly proportional to the square root of the reaction time, indicating that diffusion is a major

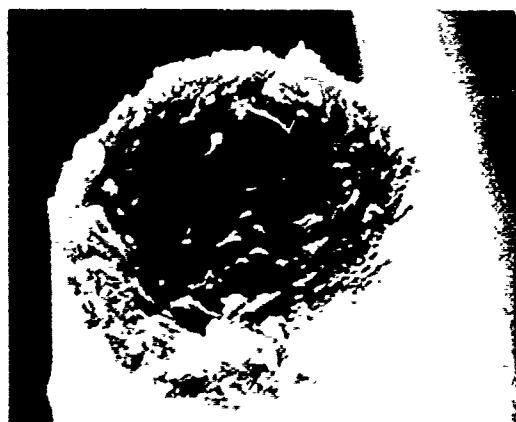
controlling mechanism (Ref 35). Mathematical modeling of oxygen diffusion in the stabilization process has been made (Ref 9,10,38). The diffusion parameters of molecular oxygen have been calculated from the observed experimental data. The fiber is assumed to consist of two components (Ref 10): aliphatic and aromatic mesophases having different reactivities and diffusion constants. Another approach (Ref 9) uses aliphatic side branches as the only active components that can be oxidized. Both modelings claim to have good agreement with their experimental observations.



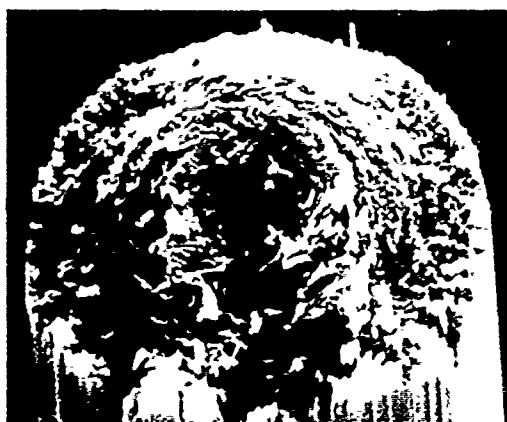
(a)



(b)



(c)



(d)

Figure 6. SEM micrographs of pitch based carbon fiber cross sections. Four types of cross sections are shown: (a) radial, (b) onion skin, (c) random, and (d) quasi onion skin. These structures are produced mainly from the mechanical stirring above the spinneret during the melt spinning process. Courtesy of Ref 6.



Perhaps due to proprietary information, oxygen profiles of commercial fibers after stabilization are rarely seen in the open literature. A similar oxygen profile obtained from a mesophase bead (Ref 35) is illustrated in Figure 7. The oxygen concentration determined by energy dispersive analyses by x-ray (EDAX) shows a gradual decrease from the surface toward the fiber center. However, the computed profile (Ref 9), in accordance with the experiment, shows a rather steep decline over a narrow width across the fiber cross section.

## FUTURE PROSPECTS

Stabilization is only one step in the fabrication of pitch-based carbon fiber. The

process parameters are essential but are the only ones affecting the final mechanical strength of the fiber. Moreover, stabilization is the most time consuming step in the entire fabrication process. With the objective of reducing stabilization time without degrading the fiber properties, various methods, such as admixtures of aliphatic branch pitches, improvements of mesophase precursors, and various oxidizing atmospheres and reaction temperatures, have been devised to shorten the required exposure time. By carefully selecting the processing parameters, the time period required for stabilization could be reduced in the near future.

