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4TH JAPAN INTERNATIONAL SAMPE SYMPOSIUM & EXHIBITION: MULTIMEDIA INFORMATION HIGHWAY "COMMERCE AT LIGHT SPEED" PROGRAM: OPTO-ELECTRONIC TECHNOLOGY RESEARCH LABORATORY

S.R. LECLAIR

SEPTEMBER 1995

INTERIM REPORT FOR 09/25/95-09/28/95

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MATERIALS DIRECTORATE
WRIGHT LABORATORY
AIR FORCE MATERIEL COMMAND
WRIGHT PATTERSON AFB OH 45433-7734

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This technical report has been reviewed and is approved for publication.

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13. ABSTRACT *(Maximum 200 words)*

A trip report composed by Dr Steven R. LeClair, Chief of the Materials Process Design Branch of the Air Force Materials Directorate. Discusses visits to 1) The 4th Japan International "Society for the Advancement of Materials and Process Engineering" (SAMPE) Symposium and Exhibition, 2) The Multimedia Information Highway "Commerce at Light Speed" (CALS) Program and 3) The Opto-electronic Technology Research (OTRL) Laboratory located in Tohkodai, Japan.

Research in material/process discovery methods was the focus of the participation in SAMPE. A copy of the presentation on "Innovations in Materials Design" by Dr. LeClair is included in addition to presentations by Dr Yoh-Han Pao, Dr Al Jackson and Mr Steve Adams.

Observations on the Internet Information Highway and the potential it may hold for materials/process research is discussed in the section on the CALS program.

Four presentations on processing technologies associated with molecular beam epitaxy (MBE) are summarized in the section on OTRL.

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Executive Summary

The following is a report of my presentation, observations, discussions and learned information as a consequence of my attending the 4th Japan Society of Material Processing Engineers (SAMPE) and co-chairing a special session of the SAMPE Symposium entitled 'Innovations in Materials Design' and visits to the Optoelectronic Technology Research Laboratory regarding research in the growth of opto-electronic films and Keio University regarding developments in the internet information highway.

The special session of the SAMPE Symposium entitled 'Innovations in Materials Design' was sponsored by the Asian Office of the Air Force Office of Scientific Research (AOARD).

Introduction

This report will cover a five day visit to Tokyo, Japan at the following locations:

24-26 Sept 95 - 4th Japan SAMPE Symposium & Exhibition, Hotel Mariner's Court, 3-1-5 Kamiosaki, Shinagawa-ku, Tokyo, 141 Japan;

27 Sept 95 - Environmental Information Department, Keio University, 5322 Endoh, Fujisawa 252 Japan;

and

28 Sept 95 - Optoelectronic Technology Research Laboratory, 5-5 Tohkodai, Tsukuba, Ibaraki, 30026 Japan.

The report will address site visits and will consist of the following sections for each site:

1) a brief overview of the author's perception of research in material/process discovery methods,

2) a description of site visited,

3) facilities and assistance,

4) research emphasis discussion,

5) progress (conference results),

6) continuing activities.

SAMPE Conference

1) Brief overview of the authors' observations of research in material/process discovery methods presented at the 4th International SAMPE Symposium & Exhibition

The SAMPE symposium is an opportunity to hear from the international materials and processing research community involving a broad range of methods from first-principle calculations to the use of empirical methods for the design and processing of materials and resultant products. Of specific interest is the opportunity to discuss further development of methods for automating empirical research of materials and/or processing in the pursuit of 'virtual' materials processing research.

A special session of the symposium, entitled 'Innovations in Materials Design' was organized by myself and Professor Shuichi Iwata of Tokyo University. The session was the second opportunity for us to exchange views and research ideas toward the development of new methods in the design of materials at the atomic-scale. My interest in this area is development of design aids for processing films and coatings. Such aids will be a prelude to the eventual development of tools for virtual materials processing research. A brochure highlighting the session and the various presentations is contained in attachment #1.

I opened the session with a presentation on the definition and perspectives of this area referred to as 'Innovations in Materials Design'. The view graphs and text of the presentation are in attachment #2. The presentations which followed included those from my own group (Dr Al Jackson, Dr Yoh-Han Pao, and Mr Steve Adams), those from Professor Iwata's group and others from France, Canada, China and Russia.

All of the presentations addressed the design of materials based upon a structure-properties data base, a computational method or both. The work presented by my group extended computational methods to structure-properties-<u>processing</u> data as our interest is 'AFFORDABILITY' of novel new materials. This was particularly interesting to the rest of the session attendees because it addressed a more attractive long term objective - 'virtual' materials research. Among the Air Force interests in this area are the implications of profound enhancements toward the acceleration and productivity of materials research.

1. There are many databases in existence that contain good data, but the formats are incompatible, making coordination of these databases difficult.
2. Computational efforts for multi-electron atoms are lagging behind needs for multi-element (ternary, quarternary, etc.) material compounds and alloys.
3. New methods are being developed and applied to real problems, including a reduced dimensional plot to capture patterns across compound structure-property data, data perusal semi-autonomous agents, density functional calculations using a modified (reduced dimension) Hamiltonian .
4. Property prediction approaches are in abundance, but because each is complex, an assessment of the strengths of each needs to be done to put them into some sort of perspective.
5. New approaches to classification schemes look good, but the limits of each need to be identified.
6. Combining computational approaches with heuristics and empirical methods may provide the most powerful approach when multi-element compounds need to be considered. How to accomplish this, of course, is a major problem.
7. Combining process data with static data in a common format or readily accessible format that has been started by us. Its advantages are only now being assessed and appreciated.
8. Interpretation of outputs (from methods) must be given more effort. Currently outputs are cryptic to all except the originator of the method. More user-friendly displays are desperately needed.

It was clear that among the attendees of this session, Professor Iwata and his group are best postured to make advances for two reasons: 1) after visiting his laboratory it is apparent that he has been given ample resources to make significant materials design contributions, 2) Professor Iwata is also keenly aware that part of his mission is an awareness of competing research in the international community.

2) A Description of the 4th International SAMPE Symposium & Exhibition

The symposium was held at the Tokyo Hotel Mariner's Court with the exhibition area in an adjacent structure. The symposium appeared to be attended by approximately 400 individuals mostly from Japanese industry. The symposium was very well organized and conducted with conscious professionalism involving 19 sessions spanning four (4) days of presentations.

