US - RUSSIAN WORKSHOP

ON

COMPUTER SYNTHESIS OF STRUCTURE AND PROPERTIES OF ADVANCED COMPOSITES

May 10-11,1994

Russian Academy of Sciences
Main Building, Blue Hall
Moscow, Leninsky Ave.32A

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13. ABSTRACT *(Maximum 200 words)*

The objective of this workshop is to discuss the results of recent studies and experience accumulated by Russian and American scientists in the development of fundamental theoretical concepts, computer programs, methodology and techniques for numerical and experimental modeling of structure and mechanical properties of advanced composite materials, in particular with polymer matrices.

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FOREWORD

Advanced composites are dispersed heterogeneous bodies whose structure and properties depend not only on the properties of the matrix and filler, but also on various kinds of interaction between the components, on their mutual arrangement and volume ratio (the geometric factor), on the parameters of their processing and production (the technological factor), etc. These very important factors, whose change causes alteration of the properties of a composite material, must be considered both when predicting the mechanical behavior, and service life of already known composites as well as when developing new ones. The involved nature of the interacting parameters, makes theoretical treatments of these systems rather complex. This has led to the appearance of empirical and semiempirical "structural and mechanical" models which are not always satisfactory. Mathematical modeling is one way of solving technical problems encountered in the development and prediction of their mechanical behavior under diverse service conditions. For the construction of various mathematical models it is necessary to develop numerical and analytical methods.

The modeling approach is especially important for advanced polymer composite materials. When speaking of the merits and shortcomings of the theoretical approaches (including the molecular approach) used to describe the viscoelastic and mechanical behavior of polymer matrix, one has to keep in mind that they deal with macromolecules far from the surface. In a composite (a heterogeneous system), near a filler surface one must consider the interaction of separate parts of a macromolecule with the surface, which could affect its mobility and the relaxation time. The equation of dynamics of a macromolecule is thus modified and becomes nonlinear. This makes use of analytical methods impossible. Numerical methods become the best approach.

The theory of viscoelasticity is based on a function which completely characterizes the relaxation spectrum of a material. In principle from this one pivotal function all other material functions may be deduced. Although this seems rather straightforward in theory, in practice serious difficulties arise, to start with, in obtaining a reliable and unique relaxation spectrum from experimental measurements.

To describe the macromechanical properties of heterogeneous composites it is very important to model their micromechanical behavior, in particular, properties of interphase layers. For polymer composites the methods of molecular mechanics, molecular and Brownian dynamics seems to be very useful. During the past few years, the concept of a nanometric cluster modeling of condensed matter, mainly of real materials has been developed. However, when formulating it qualitatively, choice of the starting structure has to be made.

The objective of this workshop is to discuss the results of recent studies and experience accumulated by Russian and American scientists in the development of fundamental theoretical concepts, computer programs, methodology and techniques for numerical and experimental modeling of structure and mechanical properties of advanced composite materials, in particular with polymer matrices.

This workshop is also expected to contribute to the new contemporary concepts of "Computer mechanics and Nano-technology".

US - RUSSIAN WORKSHOP

ON

COMPUTER SYNTHESIS OF STRUCTURE AND PROPERTIES OF ADVANCED COMPOSITES

PROGRAM

Thuesday, May 10, 1994

9.00 - 9.30 Registration

OPENING REMARKS: 9.30 - 10.00 a.m.

Prof. Yuri G. Yanovsky

Dr. Iqbal Ahmad

Acad. Ivan F. Obraztsov

KEYNOTE LECTURES: 10.00 - 11.30

CHAIRMAN: Acad. Ivan F.Obraztsov

10.00 - 10.40 ***Some Theoretical and Model Approaches to Describing of Structure and Properties of Polymer Composites Materials*** - Yu.G. YANOVSKY,Institute of Applied Mechanics, Russian Academy of Sciences, Moscow, RUSSIA

10.40 - 11.20 ***Army Research in Advanced Polymeric Composites*** - A.CROWSON, U.S. Army Research Office, Materials Science Division, USA

11.20 - 12.00 - Coffee Break

Session A. *Theoretical Simulations*

CHAIRMAN: Prof. Yuri G.Yanovsky

12.00 - 12.40 ***Mathematical Method in the Analysis and Design of Composite Materials*** - R.V.KOHN, New York University,USA

12.40 - 13.10 ***On Statistical Theory of Brittle Crack Growth*** - A.I. MALKIN, Institute of Applied Mechanics, Russian Academy of Sciences, Moscow, RUSSIA

13.10 - 13.40 ***Ill-Posed Problems of Viscoelastic Media Equations from Mathemaical Point of View*** - Yu.A.BASISTOV, Institute of Applied Mechanics, Russian Academy of Sciences,Moscow,RUSSIA

13.40 - 15.00 Lunch

Session B. *Nano-Techological Approach in Modeling of Composite Structures*

CHAIRMAN: Dr.Vladimir S.Yushchenko

15.00 - 15.30 ***Computational investigation of the Influence of the Environment on Mechanical Properties of Solids. The Cluster Approximation*** - T.A.GOLUBINA*,V.D. KHAVRYUCHENKO**, A.I.MALKIN*,E.A.NIKITINA*and V.S.YUSHCHENKO*, Institute of Applied Mechanics, Russian Academy of Sciences, Moscow, RUSSIA*,Institute of of Surface Chemistry, Ukrainian Academy of Sciences, Kiev**

15.30 - 16.00 ***Theory of Viscoelasticity and its Application for Calculation of Relaxation Properties of Polymer Composites*** - V.N. V.N.POKROVSKY*, G.V.PYSHNOGRAY**and Yu.G. YANOVSKY***,Economics and Statistics Institute*,Moscow, Altai State Technical University,Barnaul**, Institute of Applied Mechanics,Russian Academy of Sciences,Moscow,RUSSIA

16.00 - 16.30 ***Immitation Modeling Methods of Interphase Layers Properties of Polymer Composite Materials*** - S.N.LEORA*, T.V.IVANOVA**, Yu.N.KARNET**,State University,St.Petersburg*,Institute of Applied Mechanics, Russian Academy of Sciences,Moscow,RUSSIA

16.30 - 17.00 *Critical Periodics in the Nucleus Properties and Problems of Composites Calculations* (information notice)
V.I.KUZMIN, State Institute of Radio Engineering and Automation, Moscow, RUSSIA

DINNER 19.00 -
GEORGIAN RESTAURANT "ARAGVI"

Wednesday, May 11, 1994

Session C. Computer Modeling of Strength Stress Properties of Composites

CHAIRMAN: Dr. A.CROWSON

9.30 - 10.10 *Computer Synthesis of Fiber Architecture and Properties of Textile Structural Composites* - Tsu-Wei CHOU, University of Delaware, USA

10.10 - 10.40 *Asymptotic Methods for Investigation of Impact- and Explosion- Induced Wave Processes* - A.I.MALKIN, Institute of Applied Mechanics,Academy of Sciences, Moscow, RUSSIA

10.40 - 11.20 *Experimentation and Modeling of Composite Materials* - Shun-chin CHOU, U.S.Army Research Laboratory, Watertown, USA

11.20 - 11.40 *Some Approaches to Modeling of Composites Mechanical Properties with Employment of Graphs Theory* - V.U.NOVIKOV, State Open University, Moscow, RUSSIA

11.40 - 12.00 Coffee Break

CHAIRMAN: Dr. Y.D.S.RAJAPAKSE

12.00 - 12.30 *On the Entropy Damage Accumulation Model of Composite Materials* - S.A.LOURIE, State Aviation Technical University, Moscow, Russia

12.30 - 13.10 ***Concurrent Engineering*** - H.T.HAHN, University of Calofornia, Los Angeles, USA

13.10 - 13.40 ***Progress in Computational Model by Finite Element Method of Viscoelastic Heterogeneous Continua Properties*** - A.N. VLASOV*, V.N.POTAPOV*,A.V.VORONIN**and Yu.G.YANOVSKY**,State Civil University*and Institute of Applied Mechanics**, Moscow, RUSSIA

13.40 - 15.00 Lunch

<u>Session D.</u> Advanced Composites Properties and Mechanical Behavior

CHAIRMAN: Prof. Tsu-Wei CHOU

15.00 - 15.40 ***Recent Advances in Mechanics of Composites*** - Y.D.S. RAJAPAKSE, Office of Naval Research,Arlington, USA

15.40 - 16.20 ***A New Constitutive Equation for Shape Memory Composites*** - A.A.MOWCHAN, State Aviation University,Moscow,RUSSIA

16.20 - 17.00 ***Elastically Tailored Composites Analysis and Testing*** - E.A. ARMANIOS, Georgia Institute of Technology, Georgia, USA

17.00 - 18.00 ***GENERAL DISCUSSION & CONCLUSION***

19.00 - 22.00 ***CULTURAL PROGRAM***

Thursday, May, 12, 1994

8.00 - 19.00	***TECHNICAL VISIT***
	Departure: 8.00 from Hotel Rossiya
9.30 - 12.00	***Technical visit to Scientific Industrial Company "Composite",*** Khat'kovo (80 kms outside of Moscow)
12.00 - 13.00	***Lunch***
14.30 - 16.30	***Cultural Program - Visit to Zagorsk (Sergiev Posad).*** **Zagorsk is the oldest seat of Russian Orthodox Patriarchy dating back to 11th Century.**
	Return: 19.00 to Hotel Rossiya

Friday, May 13, 1994

9.00 - 18.00	***TECHNICAL VISIT***
	Departure: 9.00 from Hotel Rossiya
10.00 - 12.30	***Technical visit to Moscow State Aviation Technical University***
12.30 - 13.30	***Lunch***
14.00 - 17.00	***Technical visit to Scientific-Technical Centre and Exibition of Machine Engineering Research Institute by A.A.Blagonravov of Russian Academy of Sciences***
	Return: 18.00 to Hotel Rossiya

ABSTRACTS

AND

BIOSKETCHES

CONTENTS

KEYNOTE LECTURES

SESSION A. Theoretical Simulations

SESSION B. Nano-Technological Approach in Modeling of Composite Structures

SESSION C. Computer Modeling of Strength - Stress Properties of Composites

SESSION D. Advanced Composites Properties and Mechanical Behavior

SOME THEORETICAL AND MODEL APPROACHES TO DESCRIBING OF STRUCTURE AND PROPERTIES OF POLYMER COMPOSITES MATERIALS

Yu.G.Yanovsky

Institute of Applied Mechanics of Russian Academy of Sciences

The use of organic (polymer) matrix composites for different industrial application actively started about thirty years ago. Comparing with traditional industrial materials there are various advantages that make such composites more attractive for use in different kind of branches, in particular for aerospace, marine, automobile etc. applications. Polymer composites have excellent corrosion resistance which reduces maintenance, low thermal conductivity, they are non-magnetic. Composite materials can be modified to become radar absorbing thus enhancing their stealth capability. Advanced composites, featuring continuous reinforcing fibers in polymer matrixes, have demonstrated their ability to provide reliable weight saving structures for various applications. These can offer weight reduction of up to 25-50% in comparison to aluminum and steel.