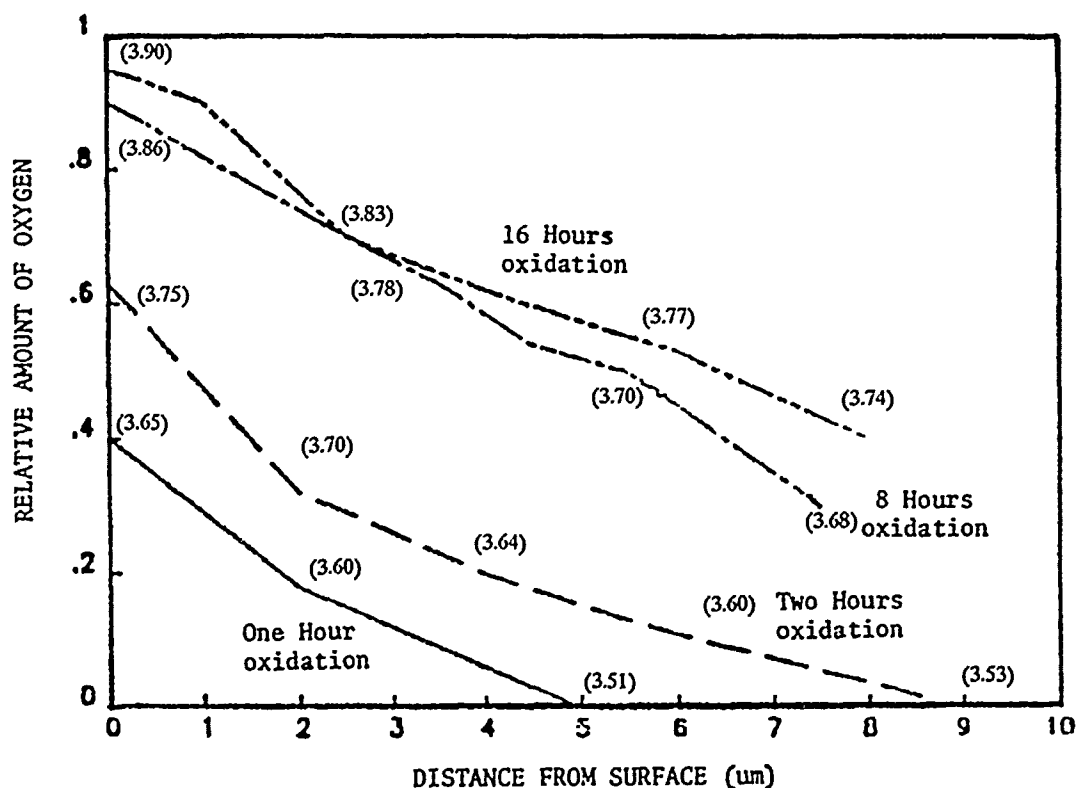


Figure 7 Oxygen profile across a mesophase particle. The semi-quantitative analysis of oxygen concentration is obtained by the EDAX technique. The relative abundances of oxygen are shown with varying oxidation times. Intermolecular distance  $d_{002}$  (Å) is shown in parentheses. Courtesy of Ref 35.

Progress has been made on the oxidative mechanisms of mesophases in carbon fibers. However, details on selective oxidation, aliphatic side chains, diffusing molecular species, diffusion barriers, and radial formation are not well established. The mechanisms involved in cross-linking mesophase molecules, leading to large carbon crystallites, are not well known. The strength of the carbon fiber in relation to locations and abundances of oxygen uptake during stabilization still remains as mystery.

Some improvements of the fiber properties tailored to specific applications are foreseeable by varying the degree of oxygen uptake during stabilization. Since higher preferred orientation occurs near the fiber circumference and assuming constant surface defects per area, higher tensile strength fiber should be obtainable by reducing the fiber diameter from today's 10  $\mu\text{m}$  to 5 to 6  $\mu\text{m}$ . By proper choice of mesophase composition and optimum processing conditions, the surface flaws that adversely affect fiber strength should be minimized. Tensile strengths of 7 GPa, roughly twice the current strength, might be obtainable within a few years. An oxygen distribution tapering at the fiber center could produce high performance fibers with high knot/loop and compressive strengths. At present, high modulus fibers up to 700 GPa, characterized by large crystallites and very high preferred orientation, are available commercially. These high modulus fibers are obtained through stabilization, which ensures homogeneous oxygen concentration over the fiber cross section, followed by heat treatment to graphitization temperatures (above 2,500 °C).

Further developments in fiber processing, especially in the stabilization step, could reduce the cost of medium grade fibers,

which in turn would expand new application fields in the immediate future. Research will continue to improve mesophase precursors and modify processing and manufacturing methods. However, low cost processing is the key factor in assuring a prosperous future for pitch-based carbon fiber.

## ACKNOWLEDGMENT

The author appreciates very much the comments and suggestions made by Dr. J.L. White, University of California at San Diego, and his help in rewriting this manuscript.