3) **4th International SAMPE Symposium & Exhibition Facilities and Assistance**

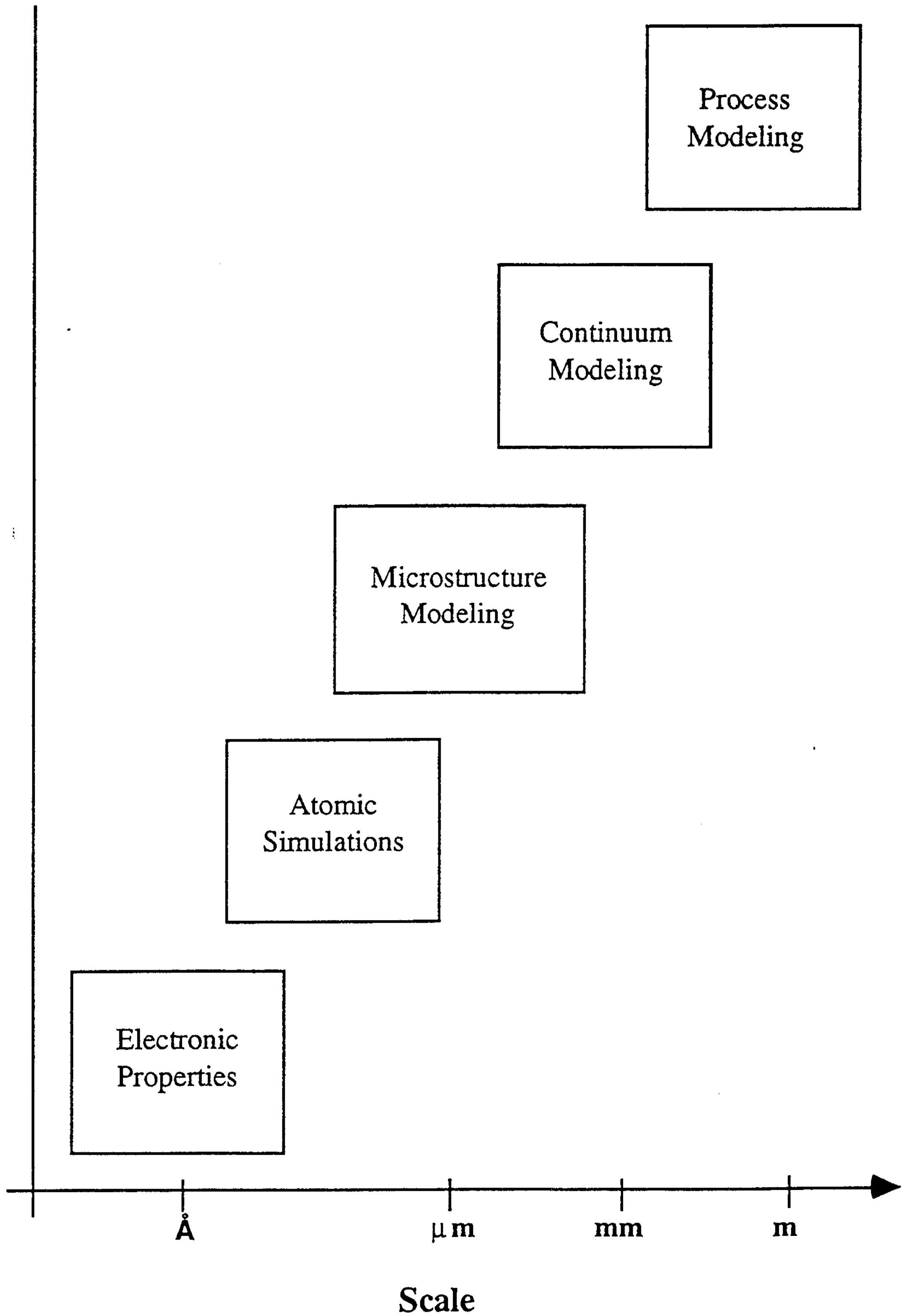
Our Japanese hosts were very hospitable and eager to assist us in any way they could. In fact, one of the individuals in my group (Dr Al Jackson) suffered an unexpected back spasm and was assisted by a Japanese doctor (at no expense) through arrangements made by the SAMPE Symposium staff.

4) **Research Emphasis Discussion**

The 4th Japan SAMPE Symposium emphasis appeared to be structural composite (organic, metal and ceramic) materials, with Titanium and Aluminum alloys of tangential interest. Also addressed were biomimetic and mechatronic materials for sensing and micro actuation, and fracture mechanics of structural composite materials. Finally, there were occasional presentations on opto-electronic materials. There were specific sessions dedicated to aerospace, automotive, rail, marine transportation; recreational materials, and civil engineering and construction. Lastly, two sessions were focused on materials design: 1) on 'Innovative Methods in Materials Design', which I co-chaired, and 2) Computer Aided Materials Design.

5) **Progress (Conference Results)**

After four days of interaction, I have acquired a clearer perspective of the research objectives, approaches and customer needs which are guiding both experimental and empirical research in Japan. The Japanese are focused on eclipsing the competition by seeking new approaches and methods to Materials Design, assuming that an evolution of current methods is not the answer. This perspective is best expressed by the wide range of methods presented at the 'Innovations in Materials Design' session involving quantum, atomic, mesoscopic (microstructure and continuum modeling), and macroscopic (process modeling) levels.



Materials Design Range of Scale

The methods presented varied in both approach and results. The most experienced in this area was the presenter from Canada (Dr John Rogers) and he explained a method for classifying compounds using a morphological metric. He also expressed that, to date, his method has merely validated, not discovered new, materials design knowledge.

The Russian presentations included one method I am familiar with (the Gladun Algorithm) and another that was conveniently not explained except that it involves a thermoconductivity metric for classifying and predicting the properties of new compounds for films and coatings. Interestingly, the metric is intended to aid in the design of a deposition process to produce the desired material.

The Chinese presentations emphasized methods based on first principle density functional calculations but aided by artificial neural networks to gain necessary computational efficiencies to extrapolate results to macroscale problems.

Finally, a Professor from the University of Paris (Prof Helene Bestougeff) presented her ideas on the development of autonomous software programs referred to as 'agents'. These programs represent yet another set of methods, which when applied to materials structure-property mappings, will add a new dimension to Materials and Processing Research as we know it.

6) Continuing Activities

As a result of the 'Innovations in Materials Design' Special Session, the organizers (Prof Iwata and myself) have secured a commitment from Elsevier Sciences and the editor of the Journal of Alloys and Compounds for a Special Issue of the Journal. (attachment #3).

In addition to the Elsevier Sciences publishing of the proceedings of the Innovations in Materials Design session of the 4th International SAMPE Symposium & Exhibition, future dates and opportunities to address progress and collaboration are as follows:

21-22 May 1996 AFOSR 'Electronic Prototyping' Initiative Review - Empirical Methods applied to Materials Design

16-22 July 1997 Australia-Pacific Forum on Intelligent Processing and Manufacturing of Materials - Workshop on Artificial Neural Networks applied to Materials Design & Processing. Professor Iwata and I have agreed to co-chair a session dedicated to 'Innovations in Materials Design'.

Now through 2000 Future Workshop and Conference Sessions focused on developing an *International* Information Highway of collaborators in pursuit of advancing knowledge and methods associated Integrated Materials-Process-Shape Design toward

'Virtual' Materials Processing Research.

Keio University - Multi-Media Information Highway

1) Brief overview of the authors' observations of developments associated with the Internet Information Highway and the potential it may hold for Materials and Process Research

The Japanese have established a collaborative program involving Nippon Telephone and Telegraph, KDD (a Japanese cable company) and American Telephone and Telegraph (AT&T) to develop applications for a high-speed (45MHz) T3 backbone to support internet communications. The backbone will direct couple major Japanese and U.S. universities. Making these resources available to students will accelerate development of applications on the internet. Obviously, the Japanese believe the internet offers long term commercial benefit and 'staying close' to the U.S. is of particular interest. Long term multi-media applications are the target and one of those applications is 'virtual' processing for both materials research and product development purposes.

Keio University Campus

2) A Description of the Multi-Media Information Highway, Commerce at Light Speed (CALS) Program

The Japanese point of contract for the CALS program is Professor Yoshiyasu Takefuji who holds faculty positions at Case Western Reserve University, Cleveland, Ohio and Keio University, Fujisawa, Japan.

Professor Takefuji has orchestrated a very ambitious program wherein the industry partners (NTT, KDD, & AT&T) will pursue the joint development of various technology areas and the universities will address various capabilities afforded by the multi-media information highway.

The to be developed by industry are the following technology areas:

- Integrated Digital Multi-media Services: to enable the integration of existing broad band services (television & telephone) and facilitate network development towards fully symmetric (bi-directional) interactive multimedia services;
- Photonic Technologies: to develop techniques for multi-gigabit bandwidth (currently 45MHx MAX) provision, optical switching technology, optical signal processing and control;
- High Speed Networking: to focus on technology and system development to support broad band services and improve the integration of networks (packet switching, routing, etc. to manage traffic on highway);
- Mobility and Personal Communications Networks: to focus on operational trials and technological aspects of fixed and mobile broad band networks, that impact on the provision of personal communication services (development of cellular phones, wrist phones, car phones, integrated computer/FAX/modem/phone, etc.);
- Intelligence in Networks and Service Engineering: to develop low cost, integrated and flexible local access network technology and advance concepts of modular standardization of service components and building blocks, as a basis for cheaper, quicker and more responsive development of services (adaptive services management);
- Quality, Security of Communication Services and Systems: to address the integrity and reliability of communications and confidentiality as well as other features such as electronic signatures (safeguards for credit cards , electronic commerce, etc.)