It is no longer a question of whether advanced composites will be used in future, but rather how to apply them more effectively. For modern polymer composite materials, which has a history more than 25 years, maximal experience has been accumulated in aerospace applications. Since aluminum has been used as the base-line material intuition and design judgment have been strongly influenced by the aluminum experience.

Fundamental difference between metallic, particularly aluminum, and polymer composite materials arise from: homogeneity versus heterogeneity and inner microstructure, isotropy versus macro- and microscopic anisotropy; elasticity versus pseudo-elasticity and microviscoelasticity; linear behavior versus non-linear behavior etc.

This paper will focus on new developments in the area of computer synthesis (design) of reinforce polymer composite materials.

For composite materials physico-mathematical models provide basic information to guide design.

The first estimates of the elastic properties of composite materials from model viewpoint were undertaken on the basis of the well known phenomenological models advanced by Voigt and Reuss. These models used the most famous rule of composite materials is the rule of mixtures. It state that a composite property as a whole is a linear function (the additivity principle) of the volume fractions of the constituents. In a very simple variant, the behavior of a two-component composite is modeled by using two Voigt or Reuss elements connected in parallel or in consecutive. Models predicting not only elastic but also viscoelastic properties were the next step in this direction. Here we must note first of all the model advanced by Takayanagi.

Analysis of phenomenological models of the above types and similar ones and verification of their adequacy has shown that at present it is difficult to recommend universal models for calculating the properties of the composites within a broad range of the change of the filler concentration and the conditions of deformation.

To be more predictive the phenomenological approaches and models need to be modified. A useful micromechanical framework can be built to model. If there is no micromechanical framework it is nearly impossible to establish quantitatively the contribution of the constituents and the interface. Empirical approach alone is not adequate. A quantitative description is important in both absolute and relative terms. It is not enough to say that an interface is good or bed. It is more important to know haw many Pascal's represent a good interfacial strength and understand what is a filler or matrix dominated behavior. With framework of micromechanics one may be able to clarify observation with quantitative precision.

It is widely known that the lack of a strictly physical substantiation of the phenomenological models was one of the main causes of the failure to describe the properties of polymer composites observed experimentally. From this standpoint, a three-element structural model can be considered more systematic and improved in this for composites. It considers not only the properties of the filler and matrix, but also the intermediate layer appearing on the boundary of the filler particles (interphase layer) and having specific properties that differ from those of the matrix.

Direct experimental results obtained by birefringence and photoelasticity techniques point to the physical substantiation of the existence of an interphase layer.

Summarized the stated above the framework of the nanotechnological ideology could be written in an appropriate for computer simulation form (see Table).

Table

Ideology of Program

"Computer synthesis of Structure and Properties of Advanced Polymer Composites"

Atomic and Molecular (Nano)-Level	Modeling of surfaces and potentials of interaction of separate phases of heterogeneous composite and dynamics of its variation by stresses and temperature (quantum approach)
Macromolecular Level	Modeling of structure, mechanical and relaxation properties of interphase layers of composites by the statistic and molecular physics and molecular mechanics methods.

Micro-Level	Modeling of structure and mechanical properties of periodicity element
Macro-Level	Modeling of mechanical properties of structure representative element, modeling of effective properties of composite media
Theoretical and Experimental Verification of Modeling and Calculation Adequacy	Test experimental investigation and mathematical correction on the base of the adaptive program packet.

The viscoelastic behavior of a deformed polymer system is a widely known experimental fact. From a physical viewpoint, such behavior is generally explained either by the existence of an internal structure, or by the heterogeneous structure of the material, or by both simultaneously. The problem of describing the properties of such systems within a broad range of variation of the magnitudes and laws of deformation, the rates (or frequencies) of deformation and other parameters generally consist in determining the time dependences of the mechanical characteristics, i.e. the material functions reflecting the viscoelastic mechanism of the behavior of these systems. The ability of a viscoelastic body to resist a mechanical load and react thereto adequately is determined by a very important characteristic of a system, viz. the relaxation time. For real viscoelastic media that generally have a rather complicated internal structure is quite natural to introduce a distribution function of the relaxation time, viz. the relaxation spectrum.

The material functions can be obtain from experimental data rather simply but a calculation of the relaxation spectrum from above functions is inverse and ill-posed problem.

Smoothing techniques based on regularization and the maximum entropy methods have been proposed recently to determine numerically the relaxation spectra of viscoelastic media from experimentally obtained material functions through the solution of Fredholm integral equations of the first kind. However, these methods show serious shortcomings in applications. We propose a new and completely different numerical technique based on the minimax method.

A large number of phenomenological relations were proposed to describe the viscoelastic behavior of polymer bodies. However a phenomenological description does not disclose the microscopic nature of materials. The considerable progress

achieved in recent years in the field of the theoretical physics of polymers also determined the achievements in the structural and molecular theory of polymers. An equation of the dynamics of a macromolecule in the foundation on which a structural theory of equilibrium and nonequilibrium relaxation phenomena can be constructed in a single molecule approximation for polymer systems. The possibility of introduction the single molecular approach is based in essence on an important experimental fact. The quantities showing the behavior of a polymer system depend in a clear and unambiguous way on the length of a macromolecule.
When speaking of the merits and shortcomings of the theoretical approaches used to description the viscoelastic behavior of polymer we must have in view that we dealt with macromolecules far from the surface. Near a surface one must consider the interaction of separate parts of a macromolecule with the surface. Here we should expect changes in the mobility of a macromolecule and the relaxation time. The equation of dynamics of a macromolecule is modified and becomes non-linear. Analytical appraisal of the results becomes impossible. Numerical method of studying come to the forefront. For this purpose, the equation of dynamics of a macromolecule must be written in a form, firstly, convenient for the modification associated with the presence of surface forces, and, secondly, convenient for performing numerical calculations, because in this case one has to work with a non-linear system of equations. One can thus state that the use of the method of Brownian and Molecular dynamics in an essential and important stage in studying the mechanism of the viscoelasticity of polymer composites in boundary layers.
Quantum chemical approach to model of the chemical activity, properties and interaction between the surface of a filler and a composite matrix is very important stage along this path too.
Quantum chemical approach has some very important advantages. Firstly, the computation of some physico-mechanical characteristics on atom level, namely, the calculated force of atom-atom interaction, the bonds strength allows to obtain the values of material parameters for continual model and to understand their sense and nature. Secondly, the energy, the electron and space structure of substance, some interphase layers singularity one can calculated more precisely than in classic molecular dynamic version. As one known molecular dynamics method are usually limited by the quality at the interatomic pair potential functions. Thirdly, the quantum chemical computation allows to determine the frequencies of phonon spectrum and the macroscopic elastic constants. Using that method the dynamic model of real substance can be calculated together with its compressibility and moduli of elasticity.
It is convenient to employ the method of finite elements to calculate the stressed state of the element periodicity and representative element of media with periodical or non-periodical structure. An object-oriented finite element programming seems to be more perspective along this path.
It has been obvious for many years that improving finite element code modularity demands a proper organization of the data. Many authors have done their best to improve data management in a Fortran context. The adequacy of the concepts of object-oriented programming for an efficient and understandable organization of the data in numerical analysis codes has only been studied recently. The

fundamental principles of the application of object-oriented techniques to the finite element method were developed by T.Zimmerman (1992). The careful design of this program resulted in a highly modular, easily understandable and extendable code. These qualities were based on data encapsulation - an object is a variable supplied with a set a protected data (its attributes) that allow it to perform operations (its methods) and to manage these operations really autonomously; class inheritance - the various types of objects (the classes) are organized in a simple and telling tree-like structure (the hierarchy) which avoids code duplications; non-anticipation - the methods of an object can be performed at any place in the program, without the constraining sequence of operations of classical codes.

An object-oriented approach was employed in the new finite-elements program pocket developed for calculation of strength-stress elastic, elasto-plastic and viscoelastic behavior of polymer composites with interface layers.

CONCLUSION

1. The structure-mechanical model of heterogeneous polymer composite with interphase layers was employed.
2. Based on this model the new approaches and computational methods of studying of strength-stress and mechanical behavior of composites including the non-linear viscoelastic response under deformation has been developed.
3. Program of calculation contains the stages which are modeling advanced composites properties at the different structure organization levels: nano- and molecular-level (quantum mechanical methods); macromolecular-level (Brownian and Molecular dynamics methods); micro-level (object-oriented finite elements method, including the viscoelastic response), macro-level (specialized pockets of adaptive computer programs).
4. Present approach is a base of nano-technological principle of the heterogeneous advanced polymer composites structure and properties constructing.

BIOSKETCH

Yuri G.YANOVSKY

Prof., Dr.Sc. Yu.G.Yanovsky is a Head of Department of Mechanics of Structured and Heterogeneous Continua and Deputy Director of Institute of Applied Mechanics of Russian Academy of Sciences.