## REFERENCES

1. E. Fitzer, editor, *Carbon Fibers and Their Composites* (Springer-Verlag, 1985).
2. S.-S. Lin, "Current status of the carbon fiber industry in Japan," *Scientific Information Bulletin* 14(2), 97 (1989).
3. J.L. White, *Pure & Appl. Chem.* 55, 765 (1983).
4. D.D. Edie and M.G. Dunham, "Melt spinning pitch based carbon fiber," *Carbon* 27, 647 (1989).
5. S. Otani, S. Watanabe, H. Ogino, K. Iuma, and T. Koitabashi, *Bull. Chem. Soc. Japan* 45, 3710 (1972).
6. T. Tomioka, "High strength pitch based carbon fibers," *Iron and Steel, Japan* 75(9), 1418 (1989).
7. I. Mochida, A. Azuma, K. Korai, and K. Kitatori, "Stabilization mechanism of petroleum based mesophase pitches," 15th Annual Meeting of the Japan Carbon Society, extended abstract 1A16, 34 (1988).
8. M. Yoshida, Idemitsu Co., private communication (1989).
9. C. Kawada, T. Komemoto, and S. Tadaki, "Model and simulation of stabilization," 16th Annual Meeting of the Japan Carbon Society, extended abstract 3A16, 196 (1989).

10. H. Arai, A. Iwashita, and T. Tomioka, "Examination of infusible reaction model by DSC," 16th Annual Meeting of the Japan Carbon Society, extended abstract 3A05, 174 (1989).
11. Otani et al., *Carbon* 4, 425 (1966).
12. U.S. Patent 4,657,753 to E.I. DuPont Co., "Stabilization of pitch fiber" (1988).
13. U.S. Patent 4,781,908 to Kawasaki Steel Co., "Process for the infusibilizing treatment of pitch fiber" (1988).
14. G.S. Bhat, F.L. Cook, L.H. Peebles, and A.S. Abhiraman, "New aspect in the stabilization of PAN based precursors for carbon fibers," 19th Biennial Conference on Carbon, extended abstract, 252 (1989).
15. E. Fitzer and G. Liu, "The effect of sulfur addition to coal tar and petroleum pitch as precursor for isotropic carbon fiber," 19th Biennial Conference on Carbon, extended abstract, 254 (1989).
16. A.C. Ma, S.H. Chen, and R.J. Diefendorf, "Oxidative stabilization of pitch carbon fibers," 128, 19th Biennial Conference on Carbon, extended abstract (1989).
17. T. Suzuki, "Air oxidation of coal tar based pitch," 16th Annual Meeting of the Japan Carbon Society, extended abstract 1A08, 18 (1989).
18. T. Takahagi and A. Ishitani, "XPS study on the surface structure of carbon fibers using chemical modification and Cls line shape analysis," *Carbon* 26, 389 (1988).
19. N. Nakamizo and Y. Adachi, "Solid state  $^{13}\text{C}$  NMR spectra of low temperature carbons," 19th Biennial Conference on Carbon, extended abstract, 148 (1989).
20. H. Arai, A. Iwashita, and T. Tomioka, "Examination of stabilization reaction model by DSC," 16th Annual Meeting of the Japan Carbon Society, extended abstract 3A05, 174 (1989).
21. I. Mochida, K. Shimizu, Y. Korai, H. Otsuka, and S. Fujiyama, "Structure and carbonization properties of pitches produced catalytically from aromatic hydrocarbons with  $\text{HF/BF}_3$ ," *Carbon* 26, 843 (1988).
22. Y. Korai, I. Mochida, and T. Matsumoto, "Stabilization process of pitch based carbon fiber," 18th Biennial Conference on Carbon, extended abstract, 411 (1987).
23. I. Mochida, S. Teng, Y. Korai, and H. Toshima, "Skin-core structure of pitch based carbon fiber derived from petroleum pitch," 16th Annual Meeting of the Japan Carbon Society, extended abstract 3A04, 172 (1989).
24. M.A. Wright, P.G. Waper, N. Murdie, P. Tlomak, and C.P. Ju, "Microstructure analysis of pitch based carbon fiber," 19th Biennial Conference on Carbon, extended abstract, 294 (1989).
25. Japan Patent 63-120112 and U.S. Patent 4,822,587, "High modulus pitch fiber," Tonen Oil Co., Japan (1989).
26. I. Mochida, Y. Korai, T. Varga, and H. Toshima, "Stabilization reactivity and chemical structure of various mesophase pitch fibers," 14th Annual Meeting of the Japan Carbon Society, extended abstract 2A01, 70 (1987).
27. I. Mochida, H. Toshima, and Y. Korai, "Acceleration of petroleum pitch in stabilization step by addition of PVC pitch," 14th Annual Meeting of the Japan Carbon Society, extended abstract 2A03, 74 (1987).
28. I. Mochida, Y. Korai, S. Nakamura, S. Inoh, and B. Rhee, "Modification of isotropic carbon fiber precursor with PVC tetraline as a solvent," 19th Biennial Conference on Carbon, extended abstract, 136 (1989).
29. I. Mochida, H. Toshima, and Y. Korai, "Changes in carbon fiber cross-sections by addition of PVC pitch," 14th Annual Meeting of the Japan Carbon Society, extended abstract 2A04, 76 (1987).