The to be explored by the universities are the following capabilities:

- Image Communications Evolution Planning: to support the introduction of digital TV, video-on-demand and multi-media interactive services across Europe;

- Digital Audio-Visual Flexible Architecture and Representation: to develop technical solutions that will improve the flexibility of communications technologies to meet different user requirements, alternative network infrastructures, terminals and operating conditions;
- Advanced Telepresence Services: to support the integration of additional sensory perceptions (e.g., touch and smell) in advanced multi-media services;
- Interactive and Distributive Multimedia Delivery: to investigate how the different network options such as satellite, terrestrial broadcast, local microwave, etc., can be exploited to provide access to a range of digital distributive and interactive audio services;
- Service Access for Advanced Multimedia Applications: to develop a range of user-friendly interfaces for multi-media services;
- Access control and Protection in Distribution Mult-media Systems: to establish a framework for the management of access and the protection of copyright and security in multi-media applications;

3) **Keio University Facilities and Assistance**

In support of general undergraduate and graduate degrees a total of 4,000 students have outstanding computing resources. The library will quickly be completely electronic for all new publications.

4) **Research Emphasis Discussion**

Professor Takefuji has not identified specific research interests as he is still in the formative stages of this program. The U.S. universities have not been identified but he did suggest Case Western Reserve as one of the candidates.

5) **Progress (Visit Results)**

The visit to Keio University has stimulated an awareness of the importance of the information highway to future materials processing research. A major source of future electronic libraries will be research laboratories, and therein, materials and processing research will depend more and more on electronic, multi-media information. It will be important to both stay abreast of the developments identified above and as well to participate where ever possible.

6) **Continuing Activities**

No continuing activities are anticipated, except Professor Takefuji has agreed to participate on the program committee for the Australia-Pacific Forum on Intelligent Processing and Manufacturing of Materials - Workshop on Artificial Neural Networks applied to Materials Design & Processing.

Opto-electronic Technology Research Laboratory

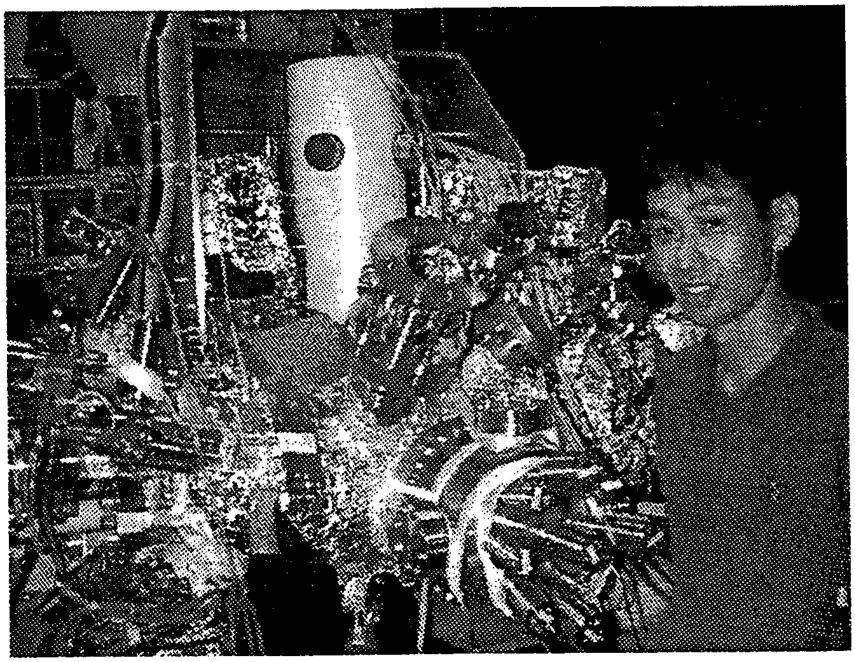
1) Brief overview of the authors' observations of research at the Opto-electronic Technology Research Laboratory

The Opto-Electronic Technology Research Laboratory (OTRL) is an excellent example of Japanese Technology Transition. The Laboratory was created in 1986 and soon will be transitioned and resources reallocated possibly to a follow-on project. It is noteworthy - the very specific focus Japanese projects have as exemplified by their limited duration and the reallocation of resources.

The OTRL research has targeted advances in processing technologies, specifically molecular beam epitaxy (MBE), for semiconductor materials. The research staff appeared to be multi-disciplinary and emphasized personnel with skills in advanced sensor and characterization methods such as scanning tunneling microscopy (STM), transmission electron microscopy, scanning electron microscopy, etc. It became apparent that these skills where needed to adapt these traditional off-line characterization methods for use as *in situ* sensors for real-time control of the MBE process.

I was given a presentation with storyboard of four (4) sub projects: 1) *μ-RHEED on MBE* - real-time observations of epitaxial growth using a scanning micro-probe reflection high-energy electron diffraction (termed μ-RHEED), 2) *STM on MBE* - STM observation between growths using ultra-high vacuum scanning tunneling microscope with atomic-scale resolution, 3) *All-UHV Processing - in situ* E-beam lithography which is capable of nanometer scale pattern fabrication and 4) *Hetero-epitaxy* - a method to suppress dislocation propagation in highly mismatched hetero-epitaxial GaAs/Si.

Each of the sub projects complemented the other toward the processing of next generation of opto-electronic devices for various applications, and specifically the information highway. The μ-RHEED will provide excellent control of thickness (with a resolution of one atomic layer), while the STM will provide information on surface roughness and uniformity, and the growth of GaAs on Si will pave the way for truly integrated opto-electronic devices on a single substrate of material.



MBE System with scanning μ-RHEED

Each of the three (3) sub projects complemented the other toward the processing of next generation of opto-electronic devices for various applications, and specifically the information highway. The μ-RHEED will provide excellent control of thickness (with a resolution of one atomic layer), while the STM will provide information on surface roughness and uniformity, and the growth of GaAs on Si will pave the way for truly integrated opto-electronic devices on a single substrate of material.

As I left the OTRL facility, I kept wondering what they were not presenting for consumption by the rest of the world. i.e.. the competition.

2) A Description of the Opto-electronic Technology Research Laboratory

The Opto-electronic Technology Research Laboratory has been conducting thin-film opto-electronic materials research for over 9 years. Their research objectives have been to advance material processing technologies for opto-electronic materials to enable the integration of optical/photonic devices and electronic devices on a single substrate, termed the 'Optoelectronic Integrated Circuit' (OEIC). The OEIC concept had been established by a MITI project called

"Optical Measurement and Control System" (1980-1986). An outgrowth of the the MITI project was the formation of a governmental organization (Optoelectronics Technology Research Corporation) including 13 industry partners. Interestingly, that each of the industry partners established branch laboratories located in their facilities during the duration of research.

The prime aim of the OTRL is to conduct such fundamental research as to produce breakthroughs in opening the new world of OEIC's where 2- and 3-dimensional superlattice structures are required. The research target of the project is best symbolized as the pursuit of, "Quantum Optoelectronic Integrated Circuits".

3) **Research Emphasis Discussion**

It is interesting to note that the OTRL had not specifically addressed *in situ* monitoring of material composition, e.g., for devices referred to as rugate filters involving varying compositions or doping of layers for specific electro-optical properties. This is probably because the Japanese industry is focused on the commercial marketplace wherein specific nonlinear optical materials have little application, at least as currently perceived.

4) **Progress (Visit Results)**

I was very impressed with both the organization and accomplishments by the research staff at the OTRL. The U.S. semiconductor industry is certainly being challenged by such efforts. It is interesting to note that many of the research staff were trained in the U.S. at such institutions as Bell Labs. It is clear that we have prepared the competition well and it is time we either begin to prepare ourselves to: 1) either define the next level of excellence in the areas of computing and telecommunication, or 2) we prepare ourselves for eventual and inevitable technological dominance by the Japanese.

5) **Continuing Activities**

None.