Yu.G.Yanovsky graduated from Department of Thermophysics of Moscow Power Engineering Institute. He received his Ph.D. degree in 1965 and Doctor of Sciences degree in 1973 from Department of Polymer Rheology of Institute of Petrochemical Synthesis of the USSR Academy of Sciences.

More than 300 papers, two monographs and series of books have been puslished by Yu.G.Yanovsky.

He is the member of British Society of Rheology, and American Society of Rheology, active member of the New York Academy of Sciences, the member of Editorial Board of Polymer Testing Journal (Elsevier), the Editor in Chief of Journal Structured and Heterogeneous Continua (New York), Chairman of International Symposia of Structured and Heterogeneous Continua. He received a number of awards including the NATO Research Award (1992), Russian Found of Foundamental Investigation Award (1993), Award for Outstanding Scientist of Russia (1994), International Science and Technology Award (1994).

His area of interests include theoretical and applied rheology, mechanics of composites, numerical simulation.

ARMY RESEARCH IN ADVANCED POLYMERIC COMPOSITES

Andrew Crowson

Materials Science Division
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The replacement of heavier metallic materials with advanced polymeric matrix composites of equal or improved structural integrity and considerable weight savings offers significant opportunities for the Army in a variety of applications. However, their use will require an improved understanding of the relationships between processing, microstructure, properties and performance derived therefrom. In order to achieve this knowledge, fundamental research is being supported within the Materials Science and Engineering Science Divisions at the Army Research Office (ARO). Program areas currently being addressed include mechanical behavior, degradation and reactivity, synthesis and processing, smart structures, and manufacturing science. In this presentation each of these areas will be described with examples of current programs being supported at ARO.

BIOSKETCH

Andrew CROWSON

Dr. Crowson received his B.S. degree in Chemistry in 1966 and his PhD in Physical Chemistry in 1971. He has worked as a materials engineer at U.S. Army laboratories conducting research in such areas as activated sintering of powder metallurgy materials, tungsten alloy processing, alloy development, powder metallurgy forging, chemical vapor deposition, physical vapor deposition, and welding. Dr. Crowson joined the Army Research Office (ARO) in 1984 where he served as the Chief of the Synthesis and Processing of Materials Branch and Associate Director of the Materials Science Division. He became the Director of the Materials science Division at ARO in 1989. As the Director, he is responsible for formulating, directing and administering the Army's extramural basic research program in materials science. In addition, Dr. Crowson is an Adjunct Professor at Duke University where he is conducting research in polymers and polymer composites. He has also served an active role in the following societies: American Society for Metals; Materials Research Society; The Minerals, Metals and Materials Society; American Welding Society; American Powder Metallurgy Institute (Editorial Board); American Ceramic Society.

MATHEMATICAL METHODS IN THE ANALYSIS AND DESIGN OF COMPOSITE MATERIALS

Robert V. Kohn

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The macroscopic properties of a composite depend in a subtle way upon the microscopic geometry. It is therefore natural to look for microstructures with advantageous - perhaps even extremal - effective behavior. There has been a lot of recent progress in this area, including an identification of the "most rigid" and "most compliant" composites achievable by mixing two materials in specified proportion. Key tools include the "translation method" for bounding effective moduli, and "sequential lamination" as a scheme for generating optimal microstructures.

A similar issue arises in the modeling of shape-memory alloys. These materials owe their special properties to a martensitic phase transformation. Martensite is actually a mixture of different crystallographic variants, so it may be viewed as a composite material. The microstructure varies with the loads and boundary conditions, driven by elastic energy minimization. Mathematical methods used in the analysis of extremal composites are also helping explain the details of shape-memory behavior.

BIOSKETCH

Robert V. KOHN

Professor Robert V. Koch received AB (1974) and Ph.D.(1979) degrees from Harvard and Princeton Universities respectively. He has since received the prestigious Sloan Foundation Fellowship, NSF Fellowships, and Charlotte Proctor Memorial Fellowship, among others. He has held many industrial and academic positions and is currently Professor and Chairman of the Mathematics Department, Courant Institute at the New York University.

He has made significant contributions and published extensively on fundamental and mathematical issues related to materials microstructure, composites and structural optimization.

Professor Kohn has trained many outstanding young mathematicians, lectured and collaborated with scientists worldwide.

He has served on the Editorial Boards of Achives for Rational Mechanics and Analysis, Proceedings of Royal Society of Edinburg, Journal of Nonlinear Science, and Progress in Nonlinear Differential Equations and Their Applications.

ON STATISTICAL THEORY OF BRITTLE CRACK GROWTH

Alex I. Malkin

Institute of Applied Mechanics, Moscow, Russia.

INTRODUCTION

At the present time there are no commonly accepted notions about mechanisms of brittle and quasi-brittle crack growth in solids. It seems to be associated not only with a host of physical mechanisms of growth but also with an imperfection of the existing system of mathematical models. Within the limits of this report it is impossible to present the growth models review of any completeness. Mention should be made of physically meaningful continual models (Barenblatt *et* al), direct computer simulation by molecular dynamics method (Yushchenko and Shchukin, Paskin, Dienes and many other investigators) and a host of dislocation models reviewed, for example, in the monograph by Vladimirov.

The vast majority of brittle crack models deals with one-dimensional rectilinear cracks and treats the growth as a sequential dissociation of interatomic bonds. These models are based on a series of experimentally found regularities such as well-known Zhurkov longevity equation. The last is taken as evidence of thermofluctuation nature of crack growth at the initial stage of fracture.

It has been known that the thermofluctuation growth of precritical cracks at brittle and quasi-brittle fracture shows the spasmodic stochastic process characteristics. Prolonged intervals of static behavior of crack are alternated with fast moving of the crack tip into a new position. The distance between the latter and the former positions of a crack tip therewith is much more than interatomic distance in a solid. By this it meant that notions of non-correlated decohesion of interatomic bonds are not true.

Theoretical "ab initio" description of stochastic growing of brittle crack is run into problems by the need of taking into account the cooperative processes in precracked zone. Therefore the development of phenomenological theory based on experimentally observed regularities as well as on the theoretical reasons of extremely common character, is of particular interest.

Here we suggest the scheme for the construction of the statistical 2-D theory of brittle crack growth. The problem considered is concerned with several phenomenological models. No consideration has been given to the detailed description of processes at the precracked zone.

GENERAL MODEL FORMULATION

Let us assume the crack at macroscopic scale can be represented by the chain of vectors $\vec{l}_i$ and hence specified by the ordered set $\mathcal{L}_n = \{\vec{l}_i, i = 0, ..., n\}$. The elementary growth act is the addition of random vector $\vec{l}_{n+1}$ to the crack tip at the arbitrary random instant of time. In order to formulate the kinetic model one should construct the probability density of $\mathcal{L}_n \rightarrow \mathcal{L}_{n+1}$ transition as a function of process prehistory.

It is clear that this problem should be solved at the intermediate and microscopic scales.

There are two causes that should be recognised for the accidental nature of crack growth. That is the random arrangement of atoms (or structure defects) and the accidental occupancy of localised vibrational modes at the precracked zone. At given atomic configuration the probability density of growth act delay time may be taken in the exponential form. This assumption is justified by the rarity of growth events at the time scale of atomic oscillations.

We shall accept that the details of the precracked zone microstructure are not very significant, so that average delay time τ_d depends on a limited number of macroparameters. It is natural to restrict our consideration to the minimal set of variables and parameters. Then the average delay time corresponding to the defined growth act $\vec{l}$ depends only on $\vec{l}$, temperature and local stresses. We suppose the average delay time to be an Arrenius function with the activation energy linear - dependent on stresses.

The required invariance of the average delay time in respect to coordinate system choice imposes the essential restrictions on the form of this function. In the isotropic medium the average delay time may be written as

$$\tau_d(\vec{l}|\mathcal{L}_n) = \tau_0 \exp\left\{\frac{E_0 - v_1(l)\sigma_{ii} - v_2(l)n_i n_k \sigma_{ik}}{kT}\right\} \tag{1}$$

where σ_{ik} are the components of stress tensor, $l = |\vec{l}|, \vec{n} = \vec{l}/l, v_1(l)$ and $v_2(l)$ are some functions of the adding microcrack length, τ_o and E_o are assumed to be constant. Expression (1) is a general form of scalar $\tau_d(\vec{l}|\mathcal{L}_n)$ fulfilling the requirements imposed.

The stress tensor entering the equation (1) depends on coordinates of microcrack nucleation point. In this connection two widely used scenarios of the crack growth should be recognised. In line with the first (microcrack addition) scenario a microcrack arises from some defect at the point $\vec{l}$ and then is added to the initial crack tip. By the second (direct decohesion) scenario a microcrack arises from the initial crack tip and then grows till stopping at the point $\vec{l}$. In that case we assume the microcrack to originate at the point $\vec{æ} = æ\,\vec{n}$ with $æ \ll < l >$. Here æ is the effective curvature at the crack tip.

Stress distribution near a crack tip can be evaluated under the assumption that linear fracture mechanics is applicable to the precracked zone description. For the case of isotropic medium it may be written

$$\sigma_{ik} \simeq \frac{K_I(\mathcal{L}_n)}{\sqrt{2\pi\, æ}} \quad f_{ik}^{(I)}(\vec{n}) + \frac{K_{II}(\mathcal{L}_n)}{\sqrt{2\pi\, æ}} \quad f_{ik}^{(II)}(\vec{n}) \tag{2}$$

where stress intensity factors (SIF) depend on the initial crack configuration. Expression (2) corresponds to scenario of direct decohesion at the crack tip. However, it is easy to check that (with minor reservation) general form $\tau_d(\vec{l}|\mathcal{L}_n)$ does not depend on the scenario of crack growth. Notice that substitution of æ does not add the number of empirical parameters as æ and $v_j(l)$ enter into eq. (1) in the form $v_j(l)/\sqrt{æ}$.