- 
30. I. Mochida, Y. Korai, A. Amazu, and A. Kitatori, "Promotion of stabilization of pitch based carbon fiber by addition of hydrogen donor solvents," 16th Annual Meeting of the Japan Carbon Society, extended abstract 3A06, 176 (1989).
  31. I. Mochida, H. Toshima, and Y. Korai, "Solubility of heat resistance polymers in mesophase pitches at their spinning temperatures," 19th Biennial Conference on Carbon, extended abstract, 208 (1989).
  32. T. Suzuki and M. Hamaguchi, "The initial stage of carbonization in the air oxidation of coal tar based pitch," 15th Annual Meeting of the Japan Carbon Society, extended abstract 3A01, 160 (1988).
  33. T. Suzuki and M. Hamaguchi, "Initial carbonization process of oxidized coal tar pitch," 19th Biennial Conference on Carbon, extended abstract, 166 (1989).
  34. Y. Yamada, K. Imamura, and Y. Honda, "Effects of carbonization and stabilization parameters on properties of pitch based carbon fibers," 14th Annual Meeting of the Japan Carbon Society, extended abstract 2A05, 78 (1987).
  35. W. Kowbel and J. Don, "Structure and oxidation studies of mesophase pitch," 18th Biennial Conference on Carbon, extended abstract, 409 (1987).
  36. T. Hamada, T. Nishida, M. Furuyama, and T. Tomioka, "Transverse structure of pitch fiber from coal tar mesophase pitch," *Carbon* 26, 837 (1988).
  37. T. Hamada, M. Furuyama, Y. Saziku, and T. Tomioka, "Orientation pattern of pitch based fiber," 15th Annual Meeting of the Japan Carbon Society, extended abstract 2A16, 106 (1988).
  38. H. Fukushima, T. Komemoto, and S. Tadaki, "Stabilization reaction of mesophase pitch fiber," 14th Annual Meeting of the Japan Carbon Society, extended abstract 2A02, 72 (1987).

---

Sin-Shong Lin, who received a Ph.D. from the University of Kansas in 1966, has been employed by the Army Materials Technology Laboratory at Watertown, MA, since 1967. Dr. Lin's research interests include chemical thermodynamics, phase diagram, high temperature syntheses, mass spectrometry-atmospheric sampling, and surface analytical techniques (x-ray photon and Auger electron spectroscopies) for material characterizations (of interest are titanium mixed oxides, silicon nitride, gun steel erosion, rubber-elastomer, and carbon fiber). Currently he is active in the fields of surface modification and characterization of carbon fibers. Dr. Lin is a member of the American Chemical Society, American Vacuum Society, Electrochemical Society, Materials Research Society, and Carbon Society.

---

---

# PROCESS DIAGNOSTICS ON PLASMA CHEMICAL VAPOR DEPOSITION OF HYDROGENATED AMORPHOUS SILICON AND RELATED MATERIALS

---

Nobuhiro Hata

---

*This paper reviews Japanese activities in process diagnostics by laser spectroscopy on plasma chemical vapor deposition (CVD) of hydrogenated amorphous silicon (a-Si:H) and related materials in the past years and discusses the future scope of process diagnostics as an important part of materials science.*

---

## INTRODUCTION

The present aims of process diagnostics are to understand the mechanisms that lead to film deposition or etching and to enable precise control of the processes for best material qualities, etching characteristics, and process efficiencies.

Valency control by impurity doping of amorphous silicon was demonstrated for the first time in 1975 by plasma CVD (Ref 1). Since then there has been numerous research on amorphous silicon and amorphous silicon alloy materials in the world. There are two reasons why process diagnostics have been intensively pursued in this field of research. First, amorphous silicon is semiconductor material, and its structure and properties need to be carefully controlled for its applications, since structural defects or impurities of ppm order concentration sometimes affect carrier transport mechanisms drastically. Furthermore, the

material is most commonly prepared by plasma CVD, in which mechanisms that relate the operating conditions, like gas pressure, discharge power, substrate temperature, electrode configuration, and so on, to the structure and properties of the deposited material are complicated and have not been understood clearly. Second, when extensive amorphous silicon research was begun, laser technologies and optical measurement technologies had matured and could be used as powerful tools of process diagnostics. Because of these reasons, the amorphous silicon research field has become one of those in which process diagnostics are intensively studied.