General Observations Regarding Trip

1. Participation in research meetings such as the 4th Japan SAMPE Symposium are crucial for benchmarking progress in our in-house program. It is clear what we must do to compete with world class materials research - our productivity must improve. The Japanese approach, as exemplified at the OTRL in Tsukuba, is to 1) focus on objectives and not to waver from them for any reason, and 2) ensure success by active participation by the customer (13 companies). Although our intent is similar, we do not follow either of these steps very closely. There is no argument that the Japanese rigid adherence to a methodical approach has and will continue to suffer from a lack of spontaneous creativity. But from my observations, if we are to compete and maintain our leadership in critical technologies we must learn from and improve upon their approach. Which, by the way, is the highest tribute one can pay to a 'teacher' in Japan.

> **Note:** To underscore my words with actions, our research group will soon commence two projects: one in advanced processing of forged materials, and the other in automating probe path generation for eddy current inspection of engine components. Wherein, we will follow the above approach, in hopes of benefiting from a more productive research effort and a smoother transition of the technology to the end-user.

2. It is clear from both the SAMPE presentations by the Japanese presenters and the visit to OTRL that software development is not something the Japanese pride themselves in. I am not saying they are not capable or that they do not build 'intelligent' processing systems, but they do not offer to exhibit or discuss the software required to implement the methods presented at the SAMPE session nor the real-time control necessary for the advances in MBE at OTRL. This lack of pride in software development may one of the reasons for the extreme interest in the internet and the information highway as noted from my visit to Keio University.

3. One last observation regarding my trip to OTRL. The *in situ* sensing (μ RHEED and STM) appear focused on morphological aspects of films, i.e., thickness, roughness/uniformity, etc., to the exclusion of film composition or stoichiometry. It was curious that given their interest in 2- and 3-dimensional superlattice devices that, at a minimum, stoichiometry might be important, if for no other reason than AlGaAs

and low temperature growth of GaAs are stoichiometric materials. Also of interest should be the doping of III-V materials is used to enhance or alter properties in opto-electronic devices. No discussion or demonstration of *in situ* sensing of composition causes suspicion as to research they are currently doing but do not wish to talk about. It appears the Air Force interest in controlling composition and stoichiometry via *in situ* ellipsometry make be both more advanced that the Japanese, and a niche in terms of achieving our research goals which is advanced processing technology to exploit nonlinear optical materials for threat and detection applications.

Acknowledgments

First, and foremost, to take an extended trip of this nature requires the back-up of a capable deputy, Dr Jim Malas, to carry out a great many responsibilities for day-to-day operation of our research group. I am indebted to Dr Malas for assuming all of my responsibilities while out of the office - particularly for responding to all of the suspense's.

Secondly, I thank Capt Paul McQuay and Dr Shiro Fujishiro of the Asian Office of AFOSR for their support and assistance in organizing our 4th Japan SAMPE session on 'Innovations in Materials Design'.

Lastly, I would like to acknowledge the editing and contributions to the 4th Japan SAMPE Conference session on 'Innovations in Materials Design' and this report made by Drs Yoh-Han Pao, Al Jackson and Mr Steve Adams.

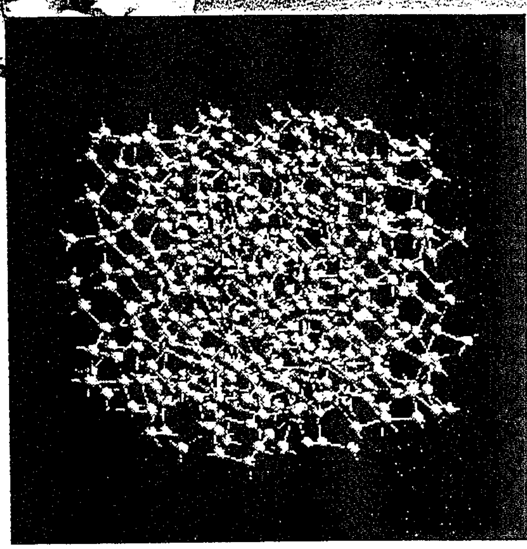
Symposia L1

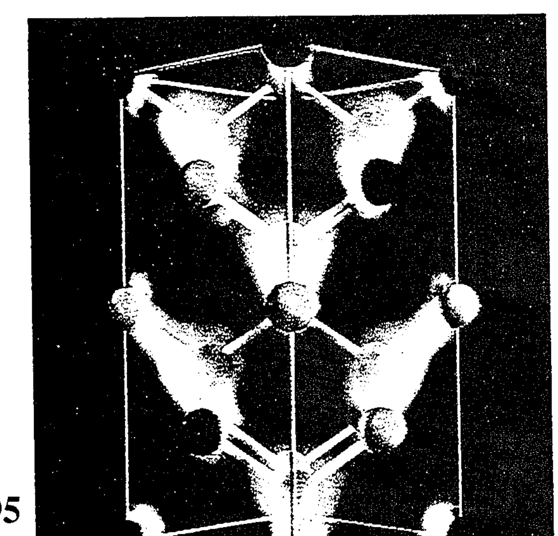
"INNOVATIONS IN MATERIALS DESIGN"

Main Theme: Discovery of Attractive Materials-Serendipity

Co-chairmen: S.Iwata(The Univ. of Tokyo), S.LeClair, Wright Laboratory(AFMC)

Sponsored by AOARD





September 25-26, 1995

Tokyo International Fair site, Tokyo, Japan

Symposia L-1:"INNOVATIONS IN MATERIALS DESIGN"
New challenges in the network eraheld during September 25-26, 1995

Hotel Mariner's Court Tokyo(SUSUKI)
Main Theme:Discovery of Attractive Materials-Serendipity

Co-chairmen
S.Iwata, The University of Tokyo
S.Leclair, Wright Laboratory(AFMC)

Objectives

It can be argued that the optimal mapping of material structure to erties, processing, and use is the principal driver for all prescriptive scientific and engineering endeavors. Given the computational intractability of abinitio materials research, the efficient and accurate prediction of yet to be made materials is an equally prominent endeavor, if not a preeminent materials research frontier. Because of the vast amounts of information to be considered in the pursuit of either, the automation of search-based methods for augmenting more analytic approaches is receiving increased attention. Discovery and invention are humanendeavors driven by sensitivity and curiousity but tempered by circumstance often characterized as 'serendipity'. The literature is replete with the accounts of human discovery in the field of engineering and elsewhere. In the 21st century, the growth of high-performance computing and more efficient reasoning methods will enable still greater opportunity for serendipity: to explore and extract useful information and accelerate the pursuit of new knowledge via advanced computing resources. Several common problems of materials design are proposed so as to test a feasibility of integrating available and useful methods through computer networks. The pre-symposia will start at http://race.u-tokyo.ac.jp/JISSE4/IMD/ !!!

Future Agenda

Establish Intentions :
How to get a new idea emerged and to discover multi-variate patterns through the mining of data;browsing of continuous, heterogeneous information via filtering/ focusing/ erasing/ selecting/reasoning to extract useful information, with fluctuating/ changing viewpoints.

Establish View :
How to define, reduce dimension of, and re-represent design space

Tentative Program

September 25 Afternoon Session (5 hours) 13:00-18:00

-Problem Definition-

Opening: Selection of issues and definitions of problems
13:00-13:30
S.LeClair(WL/AFMC), S.Iwata(Univ. of Tokyo)

Fundamentals of Mathematics for Problem Solution
13:30-14:00
Y.Shikata(Nagoya Univ.)

Cognitive Problem Solving:An Intelligent Agent Approach
14:00-14:30
H.Bestougeff

-Exemplars with System Demonstrations and Coffee Break
14:30-15:00

-New Approaches-

Prediction of Phase Stability in Al-Li Alloys at High Pressure
15:00-15:30
M.H.F.Sluiter, Y.Watanabe and Y.Kawazoe(Tohoku Univ.)