It is believed that postulated eq. (1) corresponds to some approximation of the average field type. If this is the case the reasonable interpretation of the equation (1) may be provided. This interpretation is based on the supposition that local stresses at the point of microcrack nucleation have a special form

$$s_{ik} = q_1(l)\sigma_{ik} + q_2(l)n_i n_k \sigma_{ik} \tag{3}$$

where σ_{ik} is macrostress tensor (2) (σ_{ik} proposed to be the result of the averaging over the statistical ensemble), functions $q_1(l)$ and $q_2(l)$ account for the excessive stresses caused by the structural defects. These functions should be defined at the intermediate scale. The stress-induced reduction of the activation energy of microcrack nucleation is defined by activation volumes $v_1^{(0)}$ and $v_2^{(0)}$ which does not depend on l. Activation volumes are proposed to be the material constants and should be calculated at microscale. It is easy to check that each $v_j(l)$ in eq. (1) is the bilinear form of $v_i^{(0)}$ and $g_k(l)$. Needless to say that the latter functions are difficult if not impossible to obtain theoretically.

We shall introduce the state density function $\Omega(\vec{l})$. This function represents the number of microscopic distinguishable states which lead to the elementary growth act for a vector $\vec{l}$. Let us consider the virtual set of the growth acts. Clearly the growth act to be realized has a minimal random delay time $t(\vec{l})$. Therefore non-conditional distribution of growth act delay time is defined as the distribution of random value

$$t_m = \min_{\{\vec{l}\}} \ t(\vec{l}) \tag{4}$$

where the contribution from $t(\vec{l})$ should be taken into account with a weight $\Omega(\vec{l})$. Random value (4) probability distribution is also exponential. The average value $< t_m >$ is determined from the expression

$$< t_m >^{-1} \equiv Z = \int_{\{\vec{l}\}} \frac{\Omega(\vec{l})d\vec{l}}{\tau_d(\vec{l}|\mathcal{L}_n)}. \tag{5}$$

where $\tau_d(\vec{l}|\mathcal{L}_n)$ is given by expressions (1), (2). As a result, a posteriori distribution of random vectors $\vec{l}$ is

$$w(\vec{l}|\mathcal{L}_n) = \frac{\Omega(\vec{l})}{Z\tau_d(\vec{l}|\mathcal{L}_n)} \tag{6}$$

The relations presented completely determine a set of crack growth models when the functions $v_j(l)$ and state density function $\Omega(\vec{l})$ are prescribed.

Note that if state density function does not depend on stresses, then it will be the function on microcrack length but not the direction, $\Omega \equiv \Omega(l)$. In that case $\Omega(l)$ represents only the structure properties of the solid at intermediate scale. The last conclusion is true for isotropic media.

SOME PROPERTIES OF ADDING MICROCRACKS DISTRIBUTION

Geometric characteristics of 2-D cracks contour are defined by function (6). The analysis of this function leads to some restrictions on $v_j(l)$. In particular, the typical crack contour form may by obtained with the proviso that

$$v_1(l) > 0, \qquad -2v_1(l) < v_2(l) < -v_1(l)/4 \tag{7}$$

Let us assume that the initial crack is close to rectilinear mode I one, so that $K_{II}/K_I \ll 1$. If inequalities (7) are fulfilled, then the most probable direction of growth will be close to the direction of the initial crack. The conditional probability density of growth direction becomes the simple form

$$w(\theta | l, \mathcal{L}_n) = \frac{1}{\sqrt{2\pi < \delta\theta^2 >}} e^{\frac{(\theta-\theta_m)^2}{2<\delta\theta^2>}}$$

$$\theta_m = -2\frac{K_{II}}{K_I}, \qquad < \delta\theta^2 > = \frac{4kT\sqrt{2\pi\ \ae}}{v_- K_I(\mathcal{L}_n)}$$

where $v_- = 2v_1(l) - v_2(l)$ Basing on the need to obtain the correct expression for specimen lifetime (i.e. Zhurkov longevity equation) one can conclude that microcrack length dependence of v_j is bound to be smooth. More precisely, v_1 and v_2 variation with microcrack length must be small for the range contributing significantly to the integral (5). An alternate possibility consists of a special definition of functions $v_j(l)$ and $\Omega(l)$. This possibility seems to be highly improbable.

By these means the v_j dependence on the adding microcrack length should be neglected at least at the initial stage of crack growth. It is therefore concluded that the microcrack length and direction are independent random values. As a result, the distribution density of microcrack length (6) may by rewritten as

$$w(l|\mathcal{L}_n) = w(l) = \frac{2\pi l \Omega(l)}{\mathcal{N}}, \qquad \mathcal{N} = 2\pi \int_0^\infty \Omega(l) l dl \tag{9}$$

and does not depend on process prehistory. The first order correction to the most probable microcrack length l_o is represented by expression

$$\delta l \simeq \frac{\mathcal{N}^2}{(2\pi l_0)^3 \Omega^2(l_0) kT} \frac{K_I}{\sqrt{2\pi\ \ae}} l_0 \frac{dv_+}{dl}\bigg|_{l=l_0}$$

where $v_+ = 2v_1 + v_2$ and derivation dv_+/dl appears to be always positive. The condition for formula (9) validity may be defined as $\delta l/l_0 \ll 1$.

GENERAL KINETIC EQUATION

Within the limits of statistical approach it is natural to describe the crack growth by the probability density of transition from the initial state $\mathcal{L}_o$ to the state $\mathcal{L}_n$ in a time t . We shall denote this function by $V(\mathcal{L}_n, t)$. Based on the suppositions above it is not difficult to obtain the basic equation in $V(\mathcal{L}_n, t)$

$$\frac{\partial V(\mathcal{L}_n,t)}{\partial t} = -Z(\mathcal{L}_n)V(\mathcal{L}_n,t) + \frac{\Omega(l_n)(1-\delta_{0n})}{\tau_d(\vec{l}_n|\mathcal{L}_{n-1})}V(\mathcal{L}_{n-1},t) \qquad n = 0,1,... \tag{10}$$

The initial condition for eq. (10) is

$$V(\mathcal{L}_n, 0) = \delta_{0n}\delta(\mathcal{L}_0, \mathcal{L}_0^{(0)}) \tag{11}$$

Here δ_{on} is Kronecker delta, $\delta(\mathcal{L}_o, \mathcal{L}_o^{(o)})$ is delta-function, $\mathcal{L}_o^{(o)}$ is the prescribed initial crack contour.

To solve the initial value problem (10),(11), SIF at every growth step should be known . Analytical approach is possible only in the small-angle approximation. Here we shall restrict our consideration to the more simple case of rectilinear crack growth.

RECTILINEAR GROWTH APPROXIMATION

Let us consider near-the-surface crack in a semi-infinite specimen (i.e. in a half-plane). One-dimensional approximation of rectilinear growth corresponds to the limit $K_{II} \to 0$, $< \delta\theta^2 > \to 0$. Consequently, the conditional distribution (8) transforms into delta-function, and crack configuration is characterized by the unique parameter - the length L. If the crack contour is normal to the specimen boundary then SIF $K_I \simeq 1,12\sqrt{\pi L}\sigma_\infty$.

Distribution density of rectilinear crack length should be introduced as follows:

$$V_r(L,t) = \sum_{n=0}^{\infty} \int d\mathcal{L}_n dL_y \delta(\vec{L} - \sum_{i=0}^{n} \vec{l}_i) V(\mathcal{L}_n, t) \tag{12}$$

where $d\mathcal{L}_n = \prod_{i=0}^{n} d\vec{l}_i$, $\vec{l}_o \equiv \vec{L}_o$ is a vector assigning the initial crack tip location. In order to obtain the equation in $V_r(L,t)$, one should multiply eq. (10) by $\delta(\vec{L} - \sum_{i=0}^{n} \vec{l}_i)$, integrate the product over $d\mathcal{L}_n dL_y$ and then summarize the result over all n considering $V(\mathcal{L}_n, t) \equiv 0$ for $n < 0$. In consequence of this procedure we have

$$\begin{aligned} \frac{\partial V_r(L,\tau)}{\partial \tau} = &- e^{\beta\sqrt{L/L_o}}\left(\frac{L}{L_0}\right)^{-1/4} V_r + \\ &+ \int_{L_o}^{L} dL' w(L-L') e^{\beta\sqrt{L'/L_o}}\left(\frac{L'}{L_0}\right)^{-1/4} V_r(L',\tau) \end{aligned} \tag{13}$$

with the initial condition

$$V_r(L,0) = \delta_+(L - L_0)$$

Here the dimensionless variable τ and parameter β are given by

$$\tau = \frac{2N}{\tau_o} t \sqrt{\frac{kT}{2,24\pi v\_\sigma_\infty}} \left(\frac{L_o}{2\varkappa}\right)^{-\frac{1}{4}} e^{-\frac{U}{kT}}$$

and

$$\beta = \frac{1,12 v_{+} \sigma_{\infty}}{kT} \sqrt{\frac{L_o}{2\,æ}}$$

Numerical solution of eq. (13) should not present any essential difficulties. As for the analytical studies, there is a more convenient way of treatment. This way is based on the so-called diffusion model.

DIFFUSION MODEL OF RECTILINEAR GROWTH

Equation (13) can be reduced approximately to the more readily solved partial differential equation. This equation may be obtained in the usual way when the major contribution to the integral term in eq. (13) is given by a small range near the upper limit. It can be shown that the necessary condition for the diffusion model validity is

$$< l > \ll \frac{kT\sqrt{2\pi\, æ}}{v_{+}\sigma_{\infty}}$$

The diffusion model equation of rectilinear crack growth takes the form

$$\frac{\partial V_r}{\partial \tau} = - < l > \frac{\partial}{\partial L} e^{\beta\sqrt{L/L_o}} \left(\frac{L}{L_0}\right)^{-1/4} V_r + \frac{< e^2 >}{2} \frac{\partial^2}{\partial L^2} e^{\beta\sqrt{L/L_o}} \left(\frac{L}{L_0}\right)^{-1/4} V_r \quad (14)$$

It is clear that eq.(14) represents the crack growth process at the crude scales of length and time. The results of the diffusion model are meaningful when the growth observation time interval is considerably larger than the growth elementary act expectation.