It should be noted here that process diagnostics are an important part of materials science, since it is open to a wide variety of materials and not restricted within one particular material like amorphous silicon. It makes empirical or trial-and-error material research and development more scientific

and efficient. In this paper, keeping this in mind, I will review process diagnostics on amorphous silicon related materials.

Historically, process diagnostics research was initiated as observations of the process by emission spectroscopy and mass spectrometry (Ref 2). Those techniques are rather conventional, but they triggered the succeeding activities in process diagnostics; with knowledge from this initial research, simple models of plasma CVD mechanisms were proposed and discussed, which led us to further research with laser spectroscopic and other techniques.

## EXPERIMENTAL

The experimental setup for process diagnostics by coherent anti-Stokes Raman spectroscopy (CARS) and laser-induced fluorescence (LIF) is described in our previous papers (Ref 3-5). Lasers were selected from commercial models to meet the requirements for the experiments such as peak intensity, line width, tunability, wavelength range, stability, repetition rate, etc. Optics were designed and composed so as to increase the signal intensities and reduce the background noises. Detection systems were selected considering the detectivity at the signal wavelengths. The plasma CVD chamber was designed essentially the same as that used for film deposition and was equipped with optical windows for the measurements. To enable the chamber to be moved to alter the measuring position, it was put on a large X-Z stage. For measurements, the lasers and detection systems had to be controlled coincidentally, and a computer was used for that purpose. Signal processing was required to output spectral and intensity data.

## RESULTS AND DISCUSSION

### Detection of $\text{SiH}_2$ and Its Concentration

In order to detect transient species by CARS in a plasma CVD environment, it is necessary to know at least one of the transition frequencies of the species to be detected. The literature gives the vibrational frequencies of  $\text{SiH}_x$  species, which are most probably transient species in silane ( $\text{SiH}_4$ ) discharges for amorphous silicon deposition, determined from infrared absorption spectra of flash photolysis products from silane molecules isolated in a cold argon (Ar) matrix (Ref 6). From the data, it is known that silylene ( $\text{SiH}_2$ ) has a  $\nu_1$  symmetric vibrational frequency of about  $2,032\text{ cm}^{-1}$ .

Another requirement for the measurement of transient species is that its concentration is high enough to generate a detectably strong signal. Since the detection limit by CARS is reported to be about  $10^{12}\text{ cm}^{-3}$  for a single rovibrational line,  $10^{11}\text{ cm}^{-3}$  of silylene is approximately the lower limit, which is rather high as the concentration of transient species (Ref 7). The measurement was carried out in a high discharge power, gas pressure, and gas flow rate mixed-gas discharge plasma of silane and hydrogen in which concentrations of transient species are expected to be higher than in that typically used for amorphous silicon deposition (Ref 8).

The CARS spectral structure at around  $2,032\text{ cm}^{-1}$  is shown in Figure 1 (Ref 8). The spectral structure was assigned to be the  $\nu_1$  Q-branch of  $\text{SiH}_2$  for two reasons: (1) the position of the main peak was at  $2,032\text{ cm}^{-1}$ , and (2) those peaks disappeared when the discharge power was turned off.

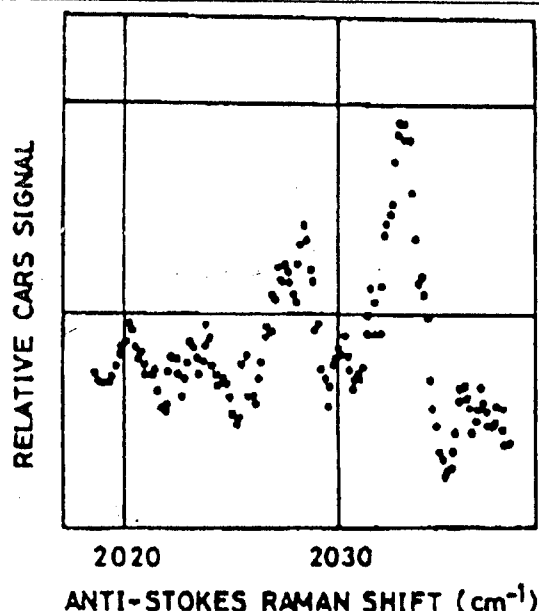


Figure 1.  $\text{SiH}_2$   $\nu_1$  Q-band CARS spectra in the high power ( $1 \text{ W/cm}^2$ ) RF glow-discharge plasma of 2.4-Torr  $\text{SiH}_4$ - $\text{H}_2$  mixture ( $\text{SiH}_4/\text{H}_2 = 1/9$ ). Reprinted with permission of Elsevier Science Publishers, Physical Sciences & Engineering Division.