Manupilating the Recipe and Job of Semiconductor Process and Device Simulations in the TCAD System VEGA
15:30-16:00
M.Yokotani, A.Kato, N.Ishihara,Y.Iriye and H.Koike(FUJI-RIC)

Analysis of Generation and Wall Loss Reactions of Plasmas in Dry Etching of Silicon Dioxide
16:00-16:30
K.Tago, H.Kazumi and K.Kobayashi(HITACHI)

Refinements of captured information to extract solutions by data bases

On the Interfacing of Material Property Databases in KBS/DSS Architectures for Life Management of Power Plant
16:30-17:00
H.Kroeckel, A.S.Jovanovic, H.H.Over(JRC-Petter,MPA Stuttgart)

(to be added at the last version)
17:00-17:30
F.Kuznetsov(IMI-Novosibirsk)

September 26 Morning Session (4hours) **8:30-12:30**
-Exemplars with System Demonstrations-
8:30-9:00

-Refinements of captured information to extract solutions
New ASpects : Eco-Materials
9:00-9:30
R.Yamamoto(Univ. of Tokyo)
-by electronic and atomistic, mesoscopic and macroscopic approaches
-First Principles

Density Functional Approach for Many Elecron Systems
9:30-11:00
H.Odaka, S.Ohnishi* and S.Iwata(Univ. of Tokyo, NEC*)
K.Rabe
B. Gu(Tsinghua Univ.)
Atomistic Approaches for Materials Design
11:00-11:30
S.Yip, M.Tang* and K.Mizushima(MIT,LLNL*,MMC***)

Virtual Materials System for Metal Injection Molding
11:30-12:00
T.Iwai, T.Aizawa and J.Kihara(Univ. of Tokyo)

Design of Metal/Oxide Interfaces by the Use of Non-equilibrium Thermodynamics
12:00-12:30
Hideaki Inaba(Kawasaki Steel Corporation)

Lunch Breack

September 26 Afternoon Session (6.5 hours) **13:30-19:00**

Refinements of captured information to extract solutions
-by reasoning-
13:30-14:00
Discovery Approaches for Materials Systems
14:00-14:30
A.G.Jackson, S.R.Leclair and S.Adams (WL/AFML)

Fundamentals of Mathematics for Problem Solution

Yoshihiro SHIKATA
Nagoya University

Sometimes mathematical theory is too rigid to be applied to practical problems, like material design. Take for example a problem to find a surface of minimal area bounding two parallel circles. Though the answer is a cylinder or two disjoint disks depending on the position of the circles, a conventional variation theory gives only a cylinder or only disks because there is a jump of topological type between the cylinder and the disk. The topological jump is natural in practice, like in material design, therefore it may be important to construct a variation theory which admits the topological jump and reduces mathematical rigidness. Thus we try to develop less rigid mathematics to treat the dendritic growth of the snow crystal and the shape of milk crown. In contrast with the rigid mathematics which starts from equations and ends with the comparison of the polution with the phenomena, we take first phenomena and extract essentials deciding its "shape" or "behaviour", then obtain type of equations necessary for the shape or behaviour.

MANUPILATING THE RECIPE AND JOB OF SEMICONDUCTOR PROCESS AND DEVICE SIMULATIONS IN THE TCAD SYSTEM VEGA

M.Yokotani,A.Kato,N.Ishihara,Y.Iriye and H.Koike
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Fuji Research Institute Corporation
Kaigan Minato-ku Tokyo,Japan

We discuss the problem usability of TCAD system that has semiconductor process and device simulators. We show a solution that such system needs PERT chart processing,ability of user customization and knowledge data base. PERT stands for Program Evaluation and Review Technique. PERT chart is a directed acyclic graph whose vertex is called a task that is a recipe for simulator. VEGA with MINERVA is an example of the solution. VEGA's recipe is a semiconductor process sequence or a control data for device simulators or an input data for a program making SPICE parameters. User customization is supported by a lisp interpleter

GPa. Electronic total energies have been computed within the local density formalism with the linear muffin-tin orbital method in the atomic sphere approximation and the phase stability properties at zero temperature have been examined.The effect of temperature was considered by solving the configurational part of the alloy hamiltonian with the cluster variation method. Both fcc and bcc based structures as well as the complicated interloper phases Al2Li3 and Al4Li9 were considered. Computation of the pressure dependence of the Al-Li phase equilibria has made it possible to examine the importance of the atomic size difference, and it also addresses the question of whether the stability of the AL3Li precipitates is affected by conditions of high stress. A critical comparison with recent experimental results and with other theoretical work is made.

a) selection of materials, precursors to provide desirable functions and acceptable efficiencies
b) selection and optimization of processes used for synthesis of materials
c) Identification of factors which regulate life-time of materials and their combinations
3. Capabilities of the thermodynamic modeling will be demonstrated by our results in field of electronic material processing: CVD and MO CVD deposition, interface reactions, oxidation of multi components compounds.
4. Type of application determines requirement to data sets used in calculation. Specific feature of problems oriented data sets are self consistency of data and completeness of data selection. Electronic Materials Properties Data Base EMPDb created at the Institute is an example of such a system. Copy of the bank will be available for demonstration.
5. At present use of different of modeling in design and optimizing of production process become very practical. However at least at the moment knowledge of modeling methods is early combined with skill in production technology. Two parts of the business is being done by different people. We believe that this separation of responsibility will stay for some time in future. One of the tasks of present meeting is to our understanding establishing working cooperation of specialists in computer and real experimenting. Our group offers it's potential in thermodynamic modeling.

DYNAMICS OF FRACTURE: A COMPUTATIONAL PERSPECTIVE

Xiaopeng Xu, Farid F. Abraham
IBM Almaden Research Center, San Jose, CA. 95120

Continuum fracture theory typically assumes that cracks are smooth and predicts that they accelerate to a limiting velocity equal to the Rayleigh speed, or surface sound speed, of the material. In contrast, experiment tells us that, in a common fracture sequence, an initially smooth and mirrorlike fracture surface begins to appear misty and then evolves into a rough, hackled region with a limiting velocity of about six-tenths the Rayleigh speed. Recent experiments have clearly shown that violent crack velocity oscillations occur beyond a speed of about one-third the Rayleigh speed and are correlated with the roughness of the crack surface. Also observations of fast crack growth in brittle solids typically reveal complex patterns of crack branching. All of these features are unexplained using conventional continuum theory.

that are useful is very difficult and costly. Applications of rough sets and pyramidal nets to these problems are presented, as are limitations to these methods and difficulties in application.

A Computational Materials Design Program

John R. Roders
NRC-CANADA

In recent years Material Science and Engineering have played an increasingly important role in dealing with issues of high visibility, such as energy efficiency, product durability/reliability and environmental sustain ability. As a result, Material Science Research has moved to the forefront of worldwide technological priorities. Currently, computer simulation is widely utilized in the mechanical design and manufacturing management areas. Materials property and process optimization, however, have continued to be pursued largely through empirical experimentation, placing increasing cost burdens on management due to rising experimental costs and ever more complex environmental and performance requirements. Recent developments in theoretical methods have, kinds of materials properties are possible. In addition, methods are now able to quantitatively predict micro structural changes by direct simulation or by simple theoretical and/or empirical analyses. By combining these new methods with already existing materials databases, atomistic simulation and carefully chosen experiments, the process of developing and commercializing new materials can be dramatically improved.

To achieve this goal, I propose a major new consortium project to be established, with companies involved in materials development, production and /or utilization to pursue four key objectives;

1. To collect, validate, integrate and package for early distribution to members, the best current predictive methods.
2. To produce, together with other affiliated research groups, enhancements which will extend current methods, strength their theoretical base and broaden their applicability to important commercial problems.
3. To combine these methods into an integrated materials design tool set suitable for use by engineers and scientists.
4. To link these methods to currently used mechanical design and process management models.

and so on. However if we want to simulate a large group of atoms in dynamic motion, this conventional procedure becomes inefficient as the numbers of atoms increase. To overcome this problem, we are studying and developing approximate kinetic-energy functional of electron density, because the solution of the Kohn-Sham equation for a large number of bands and k points can be reduced to the calculation of a single function by using the kinetic energy functional. The accuracy and efficiency of this method will be discussed.