GROWTH KINETICS IN THE DIFFUSION MODEL

It is convenient to conduct growth kinetics consideration by the use of the equation in the integral distribution function $U'(V_r = \partial U/\partial L)$. Substitution $x = -1 + L/L_o$, $\tau \rightarrow < l > \tau/L_o$ leads to the following form of this equation:

$$\frac{\partial U}{\partial \tau} = -e^{\beta\sqrt{1+x}}(1+x)^{-1/4}\frac{\partial U}{\partial x} + D\frac{\partial}{\partial x} e^{\beta\sqrt{1+x}}(1+x)^{-1/4}\frac{\partial U}{\partial x} \quad (15)$$

where $D = < l^2 > /2 < l > L_o$.

The initial and boundary conditions for U are

$$\begin{aligned} &U(x,0) = 1, \quad x > 0 \\ &U(0,\tau) = 0, \quad U(\infty,\tau) = 1, \quad \tau > 0 \end{aligned} \quad (16)$$

The solution of boundary-value problem (16),(17) can be obtained by numerical simulation only. However, if $D \gg 1$, the approximate solution is constractible. This solution is represented by the asymptotic expansion over small D which is uniformly suitable at a wide range of independent variables.

Some notions of the crack growth kinetics can be gained from the first statistical moments. The calculations were carried out by the use of approximate solution. In the most interesting case $\beta \gg 1$, for the dimensionless average crack length $1+ < x >$ and dispersion $< \delta x^2 >$ we obtained the following expressions

$$\begin{aligned} 1+ < x > &= \frac{1}{\beta^2} \ln^2 \frac{\beta(\tau_* - \tau)}{2} \left[1 + O(\frac{1}{\beta})\right] \\ < \delta x^2 > &= \frac{4De^{-2\beta}}{\beta^5 (\tau_* - \tau)^2} \ln^2 \frac{\beta(\tau_* - \tau)}{e^{-\beta}} + \ldots \end{aligned} \tag{17}$$

where

$$\tau_* = \frac{1}{\beta} e^{-\beta} \left[1 + \frac{3}{2\beta} + O\left(\frac{1}{\beta^2}\right)\right]$$

Expressions (17) are the dominant parts of the moments expansion over small D.

It should be recalled that the considered model is suitable for initial stage of the crack growth. Therefore, expressions (17) *do not* describe the growth at the $\tau \to \tau_*$ limit. The crack tip tends to infinity at the finite instant of time is due to the neglecting of growth elementary act duration.

It is of interest that the crack length dispersion shows an extremely rapid increasing. The ratio of distribution half-width to average length diverges as $(\tau_* - \tau) \ln^{-1} (\tau_* - \tau)$.

CONCLUSION

Here we have tried to formulate the phenomenological approach to the statistical description of brittle crack growth. We discussed the limiting case of an extremely localized growth. Furthermore, our consideration was restricted to the minimal number of statistical degrees of freedom. The growth elementary act was assumed to be defined by geometrical parameters of adding microcrack only.

Apparently, the suppositions used are rather limiting for real crack growth processes. However, the number of generalisations is possible by the method given above without essential modifications. This is particularly true for substitution of added statistical variables which specify the growth elementary act. It is desirable that the method which is under discussion, can be used for the construction of more realistic statistical models.

BIOSKETCH

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ILL POSED PROBLEMS OF VISCOELASTIC MEDIA EQUATIONS FROM MATHEMATICAL POINT OF VIEW

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The linear theory of viscoelasticity is based on one function which completely characterizes the material, the relaxation spectrum. In principle, from this one pivotal function all other material functions may be deduced. Although this seems rather straightforward in theory, in practice serious difficulties arise, to start with in obtaining a reliable and unique relaxation spectrum from experimental measurements.

The difficulties encountered are two fold. Firstly, considerable noise is superposed on the discrete values measured depending on the method, and secondly the domain of the discrete values is certainly restricted in any experiment. Further, the inverse problem of finding the relaxation spectrum, the kernel of a Fredholm equation of the first kind, from measured data is an ill-posed problem. Inverting this integral equation is not an easy task because the solution to the inverse problem is not unique. It can be made unique only by introducing additional assumptions or additional a priori information. Recently, Tikhonov regularization and entropy functional methods have been applied to the inverse problem of finding the kernel of the Fredholm equation. Both methods allow unique determination of the kernel by introducing a priori error estimates and optimizing a regularization functional. Introducing error estimates and assuming a certain error distribution makes the solution unique, but not necessarily the correct solution as it depends on the a priori estimates. Further, in any experimental data, in addition to the inherent noise, there is embedded another set of experimental values which are not accounted for by any error estimate and distribution, called outliers. The answer to the question as to how large is this set depends on many factors. But it is certainly not negligible by any means. Lastly, we remark that if the data has been obtained in a restricted region, which it is almost always, extending the relaxation spectrum deduced from it by whatever to a larger range, which is always necessary in practice, is a moot question by definition if the method used to obtain the spectrum in the limited range has shortcomings to begin with.

The new algorithm based on the minimax method we develop does not require a priori error estimates and the set of outliers are taken into account. We construct the algorithm, give several hypothetical examples to test the reliability and exactness of the method, and finally end the paper with a concrete example of relaxation spectrum we determine for a polymeric liquid.

BIOSKETCH

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COMPUTATIONAL INVESTIGATION OF THE INFLUENCE OF THE ENVIRONMENT ON MECHANICAL PROPERTIES OF THE SOLIDS. THE CLUSTER APPROACH.

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INTRODUCTION

The phenomenon of the sharp decrease of the strength of solids in some environments (specific for each material) is well-known and finds many applications in various branches of engineering. Sometimes (especially for liquid metal embrittlement) the reduction of strength may be some tens or hundred times. This effect appears immediately after the contact of solid with such active media and is quite different from usual corrosion or stress-corrosion. Obviously the active medium participates in the process of the fracture - if the active medium is removed, the strength returns to its initial value. This phenomenon has been studied for many years from pioneering work of P.A.Rehbinder (1928) who related the effect with the reduction of surface free energy of solid in contact with the active medium and the decrease in the work of fracture because the fracture always is the creation of new surfaces. This idea has found various confirmations at least as a necessary condition of the phenomenon that is often named as the Rehbinder effect (RE). Such thermodynamic approach may be used as the basis of the macroscopic analysis of the RE, but it leaves aside the mechanism of the phenomenon.

There are various hypothesis about the atom-scale mechanism of the RE, but none of them is able to include all cases of its manifestation. In last decade the understanding appeared that the RE is the complex phenomenon that may be caused by various processes at the boundary between the solid and the active medium and it is more correct to speak about the possible specific mechanisms of the fracture in active medium and their role in total influence of environment on the mechanical behavior of the solid.

It is commonly supposed that the most "direct" and obvious mechanism RE is decohesion - reduction of the strength of interatomic bonds in the surface layer of the solid interacting with active medium (and active media are those that weaken interactions in solids). The quantum-chemical calculations of various level seem to be the only way of theoretical investigation of this mechanism.

The complex nature of the effect makes it very difficult to use first-principles approaches to study the processes of deformation and fracture. There are two ways to overcome this problem: (1) to choose the system simple enough that really may be considered from the first principles and (2) to use some of semiempirical methods that allow to deal with larger systems and to consider more or less large clusters of atoms.

It seems that most if not all of the known quantum-chemical calculations have been done by the first method. In particular, methodical *"Ab initio"* calculations are fulfilled (V.S. Yushchenko, E.D. Shchukin et al.) for rather small systems with the $C-C$ and $C=C$ bonds.

This way is somewhat substantiated at least for qualitative or, at best, semi-quantitative description of the effect in solids with covalent (or predominantly covalent) bonds. In that case the properties of the interactions are determined by the interacting atoms and their nearest neighbors. A different situation is realised in the metallic solids characterised by the completely non-local interatomic interactions. It is apparent that metallic solids should not be studied with the usage of small-scale atomic systems. Because of this the second way is preferable over the metallic and ionic solids. However even in the case of covalent solids it is questionable whether the results obtained for small molecules are useful in the description of fracture processes in the crack tip. The point is that even a single act of adsorption may produce the significant atomic rearrangement in a moderately large domain of the stressed solid. This kind of instabilities seems to be important in fracture processes.

By these means the semiempirical cluster methods are required for quantum-chemical investigations of RE despite their obvious pitfalls. Cluster approach has the advantage that the adsorption-induced rearrangement of the precracked zone can be calculated directly. Here we apply semiempirical $AM1$, $MNDO/H$ and $NDDO$ methods able to operate with 500-orbital systems with complete optimisation of atomic structure for the investigation of the adsorption-induced breakage of stressed hydrocarbon chains, clusters of aluminium of different size as well as with the clusters on immovable substrate and with bulk silica systems.

To test the validity of these methods for the problem under consideration the comparison between *"ab initio"* calculation results, and semiempirical ones was performed for the simplest systems.

THE CALCULATION METHOD

The quantum chemical methods $MNDO/H$ and $AM1$ applicable for $s-$ and $p-$ elements have been offered by Dewar in 1985. These methods are based on selfconsistent semiempirical approach giving the precision comparable with the *"ab initio"* method $STO-4-31GF$ but 10^3 times quicker. We suppose these methods (with the modifications required) to be the most convenient for the RE studies. The modifications include "energetic" parametrisation, the opportunity of the d-orbitals involving for transition elements and the algorythm for the deformed states simulation.

The suggested cluster approximation makes it possible to fulfill the total optimization of the space structure of systems containing up to 150 - 300 atoms using PC computers based on $INTEL$ 486/487.

The computer simulation of RE in the cluster approach includes two main stages. The preliminary study involves the modelling of the systems with various initial configurations in order to reveal the set of low-energy cluster structures. The latter is very important for simulation of the slow adiabatic decohesion processes because it is natural to expect the finite configurations to be the most stable low-energy ones.