The signal intensity was compared with that from  $\text{SiH}_4$  of known concentration, and the concentration of  $\text{SiH}_2$  was estimated, assuming the nonlinear electric susceptibility of  $\text{SiH}_2$  is almost the same as that of  $\text{SiH}_4$  at  $2,187 \text{ cm}^{-1}$ , and the sensitivity of the detection system is almost the same between the two frequencies. The estimated concentration of  $\text{SiH}_2$  was  $1.7 \times 10^{14} \text{ cm}^{-3}$ .

The concentration of  $\text{SiH}_2$  was estimated also by another method. From the slope of the semi-logarithmic plot of the CARS signal of  $\text{SiH}_4$  in a discharge plasma, the loss rate of  $\text{SiH}_4$  was determined (Ref 4). Then, the creation rate of  $\text{SiH}_2$  was calculated assuming the branching ratio of  $\text{SiH}_4$  molecules dissociate into  $\text{SiH}_2$ . The creation rate was introduced into the rate equation representing the balance between the creation and loss by diffusion to the substrate or wall surface. At the steady state

conditions, the equation was solved, and the obtained value of  $\text{SiH}_2$  concentration is a steady state discharge was  $2.9 \times 10^{15} \text{ cm}^{-3}$ . It is found that this value is about 17 times larger than that obtained from  $\text{SiH}_2$  using the CARS signal intensity. The rate constants of  $\text{SiH}_2$  insertion reaction into  $\text{SiH}_4$  are reported to be  $2.3 \times 10^{-12} \text{ cm}^3/\text{s}$ ,  $5 \times 10^{-11} \text{ cm}^3/\text{s}$ , and  $1.1 \times 10^{-10} \text{ cm}^3/\text{s}$  by different authors (Ref 9-11). Even if the smallest value is adopted, the average time to the reaction, which is obtained by multiplying the rate constant by  $\text{SiH}_4$  concentration and taking the inverse of the product, is  $5.4 \times 10^{-5} \text{ s}$ , which is much shorter than the average time of 0.12 s of diffusion to the surface.

The result means that gas-phase chemical reactions dominate the loss of  $\text{SiH}_2$ . A large number of constants and coefficients are required to solve the gas-phase chemistry, which will not be discussed here. But it can at least be said that the discharge system is complicated and cannot be solved by a simple dissociation and diffusion model, but should be treated considering chemical reactions in the gas phase and probably on the surface as well.

## Concentration Gradient of Source Gas Molecule

Source gas molecules and some product molecules are more abundant in discharge plasmas and therefore easier to be detected by CARS. From the signal intensity and spectral shape the concentration profiles of these source gas molecules can be obtained.

We have already published many data on concentration profiles of source gas molecules, especially of silane (Ref 3,5,12-14). Among them, Figure 2 (Ref 5) shows a lateral concentration profile of silane and germane. The concentration gradient of source gas silane is obtained from the data

by taking the slope of the concentration profile. Since axial symmetry can be assumed in this system, the number of silane molecules entering the discharge volume from outside per unit time is calculated by multiplying the concentration gradient by diffusion coefficient and columnar area. That value is then divided by the total area of the electrode surfaces and density of amorphous silicon film. The obtained value is 2.4 A/s, which corresponds to the film growth rate, and the value is in good agreement with the actual film growth rate.