First principle calculations of the electronic structure of C60, C58BN solids and Carbon nanotube

Bing-Lin Gu
Dept. of Phys., Tsinghua Univ., Beijing 100084, China

Using a self-consistent mixed-basis all-electron and full-potential approach within the local density approximation,we have investigated the effects of molecular orientation on the electronic structure of C60 solid and C58BN hetero-fullerenes in fcc phase. The degeneracies at special **k** points, the dispersion, and the widths of bands and the location of the valence-band maximum and the conduction-band minimum have been found to be sensitive to the orientation of the fullerenes in fcc lattices. In addition, the filling of Carbon nanotubes is discussed by use of DV-X*alpha* method.

Role of Atomistic Simulations in Materials Design: Structural Stability of Si and SiC under High Compression

Kazuki Mizushima
Central Research Institute, Mitsubishi Materials Corporation 1-297
Kitabukuro-cho, Omiya, Saitama 330, Japan

Meijie Tang* and Sidney Yip
Department of Nuclear Engineering, Massachusetts Institute of Technology
Cambridge, Massachusetts 02139, U.S.A.

Current developments in molecular dynamics simulation for analyzing the structural responses of solids under an external stress point to a capability which is potentially useful in materials modeling. Using many-body potential functions one can now investigate thermomechanical behavior of covalent solids at finite temperature and deformation; moreover, the resulting atomic configurations can serve as inputs for the theoretically more rigorous appoaches such as tight binding

Virtual Materials System for Metal Injection Molding

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7-3-1 Hongo,Bunkyo-ku,Tokyo 113

The metal injection molding(MIM)is expected to be the most promising powder forming technology to realize near-net shaping of complex parts and members. Different from the molding technology for plastic polymers,metallic powders are pre-mixed into a compound with high loading ratio. Hence,its mechanical properties are completely dependent on the loaded powder characteristics and distribution;i.e. since the density of powder particles distributes in molded compound,a green molded part has intrinsic ambiguity with respect to its mechanical properties, and the measured strength and toughness by experimental testing is only a sampled result in this statistics. Then,materials design for high reliability and quality assurance requires for new methodology to describe the configurational change of powders in molding and to predict mechanical behaviors of molded materials.

In the present paper,authors propose and develop a virtual materials system: 1) Our developed granular modeling is utilized to make direct simulation of compound flow and consolidation in MIM process, 2) Our proposed micromechanical model is applied to deduce microscopic mechanical properties of consolidated compound,and 3) Macroscopic distribution of mechanical properties is estimated by the homogenization method. Main feature is that the mechanical properties and their ambiguity for molded parts and members are quantitatively described by the present approach only with use of the mechanical properties of polymer binders and metallic powders and the powder loading ratio.

Design of metal / oxide interfaces by the use of non-equilibrium thermodynamics

Hideaki Inaba
Technical Research Laboratories, Kawasaki Steel Corporation
1 Kawasaki-Chou, Chuo-Ku, Chiba 260, Japan

When we are doing research or manufacture of materials including metals, semiconductors and ceramics, we often meet the problems of interface reactions involving more than two phases and multi-component diffusions. However, the studies analyzing these problems in terms of multi-thermodynamic and diffusional data and the method of analysis for

APPLICATION OF ARTIFICIAL INTELLIGENCE METHODS IN INORGANIC COMPOUNDS DESIGN

N.N. KISELYOVA

A.A.Baikov Institute of Metallurgy of Russian Academy of Sciences
Leninski Prospect, 49, 117334 Moscow, Russia

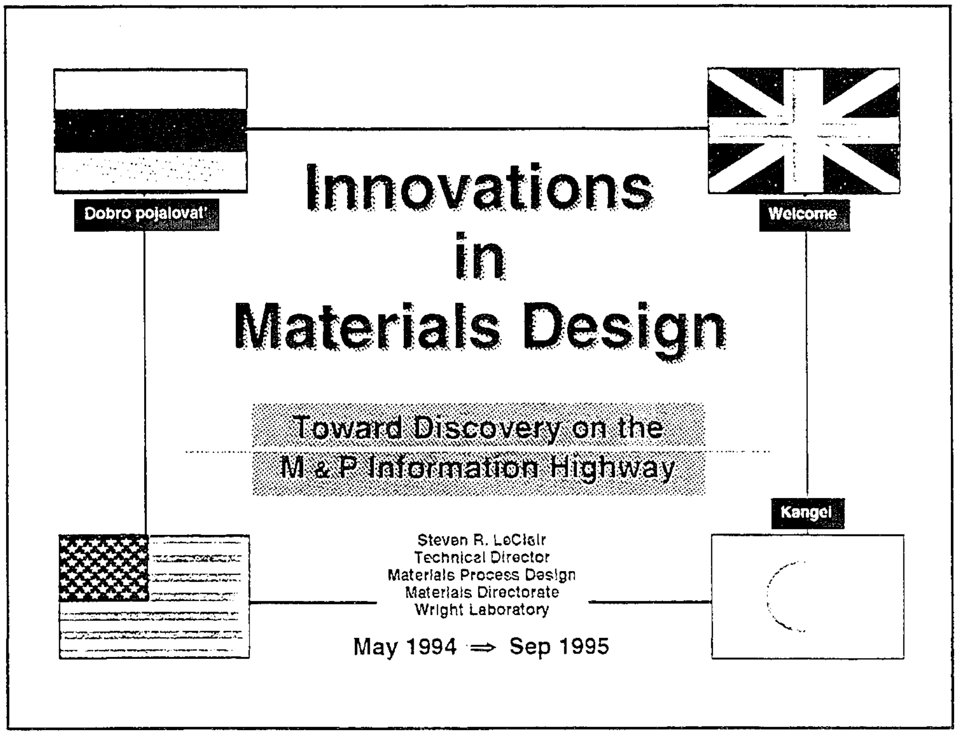
The most difficult problem of inorganic materials science and chemistry - calculating the intrinsic properties of multicomponent compounds starting from the knowledge of their constituent components' properties - still remains unsolved. We apply the methods of the artificial intelligence (learning of computer) for solution of this problem. Tha data for computer learning are extracted from the data-bases of known inorganic compounds' properties. The computer learning allows to find the complicated periodical regularities for certain classes of inorganic compounds. The prediction of the unknown properties of the compounds requires only the knowledge of the values of the component properties. By applying this approach we have predicted the formation of thousands of new compounds in ternary, quaternary and more complicated systems. These compounds were then searched for new semiconductors, superconductors, ferroelectrics, magnets
and other materials required for new technologies. The comparison of these predictions with the experimental data, obtained later, showed that the average reliability of predicted ternary phases exceeds 80 percent.

The 2-Dimensional Episodal Associative Memory: A New Way of Structuring andUtilizing Pattern-Based Knowledge Bases.

Yoh-Han Pao
Case Western ReserveUniversity, USA.

The new information processing methodology described in this paper consists of constructing a reduced-dimension representation of a body of data items, each of which might be a listing of the feature values of a material composition. A vast amount of data can be displayed visually in a 2-D display which is a 'self-organised' memory of all those known items. Correlations, associativity, sensitivity and likely causal relations are readily explored in that representation. Categorization rules can also be learned and imposed on such displays as 'overlays'. This methodolgy has close ties with the concepts and practices of principal component analysis, feature extraction, feature mapping and so on, but in fact embodies significant departures from previous practices. The nature and use of such reduced-dimension assosiative memory data-bases are illustrate with three sets of data, one of benchmark nature, another of the nature of real-world

powder form, is mixed with a plasticizing binder, dispensed as a thin layer on a carrier tape, and dried on the tape in a continuous process. The binder formulation and the casting parameters must be optimized to enable precise laser cutting and uniform densification during a subsequent sintering operation. Using sheet material so produced, a laser cuts successive layers of a part, as derived from a CAD model description. A material-handling robot uses a selective-area gripper to extract only the desired part outlines from the surrounding waste material, then stacks the slices to build the part. Finally, the "green" assemblies are postprocessed to burn out the plasticizing binder and densify the powder material.The result is a system that enables rapid manufacture of functional engineering components with arbitrarily complex internal and external geometries. By separating the process steps into a sheet-fabrication pre-process, a mechanical cut-and-stack assembly process, and a binder burn-out and densification post-process, the materials-processing aspects are kept virtually independent of the geometric formation process. This decoupling offers the potential to simultaneously optimize for both geometric precision and structural performance of parts thus produced. This decoupling also offers the prospect of extending the process to virtually any material available in sheet form, as well as the manufacture of components with functionally-graded materials. Characterization results of geometric and mechanical properties of alumina parts produced to date are reported.