One of the main difficulties of the cluster approach comes from the problem of the base cluster choice. We should search for the smallest suitable configuration in order to simplify the calculations. At the same time the cluster must be large enough, capable not only to describe the properties of the surface but also to model all the possible adsorption sites for different types of adsorbates. In accordance with the theory of the "active ensembles" the problem is to reveal how many atoms should be taken into consideration.

The problem of the cluster choice differs for different types of systems. For the covalent silica system the cluster should contain the combination of several silicon - oxygen tetrahedra surrounding the $Si - O - Si$ bond. For the metallic systems the cluster can be chosen on the base of the bulk crystal structure or the definite crystallographic face. In this case the number of atoms of the upper layer necessary to be taken into account, depends on the origin of the metal and the adsorbate as well. It is also not clear how many layers take part in the adsorption and deformation process especially for the metals for which the strong adsorbate induced surface reconstruction is observed.

The second stage includes the study of the influence of adsorbates on the deformation properties of the systems. In order to solve the main problem, the basic method was adapted for calculating of different types of mechanical deformations of clusters such as uniaxial deformation and bending.

The computational experiment consists of sequential step-by-step deformation from the initial stable state to rupture. The elementary deformation step is chosen according to the value of interatomic distances in the non-deformed cluster. The proper step length is found to be $10^{-2}...10^{-1}$ of the bond length. The complete optimisation of space structure is performed at each step.

It is clear that such a method is able to describe a sequence of stable states but not the kinetics of rupture. In order to obtain the kinetic characteristics one should turn to well-known models of the reaction rate theory. As we are able to calculate the vibrational spectra and saddle points parameters the kinetic characteristics can be estimated.

The method described was applied to the investigation of the mechanical properties of hydrocarbon chains, bulk silica systems and aluminium clusters under the adsorption of several water molecules, proton, hydroxyl, hydroxonium ions.

THE APPLICATION TO HYDROCARBON CHAINS

In order to compare the results obtained for RE by the method under discussion with those obtained by *ab initio* calculations we have reproduced the energy and interatomic forces calculations of double $C - C$ bond in ethylene. The influence of the hydrogen cation on the bond weakening was also studied. The results obtained by the semiempirical and *ab initio* calculations are in good agreement.

The scheme of the modelling of different deformation types (the uniaxial deformation and the bending) was tested on a heptane molecule. The dependence of the space and electronic structure and the heat of formation on mechanical deformation of the heptane molecule were obtained as well as the vibrational spectra for the free and stretched heptane molecule. The obtained low frequency shift for the stretched molecule is in qualitative accordance with experimental data for polymers.

THE APPLICATION TO SILICA SYSTEMS

One further example of the application of the method under discussion to the covalent systems is the study of the mechanical properties of silica dioxide in active media. The mechanical stretch of the $Si-O-Si$ bond was examined in vacuum and in the presence of several reagents (water, the hydroxonium ion, some surface-active organic molecules, etc.). The cluster containing two silica-oxygen tetrahedra modelling the active center of silica dioxide was chosen. The alteration of the heats of formation, the changes in the structural and electronic configurations of the clusters, and the force characteristics of deformed systems were obtained (Fig.1). The hydroxonium ion was shown to have the greatest influence on the rupture of the $Si-O-Si$ bond. It may be concluded that the bond decohesion force in the slightly acidic medium is reduced approximately three times and the work of rupture - almost ten times being compared with that for the free cluster. The close results were obtained in the presence of the surface active substances (SAS).

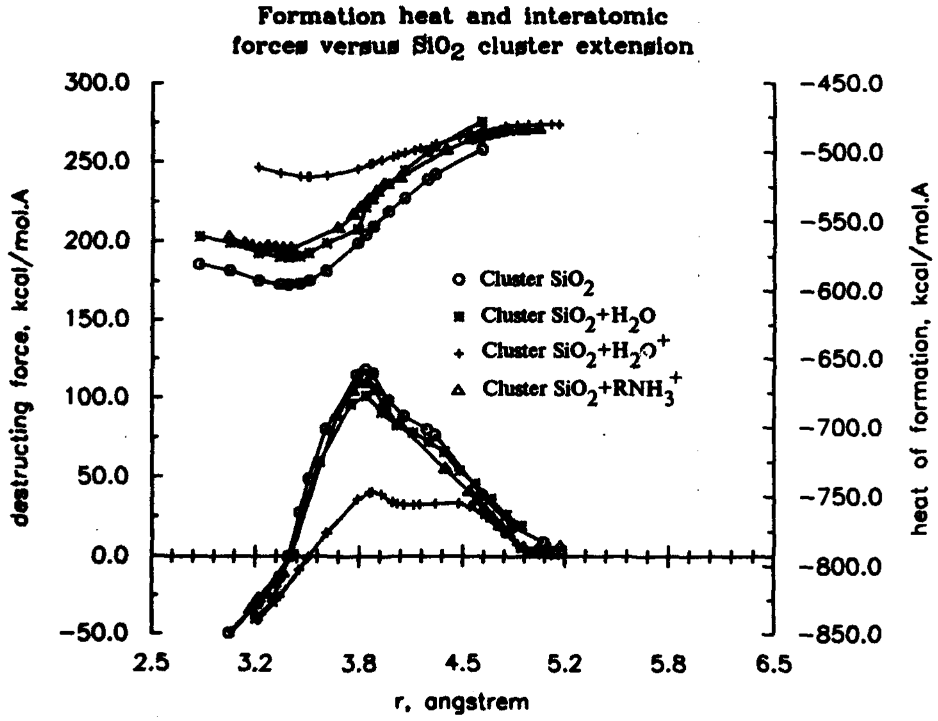

Fig. 1

THE APPLICATION TO METALLIC SYSTEMS

The preliminary stage of the investigation including the selection of the cluster size and structure becomes for metallic systems very important. The cluster should be large enough to possess the properties (ionisation potential, the face crystallography, etc.) close to the bulk metal ones. On the other hand the system should be sufficiently small to be accessible for serial calculations.

Total optimisation of clusters containing from 2 to 26 *Al* atoms give us an opportunity to make certain conclusions:

(1) several isomers can be obtained for almost all of the clusters of each size;

(2) the most low-energy modifications of small aluminium clusters, containing from 2 to 7 atoms, are planner;

(3) the stable clusters containing from 8 to 11 atoms are transitional between planar and 3-dimensional structures;

(4) the bulk structures are obtained for the clusters with the number of atoms more than 12;

(5) the cluster of Al_{13} possess the lowest heat of formation and the total energy related to one atom among all the clusters from Al_2 to Al_{26}, it appears to be a stable system of tetrahedra connected in twos by sides and by two common tops, the hybridisation of the orbitals of the central atom is sp^3;

(6) all the bulk clusters seem to be built from stable Al_{13} block by filling the successive coordination shells by *Al* atoms forming the additional tedrahedra.

According to the reasons above we have chosen the cluster as the main object for investigation of RE for aluminium systems. Al_{26} looks like two blocks having a common quadrangular side.

Under the influence of external stresses the Al_{26}-block is deformed, the reconstruction of all the bonds occurs. We have found several sones of elasticity separated by the "plastic" sones of two types: the sharp reduction of stresses corresponding to significant structure rearrangement and the sones where the inner stress doesn't depend upon the cluster extension. The spasmodic transitions from one sone to another (fig.2) reflect the spasmodic transformations of the system of the bonds.

For aluminum system we investigate the influence of media *pH* on its deformation properties. The interaction of Al_{26}-cluster with water molecules, as well as with the additional protons or hydroxyl groups is examined.

The electron-donor adsorbates (like water or hydroxyl) can coordinate in the *"on -top"* position on aluminium atoms with sp^2-hybridisation of orbitals (like (111) and (100) faces) or in the "bridge" or the so-called "slanting bridge" position on the atoms with the proper sp^3- hybridisation of orbitals (like the (110) face). In order to realise the adsorption of electron-acceptor adsorbate (like hydroxonium) the complete rearrangement of electron density is needed.

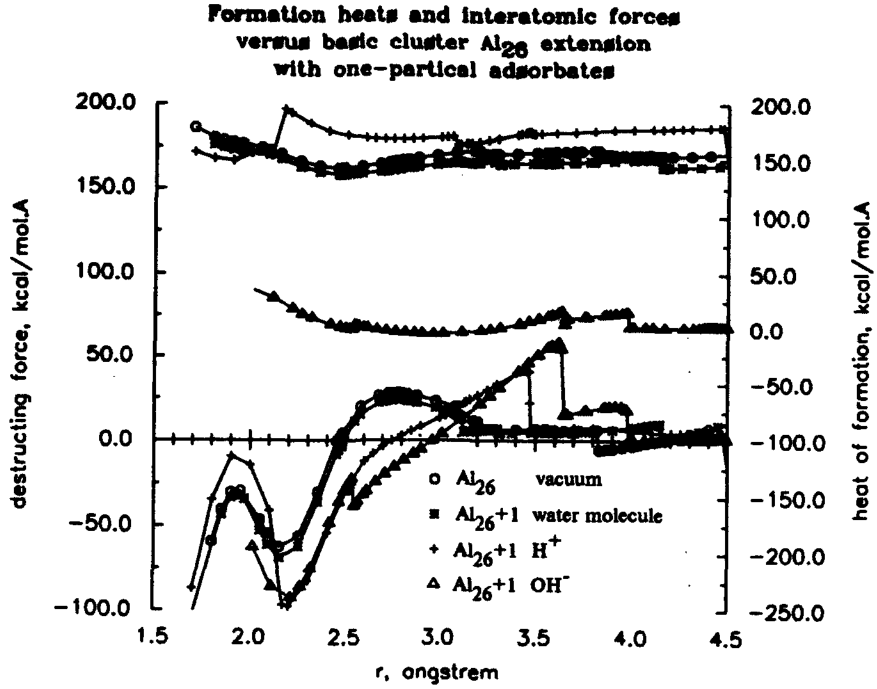

fig. 2

The comparison of the properties of the systems containing 1 - 4 water molecules shows that though the stability of the clusters under investigation increases in the presence of the additional water molecules; system behavior under deformation does not depend upon the number of water molecules if it is greater than 3. The thing is that the optimized cluster $Al_{26} - nH_2O$ can make chemical bonds only with 3 water molecules while the forth one is coordinated by the hydrogen bond in the second sphere.