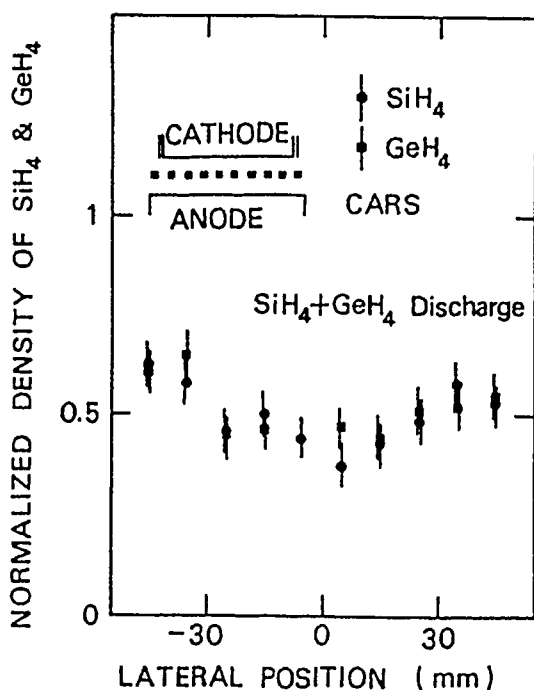


Figure 2. Distributions of  $\text{SiH}_4$  and  $\text{GeH}_4$  molecules are determined by CARS measurements in a  $\text{SiH}_4 + \text{GeH}_4$  steady-state discharge. They are normalized to the values of the density when the discharge is off and plotted against the lateral position, as shown by the inserted sketch in the figure. The rf-power density, total gas pressure,  $\text{GeH}_4/\text{SiH}_4$  ratio, and  $\text{SiH}_4$  flow rate are  $80 \text{ mW/cm}^2$ ,  $10 \text{ Pa}$ ,  $1/1$ , and  $2 \text{ sccm}$ , respectively (from Ref 5). Reprinted with permission of the American Institute of Physics.

The conclusion from this discussion is that most of the silane molecules entered into the discharge volume are involved in the deposited amorphous silicon film. This also suggest that CARS measurements of the source gas molecules are effective in discussing the mass transport in plasma CVD systems.

## Temperature Profile

The other information obtained from the CARS signal is the distribution in the internal states. Under the gas pressure (0.1 to 1 Torr) typically used for plasma CVD of amorphous silicon, rotational distribution of molecules is thermalized to the translational temperature of molecules. Thus, gas (translational) temperature is obtained from the CARS spectral shape or ratio of CARS signal peak intensities, which are determined by the rotational distribution. We have reported two ways to determine temperature by CARS in a plasma CVD environment for amorphous silicon. One is from the  $\nu_1$  Q-branch CARS spectrum of silane (Ref 15). The CARS spectral shape was compared with those calculated theoretically to find the best fitting value of the rotational temperature. The other is from the rotational CARS signal of hydrogen molecules (Ref 16). The intensities of the signal peaks from different rotational states were compared to each other to find the value of the rotational temperature.

Figure 3 (Ref 16) is the gas-phase temperature profile between the two electrodes of a plasma CVD system. The profile shows a monotonous increase of the gas-phase temperature from the cathode to the heated anode when the substrate heater is turned on; it is flat at room temperature when the heater is off. It should be noted that the temperature profile does not change considerably even if the gas pressure, flow



rate, or discharge power are varied in the range of typical plasma CVD conditions.

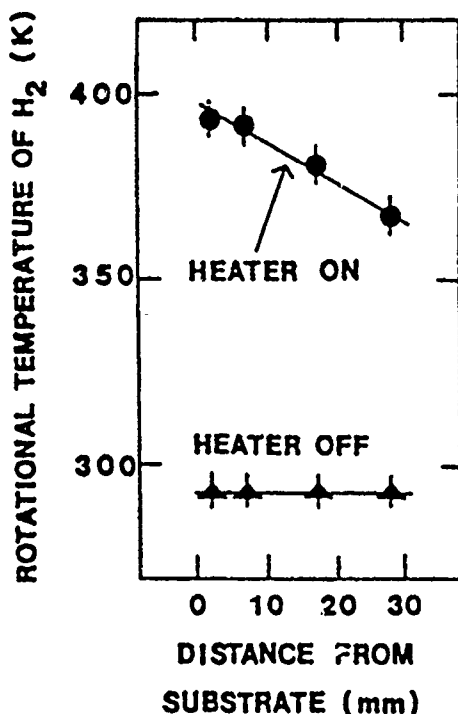


Figure 3. Gas-phase temperature profile determined from the pure-rotational CARS spectra of hydrogen in rf discharges with substrate heater turned on and off (from Ref 16).

The relaxation time of the gas-phase temperature profile is calculated from the ratio of thermal conductivity and heat capacity of the gas, and it is much shorter than the gas residence time under the present values of operating conditions. That is the reason why the temperature profile does not change very much with the gas pressure and flow rate. The gas-phase temperature rise due to discharge rf power is smaller in the hydrogen-diluted discharge than in the silane discharge because of the much higher thermal conductivity of hydrogen molecules.