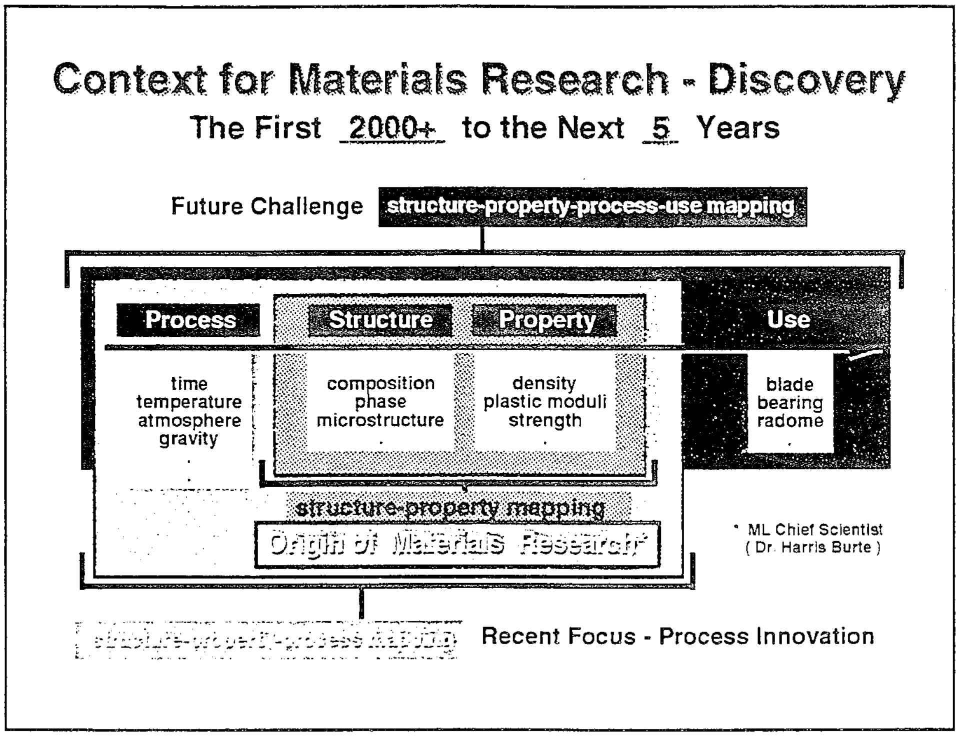
In 1994, a small group of scientists (England, Russia, Japan & the U.S.) gathered for the first time to explore and compare **new** *innovative* methods for the design of materials.

We are here today to continue that exploration . . . and for purposes of setting context there are two (2) perspectives I need to establish:

1) fundamental to **Materials Design** is the mapping of material structure, with properties, with processing parameters and use,

2) ultimately the goal is to improve research productivity by automating the process of discovering those mappings, i.e.,

Automated Materials Research on the M&P Information Highway



There is a saying, *" the more you know, the more you know what you don't know "* - when applied to materials design it may be said,

"as the growth in material complexity (monolithic alloys, fiber reinforced composites to multi or gradient materials) continues, our awareness of computational limits becomes ever more painfully apparent "

Worldwide efforts in Materials Research over the century, if not 2+ millinea, has at a minimum established a science of 'structure-property' mappings, but in spite of a science and attendant tools when considering 'structure-property-process' mappings it is apparent that we are already computationally bound, e.g.,

- **No one can afford the cost/time to generate phase diag. - thermodynamic data of ternary+ compounds**
- **FEM/FEA are, and for the foreseeable future remain, validation, not design tools.**

Materials & Process Challenge

"It is estimated that the amount of information in the world
(currently) doubles every 20 months"

William J. Frawley, Gregory Piatetsky-Shapiro, and Christopher J. Matheus
Knowledge Discovery in Databases: An Overview
AI Magazine, Fall 1992

Example: "It has been estimated that in 1965, a mechanic who understood about 500 pages of various repair manuals could fix just about any car on the road. Today, that same mechanic would need nearly 500,000 pages of manuals - equivalent to roughly 50 New York City telephone books"

National Center for Manufacturing Sciences, Focus, August 1992

NEED:

In addition to organizing available knowledge to avoid re-learning how to design, manufacture and repair existing technology,

we must *also* find ways to automate the organization of new knowledge.

In the Sep 95 issue of Scientific American (An issue dedicated to Information Technologies for the 21st Century), it was stated that,

" every 18 months microprocessors double (2X) in speed "

meanwhile information is also doubling **every 20 months in 1992** and at an increasing rate if you consider the car repair manual example (1965-1992) the average doubling was ~26 months.

As a world **awash in information** we are in desparate need of new, more efficient methods to ORGANIZE knowledge (existing and new), most importantly, Materials and Process knowledge because it is the principle driver for all scientific and engineering endeavors - and therein in our competitiveness.

Problem:

What might researchers do
to improve their productivity
and how (what methods) do we,
as scientists and engineers,
propose to address this problem?

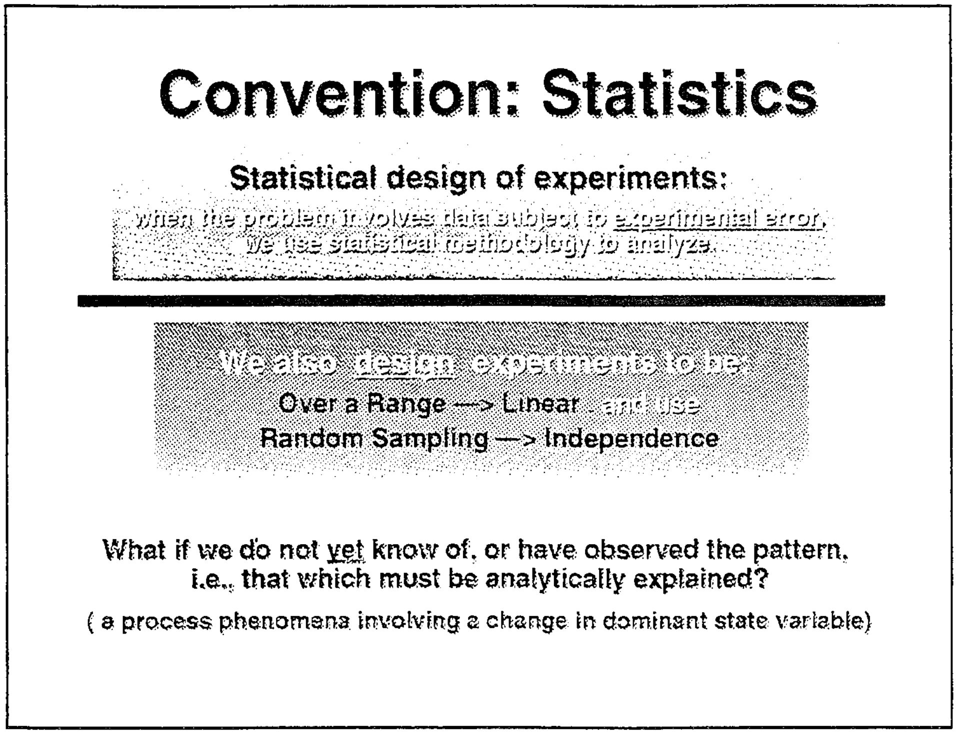
When considering the issue of **productivity** - most, if not all, of us think of 'manufacturing productivity'. It is clear that near term competitiveness depends largely, if not exclusively, on manufacturing productivity.