The adding of a proton to a basic cluster makes the latter less stable (fig. 2), and as it occupies the "*bridge*"-position on two aluminium atoms the bond between them is broken and the distance $Al_1 - Al_{12}$ in the free protonised cluster is a little bit longer than in the basic one (fig.2). The first zone of elasticity as well as the decohesion energy is also perceptibly larger.

In the cluster modelling the acidic medium the H_3O^+ -ion does not make a chemical bond with any aluminium atom and the interaction is reduced to a hydrogen-like coordination. The character of the force-curve (fig.3) is very close to that for the basic cluster and in the stretching zone of deformation almost coincides with the curve for the cluster, connected with 2 water molecules: so the acid medium seems to make no principle influence on the stretching of the cluster. In the compression zone, on the contrary, the work of deformation is visibly smaller than both for basic and for water-containing clusters.

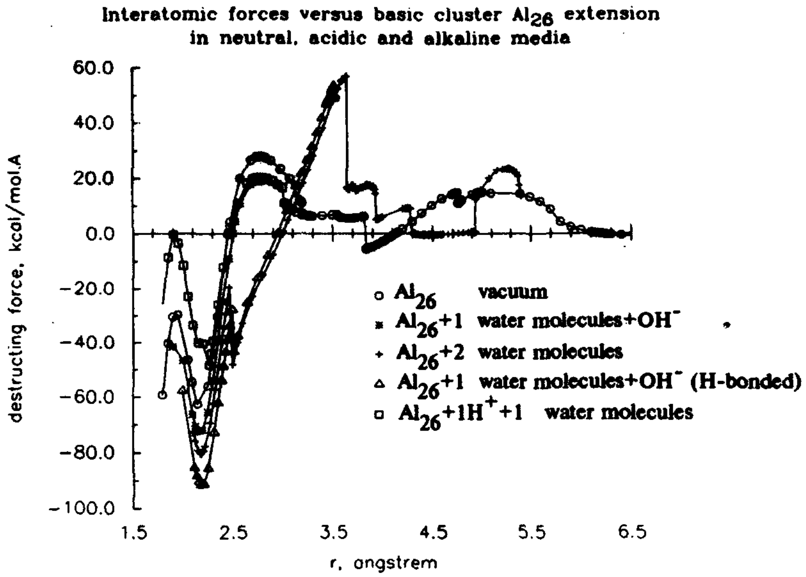

Fig. 3

The alkaline medium greatly influences the deformation properties of the aluminium cluster. Though the arid hydroxyle group greatly increases the stability of the cluster, the deformation properties are similar to that of the protonized cluster (fig.2). The situation completely changes when we model the slightly-alkaline medium by adsorbing on the base aluminium cluster a hydroxyle ion together with a water molecule. In this case the first zone of elastic deformations is spread on the large interval of external tensions (fig. 3) and the work of deformation is much higher than for all the previous systems.

So while the acidic medium reduces the work necessary for the aluminium cluster destruction, the alkaline medium expands the zone of elastic deformations.

CONCLUSION

Here, the object was to demonstrate the potentialities of semiempirical cluster approach to quantum-chemical calculations of RE. The results presented above should be treated as the examples. The semiempirical cluster methods have an advantage over the "*ab initio*" ones, because the former allow to deal with significantly larger systems containing up to 350 atoms. This enables to calculate directly the structure rearrangement effects in the crack tip under the influence of different environments and external stress.

However, care must be exercised in the interpretation of the results obtained by semiempirical methods. It should be recognised that the last are no more than rough approximation. Nevertheless, due attention should be given in our opinion to the application of semiempirical cluster methods to RE investigation.

BIOSCETCH

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THEORY OF VISCOELASTICITY AND ITS APPLICATIONS FOR CALCULATION OF RELAXATION PROPERTIES OF POLYMER COMPOSITES

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The report consists of three parts. First of all, the dynamics of a single macromolecule in a system of entangled weakly-coupled polymer chains as a foundation of theory of viscoelasticity for polymer solutions and melts are considered. In the second part consequences of macromolecule dynamics for the theory of constitutive equation for a system in whole are discussed. In the third part method of calculation of relaxation properties of surface layer in polymer composites is demonstrated.

DYNAMICS OF MACROMOLECULES

The thermal motion of macromolecules in the non-dilute solutions and melts and its connection with irreversible processes in systems of entangled polymer chains were investigated over the last decades. Different research groups have made valiant attempts to find a unite approach to polymeric systems that would provide an explanation and description of nonequilibrium phenomena in entangled polymers from a unified point of view.

Essential progress in understanding the thermal motion of the macromolecules was achieved by de Gennes [1] and by Edwards [2] during the last two decades. In the last years it was understood that the localization of a macromolecule in "a tube", postulated by Edwards and de Gennes, follows from a formal approach based on the most general assumptions in the dynamics of a macromolecule due to Russian researches. Apart of the localization effect the approach appears to be rather broad to give explanations to all known facts of dynamics of weakly-coupled macromolecules (viscoelasticity, optical birefrengence and so on) that was demonstrated earlier (see review [3]).

It is convenient as the starting point of the analysis to take an approach which appeared in the papers by Russian researches [3]. According to the Russian theory the neighbours of the chosen macromolecule form on average a deformable relaxation medium. The chosen starting point is based on the most general assumptions and determines the first - order approximation to the dynamics of macromolecule.

We consider concentrated solutions and melts of linear polymers as systems of weakly connected macromolecules: every chain can change its neighbours and moves among the other chains. When we consider relatively slow motion of system, each macromolecule is schematically described as consisting of $N+1$

linearly coupled Brownian particles, so that we shall be able to look upon the system as on a suspension of many interacting Brownian particles suspended in a viscous "monomeric liquid".

We consider the motion of the described system under deformation with a constant velocity gradient tensor

$$v_{ij} = (\partial v_i)/(\partial x_j) \qquad (1)$$

so that a particle located at r_j^α is dragged with mean velocity $v_{ij} r_j^\alpha$.

A force acting on any part of the system gives rise to the excitation of the entire ensemble of Brownian particles, so that when behavior of the system is investigated we have to consider the collective motion of all the particles in the same way that, for example, we examine the motion of the ensemble of atoms in solids. Our task is therefore to find the normal coordinates of the polymer system, i.e., the variables that vary independently of one another.

The identification of the normal coordinates can be carried in two stages, bearing in mind the particular properties of the system (strong interaction along the chain and weak interaction between the macromolecules). The task of the first stage is to determine the dynamics of a single macromolecule, surrounded by all the others. To implement the first stage, we must eliminate all variables, other than those that refer to the chosen macromolecule. This procedure is not too simple, but we can imagine the general form of the final results before the calculations are carried out. The requirements of proper covariance and of linearity in coordinates and velocities determine [3] the general form of the equation for the dynamics of the chosen macromolecule.

This is followed by the second stage in which the normal coordinates of an individual macromolecule are determined [3].

The implementation of the program gives stochastic equations for diffusion and relaxation modes, respectively

$$m(d^2\rho_i^0)/(dt^2) = -\int\beta(s)(\rho_i^\alpha - v_{il}\rho_l^\alpha)\, ds + \sigma_i^0(t) \qquad (2)$$

$$m(d^2\rho_i^0)/(dt^2) = -\int\beta(s)(\rho_i^\alpha - v_{il}\rho_l^\alpha)_{t-s}\, ds -$$

$$-\int\varphi(s)(\rho_i\alpha - \omega_{il}\rho_l^\alpha)_{t-s}\, ds - 2\mu T\lambda_\alpha\rho_i^\alpha + \sigma_i^\alpha(t),$$

$$\alpha = 1, 2, \ldots, N \qquad (3)$$

where m is the mass of a Brownian particle associated with a piece of the macromolecule of length M/N, $2\mu T$ is elasticity coefficient, T is temperature, $\omega_{il} = 1/2(v_{il} - v_{li})$. For large N and small α the eigenvalues are then given by

$$\lambda = (\pi\alpha/N)^2, \qquad \alpha = 1, 2, \ldots, << N \qquad (4)$$

The first terms on the right of the Eqs.(2) and (3) are the hydrodynamic drag forces, the second term in Eq.(3) represents the intramolecular resistance due to the change in the shape of the macromolecular coil (kinetic stiffness) the third term in Eq.(3) represent the elastic force due to nearest-neighbour Brownian particles along the chain. The last terms in Eqs.(3) and (4) are the random thermal forces whose statistical properties are, as usual, defined so that the equilibrium values of the calculated quantities are the same as those already known.

According to [4] we should also write down the drag and resistance forces in Eqs.(2) and (3) in the form of nonlocal expressions, since exitation directly through the chain propagates to a distance $<R^2>$, i.e. a distance that is large in comparison with the size of the Brownian particle under consideration. However, for the sake of simplicity, this will not be done here, although the consequences of a nonlocal effect be noted latter. Equations (2) and (3) also rely on the questionable assumption that each particle in the chain is in the same isotropic situation.

Apart of these notes, Eqs.(2) and (3) are the most general equations for the low-frequency modes of the system in the case of a linear dependence on variables.

However, the memory functions $\beta(s)$ and $\varphi(s)$ can not be determined from general considerations: they must be found by calculations such as, for example, those reported in [5], or simple heuristic consideration must be abandoned as was observed in [3].