The conclusion from the temperature profile study is that the gas-phase temperature profile is mostly determined by the temperatures of the electrodes and chamber wall and not affected by the operating conditions very much. It is often the case that the substrate temperature is monitored by a thermocouple, which is attached to the substrate heater, and so the exact temperature of the surface is not obtained. The extrapolated gas-phase temperature to the substrate surface is a much more accurate temperature of the film growing surface, which is important information on surface processes of the film deposition.

## SUMMARY AND FUTURE SCOPE

Three typical examples of process diagnostics by CARS on plasma CVD of a-Si:H and related materials were shown, and it was demonstrated that the techniques are quite powerful in studying concentration and temperature profiles of molecules and discussing the process mechanisms.

Process mechanisms now can be studied by more complicated diagnostics than mere observation with simple techniques. The next step of this series of work is to focus on the key species and key mechanisms that govern the process and to analyze them systematically (Ref 17). This kind of work will lead to accurate process models, which will provide guiding principles for better process conditions. As process diagnostic techniques become more developed, in-process monitoring for real-time control of the system will become practical in the future.

The process diagnostics discussed in this paper were mainly related to the gas-phase processes, but those related to the surface processes will also be very important (Ref 18). Surface process diagnostics

look more difficult at the moment and have not yet been developed fully. Therefore, emphasis also should be placed on the surface processes.

The research presented in this paper was on amorphous silicon deposition but, as is obvious, process diagnostics are commonly used in research and development of many different materials and will be more important in the future. Therefore, it is strongly desired that this interdisciplinary area of research be developed through cooperation of researchers from many research areas and many countries.

## REFERENCES

1. W.E. Spear and P.G. LeComber, *Solid State Commun.* 17, 1193 (1975).
2. A. Matsuda and K. Tanaka, *Thin Solid Films* 92, 171 (1982).
3. N. Hata, A. Matsuda, K. Tanaka, K. Kajiyama, N. Moro, and K. Sajiki, *Jpn. J. Appl. Phys.* 22, L1 (1983).
4. N. Hata, A. Matsuda, and K. Tanaka, *Jpn. J. Appl. Phys.* 25, 108 (1986).
5. N. Hata, A. Matsuda, and K. Tanaka, *J. Appl. Phys.* 61, 3055 (1987).
6. D.E. Milligan and M.E. Jacox, *J. Chem. Phys.* 52, 2594 (1970).
7. M. Pealat, J.P.E. Taran, and J. Taillet, *J. Appl. Phys.* 52, 2687 (1981).
8. N. Hata, A. Matsuda, and K. Tanaka, *J. Non-Cryst. Solids* 59&60, 667 (1983).
9. P. John and J.H. Purnell, *J. Chem. Soc. Faraday Trans.* 169, 1455 (1973).
10. J.M. Jasinski and J.O. Chu, *J. Chem. Phys.* 88, 1678 (1988).
11. G. Inoue and M. Suzuki, *Chem. Phys. Lett.* 122, 361 (1985).
12. N. Hata and K. Tanaka, *J. Non-Cryst. Solids* 77&78, 777 (1985).
13. N. Hata, A. Matsuda and K. Tanaka, *Proc. Int'l Ion Eng. Congress - ISLAT'83 & IPAT'83* (Inst. Electrical Eng. Japan, Tokyo, 1983), p. 1457.
14. N. Hata, *J. Vacuum Soc. Japan* 31, 208 (1988).
15. N. Hata, A. Matsuda, and K. Tanaka, *J. Appl. Phys.* 59, 1872 (1986).
16. N. Hata, A. Matsuda, and K. Tanaka, *Symp. Proc. 8th Int'l Symp. Plasma Chemistry*, edited by K. Akashi and A. Kinbara (IUPAC, Tokyo, 1987), p. 500.
17. F.G. Celii, P.E. Pehrsson, H.-T. Wang, and J.E. Butler, *Appl. Phys. Lett.* 52, 2043 (1988).
18. K.B. Koller, W.A. Schmidt, and J.E. Butler, *J. Appl. Phys.* 64, 4704 (1988).

**Nobuhiro Hata** is a senior researcher at the Electrotechnical Laboratory, Japan, and is now visiting the Department of Electrical Engineering, Princeton University, for a joint research project on amorphous silicon alloys. He received his B.Sc. and M.Sc. degrees in physics and his Ph.D. in chemical engineering from the University of Tokyo. His research efforts are directed toward amorphous semiconductors, process diagnostics, and materials for solar cells. Dr. Hata is a member of the Materials Research Society and the Japan Society of Applied Physics, and he has received the Japan Society of Applied Physics Award.