I believe the severity of the computational limits we are confronting in **Materials Research** and the central role materials and processing technology plays in manfacturing productivity - it is only a matter of time before comparative

measures of 'research productivity'

will begin to discriminate product technology leaders,

particularly in the 'high-tech' marketplace.



I am ***not*** suggesting the **conventional approach** which, from my view, is nothing more than statistics and require considerable 'tweeking' or human intervention, i.e.,statistical trial and error of **model development - validation cycle**.

Although these methods have and will continue to serve us well, we need more autonomous methods if we are to address the information explosion before us. Most recent materials development (TiAl) has resulted in up to 15 years from concept to adequate knowledge of properties, processing and failure mechanisms. We need to augment statistical methods to accelerate this cycle **10X**.

A History Lesson in
Scientific Discovery *

Oersted, had been looking for the connection between electricity and magnetism for thirteen (13) years, but his actual discovery was not the result of any deliberate planning. In 1820, at a lecture-table, he accidentally deflected a compass needle with an electric current.

Faraday, using Oersted's discovery, deliberately discovered electromagnetic induction (a dynamic relation) between an electric current and a magnetic field.

→ **Maxwell**, formulated Faraday's work into a precise mathematical theory of electromagnetics

* Source: J.D. Bernal, 'Science in History', Hawthorn, 1965

In the discovery of electro-magnetism, few of us remember Oersted, mainly because we focus our attention on the latter steps of the **'scientific method'**.

Aside from this example of the steps in the method and the importance of each. What is equally significant is the time it took Oersted to make his **discovery**.

i.e., In the 1800's, thirteen (13) years may have been acceptable, but today we have a vastly larger set of observations to consider - what can, and must, we do to improve our productivity ?

Discovery Methods

Bernal states, "The real difficulty in science is often not so much how to make the discovery but to know that one has made it"

(i.e., separating extraneous from significant effects).

Interestingly, Bernal later states, "Sooner or later, however, if enough people concentrate on the field, someone will be found sufficiently observant, sufficiently broadminded, and sufficiently critical or ignorant of orthodox theories to make **the discovery.**"

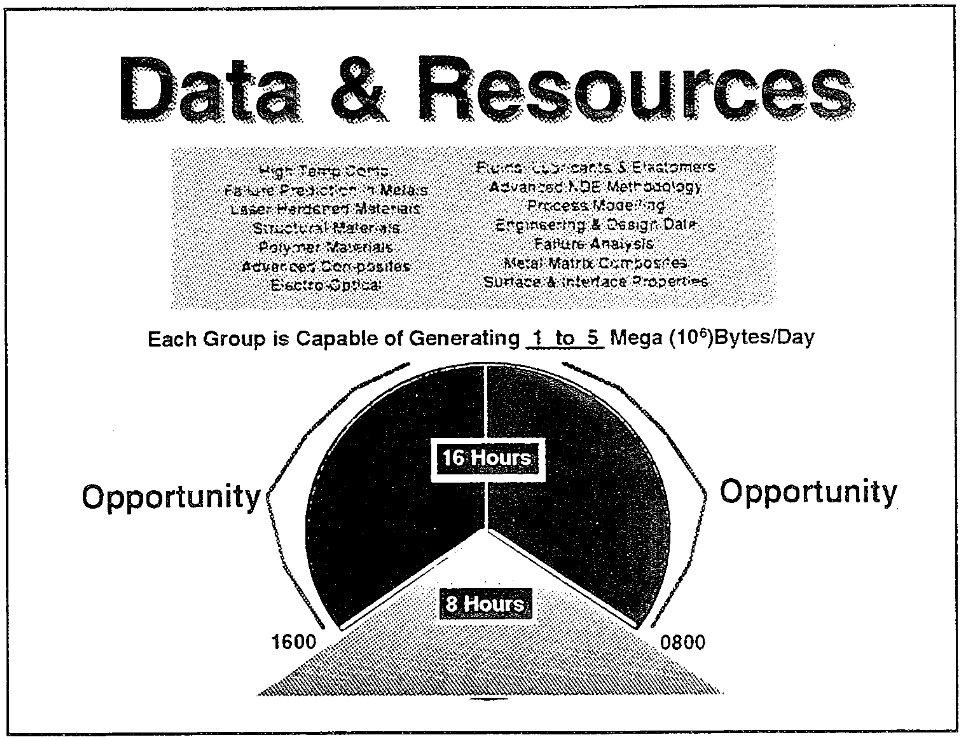
↓

suggest that COMPUTERS might make better RESEARCHERS than HUMANS.

Bernal, and apparently all of us, believed that the real difficulty in science is "separating extraneous from significant effects", i.e., the latter steps in the scientific method. And he goes on to say that discovery of the phenomena (pattern) will eventually occur.

I argue, for two (2) reasons, one of which he states, that more emphasis must placed on the first step in the method:

- **the rate of information explosion, inspite of continual advances in computing technology, is overwhelming us all,**
- **there is far more opportunity for computing technology to improve our productivity in the first step, as Bernel unknowingly suggests.**



Back-Up Chart

A closer look reveals the problem of info doubling

1990 (**effectively no electronic storage of experimental data**)

1995 (**nominal data acquisition is 1-5MBytes**) and scale of problem is to deal with 10X that amount by the turn of the century.

But there is also opportunity - if we able to develop methods, 'intelligent methods' which are

self-navigating schema generators

then we have 'after-hours' opportunity to commission our computing resources.

Concluding Thought - Why the concern?

As we enter the 21st Century . . . . " the rate at which organizations learn may become the only sustainable source of competitive advantage, especially in knowledge-intensive businesses."

Source:
Ray Stata, President & CEO
Analog Devices, Inc.
"Organizational Learning - Key to
Management Innovation"
Sloan Management Review
Spring, 1989, pp 63-74

It is my hope that I have conveyed sufficient background and perspective to adequately define

"the issues and definitions"

central to the theme of this session on

Innovations in Materials Design.

In closing I would like to leave you with this thought, I believe in a few short words, ... Mr Stata has captured the essence of why we are all gathered here today.

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7 September 1995.

Re: Proceedings of the Japan International SAMPE Symposium and Exhibition-4 (JISSE-4), "Innovations in Materials Design", to be held on September 25-28, 1995 in Tokyo, Japan.

Dear Professor Iwata,

Kindly find herewith two copies of the draft agreement for your consideration. Please go over it carefully and complete Point 4 (1,2 and 3) and Point 11 (4 only), and return one to this office with your comments/or criticisms. Once in my possession I will duly contact you to discuss and agree upon Point 11 (5) prior to establishing and sending you the agreement in final form, duly signed by our Managing Director, Drs. A.H.E. Frank.

I look forward to collaborating with you on this project for the *Journal of Alloys and Compounds* and trust to be hearing from you in the near future.

Yours sincerely,

Albert

Dr. Albert Fischer
Publishing Editor

Enc. ment.

cc: Dr. Steven Leclair

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1. Elsevier Science SA, hereinafter called the Publisher, undertakes to publish the Proceedings of the **Japan International SAMPE Symposium and Exhibition-4 (JISSE-4), "Innovations in Materials Design", to be held on September 25-28, 1995 in Tokyo, Japan.**

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3. The Proceedings will be edited by **S. Iwata and S. Leclair** who, for this special issue, will be named as Guest Editors of **Journal of Alloys and Compounds**. The name of the Guest Editors will be listed on the cover and title page of this special issue of **Journal of Alloys and Compounds.**

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Symposia Coordinator

S. Leclair
Symposia Coordinator

The Publisher:
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Dr. A.E.M.J. Fischer
Publishing Editor

Drs. A.H.E. Frank
Managing Director

cc: **Professor K.H.J. Buschow**

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3. Papers are not automatically accepted because they are part of a conference. The Guest-Editors have to check whether the author(s) have complied with all criticism raised by the referee. The Guest-Editor should feel free to reject inferior papers.

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The final decision of acceptance or rejection rests with the Editor-in-Chief of *JALCOM*. He communicates his decision to the Guest Editors as well as to the publisher.

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