In a simple case, the one-sided Fourier transforms of the memory functions were found

$$\beta[s] = \zeta(1 + B/(1-i\omega\tau)), \qquad \varphi[s] = \zeta E/(1-i\omega\tau) \qquad (5)$$

where ζ is the monomer friction, B is the measure of increasing of friction due to neighbouring macromolecules, E is the measure of "internal viscosity" due to entanglements of macromolecules in the system. The relaxation time τ in (5) is the relaxation time of the matrix which we later calculate as the main viscoelasticity relaxation time of the entire system in a self-consistent manner.

The parameters ζ,B,E and τ are the phenomenological parameters in the theory.

We can find $B \sim M^{\delta}$, where M is the length of macromolecule, if we take the non-locality of medium into account. According to [4] δ=2, experiments give a value of the exponent slightly more than 2, consistent with model.

Equations (2) and (3) can be looked upon as the first-order approximation to nonequilibrium phenomena in undilute polymers. This excludes effects due to nonlinear terms, e.g., the reptation phenomena noted by de Gennes [1], which appear when the difference between mobilities along and at right angles to the chain is taken into account. This can be described by terms of order greater than the first in a rigorous theory of motion of a macromolecule in a concentrated system. However, before we turn to this problem, we must examine the effects represented by linear terms.

MOLECULAR NON-LINEAR THEORY OF VISCOELASTICITY

The described results form a basis on which the rheological behavior of polymer liquids can be considered. Now we are in position to formulate constitutive equations for polymer liquids. In fact we have a set of constitutive equations due to various approximations.
The equations of motion for a set of Browning particles suspended in a viscoelastic liquid are formulated, which is equivalent to the derivation of the expression for the stress tensor which we write in terms of modes (3) in the following form [3]

$$\sigma_{ik}(t) = -p\delta_{ik} + nT\sum\{2\mu\lambda_\alpha <\rho_i^\alpha(t)\rho_k^\alpha(t)> - \delta_{ik} +$$

$$+ (1/T)\int\varphi(s)[<\rho_i^\alpha(t)\rho_k^\alpha(t-s)> - \omega_{kl}(t-s) <\rho_l^\alpha(t-s)\rho_i^\alpha(t)>]ds\} \qquad (6)$$

where p is the pressure, n is the macromolecular number density.
The angle brackets represent averaging over the ensemble of realization of random forces in the mode equations (3).

It is convenient to introduce internal relaxate variables x_{ik}^α and u_{ik}^α to rewhrite stress tensor in another form

$$\sigma_{ki} = -p\delta_{ik} + 3nT\sum(x_{ik}^\alpha - 1/3\delta_{ik} - u_{ik}^\alpha) \qquad (7)$$

The first set of variables is connected with deformation of macromolecule in the system. The second set of variables reflects stresses under deformation of "the tube". It was shown that two sets of relaxate variables give the adequate picture of relaxation of polymer systems [3].

It was shown [6,7] that relaxation equations for x_{ij}^α and u_{ij}^α follow from mode equation (3)

$$(D/Dt)x_{ik}^\alpha - (B\tau_\alpha^R/\tau_\alpha)(x_{ij}^\alpha\gamma_{jl}c_{lk}^\alpha + x_{kj}^\alpha\gamma_{jl}c_{li}^\alpha) =$$

$$= -1/\tau_\alpha[(x_{ij}^\alpha - 1/3\,\delta_{ij})b_{jk}^\alpha + (x_{kj}^\alpha - 1/3\,\delta_{kj})b_{ji}^\alpha] \qquad (8)$$

$$(D/Dt)u_{ik}^\alpha - (B\tau_\alpha^R/\tau_\alpha)e_{ij}^\alpha\gamma_{jl}u_{lk}^\alpha = -(1/\tau\,\delta_{ij} + 1/(2\tau_\alpha)b_{ij}^\alpha)u_{jk}^\alpha +$$

$$+ (E\tau_\alpha^R/\tau\tau_\alpha)((x_{ij}^\alpha - 1/3\,\delta_{ij})d_{jk}^\alpha - 2B\tau_\alpha^R x_{li}^\alpha\gamma_{lj}f_{jk}^\alpha) \qquad (9)$$

Auxiliary quantities b_{jk}^{α}, c_{jk}^{α}, d_{jk}^{α}, e_{jk}^{α} and f_{jk}^{α} are defined [7] as functions of parameters of the theory and anisotropy tensor

$$a_{ij} = \Sigma\,(x_{ij}^{\nu} - (1/3)\,\delta_{ij})$$

Relaxation equations (8) and (9) contain relaxation times

$$\tau, \qquad \tau_{\alpha} = \tau/2 + \tau_{\alpha}^{R}(B+E), \qquad \tau_{\alpha}^{R} = \tau^{*}/\alpha^{2}.$$

It was shown [3,6,7] that the system of constitutive equations (7), (8) and (9) describes various no-linear effects, in particular anisotropy of relaxation.
The constitutive equation takes a simpler form for fluid polymer system [7].

MACROMOLECULE IN A SURFACE LAYERS

The properties of polymer near the surface of solid is quite different from properties of bulk polymer. It is necessary to take into account this effect under the constructing of polymer solid composite with large content of solid phase. In the last case almost all amount of polymer is in modified state in surface layers. We can use the described theory of viscoelasticity to determine the alternation of polymer properties in a surface layer.
As a starting point we take the dynamics of macromolecule (2) and (3), whereby the interaction of particles with surface is taken into account. The modified equation of dynamics is non-linear now and we have to use computer simulation methods to came to results. Computer methods allows us to follow the stochastic trajectory of every Brownian particle (bead) of chain.
The data obtained from computer simulation are used for calculation of the correlation functions and mean square displacement of separate beads in the macromolecule. The results should yield diffusion coefficient and relaxation times of the macromolecule.

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BIOSKETCH

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From 1979 to 1987 he worked as a professor, Head of Department of Applied Mathematics at Altai Polytechnic Insitute in Siberia. From 1987 up to now he is professor of Moscow Institute of Economics and Statistics.
His area of interests include mechanics, physics, chemistry, biology and economics. He considers the Method of Mathematical Modeling as the main stream of his interests. V.N.Pokrovsky published more than 90 papers on molecular physics of suspensions, polymers and liquid crystals and two monographs.

IMITATION MODELING METHODS OF INTERPHASE LAYERS PROPERTIES OF POLYMER COMPOSITE MATERIALS

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INTRODUCTION

Computer simulation is widely used for studying the mechanical properties of polymers because of their practical applications and there is a strong need for accurate prediction of properties without resort to expensive experiments.

It is well-known three methods in the modeling of polymer materials. They are the stochastic dynamics methods (SD). The Brownian dynamics methods (BD) and the molecular dynamics methods (MD).

The most accurate treatment in principle, ought to be MD method, because of the explicit description of atomic motions; it takes into account the interactions between polymers chains, the interaction with solvent particles and surfaces. It is very impotent for investigation of polymer composite materials.

Our aim is to present the original molecular dynamics program MOLSIM and discuss their applications.

DETAILS OF ALGORITHM

The technique of molecular dynamics simulations is well-known. The classical equations of motion are solved for a system of interacted particles. Basic principles of the method have been described by Raman, Parrinello (constant-pressure technique), Nose, Hoover, Andersen (constant temperature algorithm). Then this method have been developed by Berendsen (loose-coupling, constant-pressure technique) and extended by Brown and Clarke for use on polymer samples.

This ideas form the basis of the MOLSIM program.

The most important features if the MOLSIM program are original algorithm of searching neighbors for evaluating nonbonded interactions and database FIELDS of empirical parameters of the Force Field of interatomic interactions.

Original algorithm of effective regional search of neighbors is realized in MOLDYN module of MOLSIM program. Operational feature of program are the core memory requirement depends only on the number of particles and not depends on the value of cutoff radius. This makes it possible to simulate efficiently very large system and use long-range potential.

The database program FIELDS provide to formation a force field describing interactions between atoms (particles) generally contains term of covalent bond interactions, bond-angle interactions, torsion angle interactions, and nonbonded interactions. The database contains variable potential functions. And widely range of potential function are also realized in MOLDYN program.

MOLSIM PROGRAM DESCRIPTION

Program MOLSIM has been developed to provide Interaction Force Fields Formation for given molecular structures and molecular dynamics simulations. This program consists of SUBGR, FIELDS and MOLDYN modules. Functional scheme of program:

File *.MOL → SUBGR → FIELDS → MOLDYN.

SUBGR module is used for analyzing given molecular structures and determination all isomorphic subgraphs (uncolored) of certain topologies and the colored subgraphs of the same topologies in a colored graph, which represent one-, two-, tree- and four-body atomic chains. "Color" is connected with an atomic name or an atomic group name.

FIELDS module provides access to the Data Base of empirical interatomic potential fields to allocate the force fields parameters for the constants in the potential energy function for given molecular structure. It may be used also to create a new potential fields for users. Database provides to create a Force Field which involves valence and nonvalence interactions

$$E = E_{val} + E_{nb},$$

where E_{val} includes the terms arising from covalent bond formation and E_{nb} includes the longrange noncovalent interactions.

As usual, E_{val} includes bond stretch, angle bend, dihedral angle torsion, one-center angle-angle cross terms, while the nonbond terms consist of van der Waals and electrostatic terms.

The MOLDYN program has been developed for molecular dynamics simulations. The computer simulation techniques based on the well-known molecular dynamics (MD) method and can be used for studying the thermodynamical, structural and dynamical properties of polymer materials. The program MOLDYN solves the classical equations of motion of a 3D-system of mutually interacting particles.

The equations of motion is solved by using of the Verlet algorithm. The desired temperature is controlled via scaling periodically the velocities of the atoms.

The program MOLDYN calculates the thermodynamic quantities: kinetic, potential and total system energy, temperature ant other mechanical values of the system.

Programming language is FORTRAN 77. The computations may be performed on the VAX hardware as well as on IBM PC AT/XT computers.

SIMULATION

Molecular dynamics computer simulations have been used to study the extantional (Young's) modulus of oriented linear polymer chains and polymer samples generated by using a modified self-avoiding random walk technique. Investigations were performed under constant tension at a range of temperature.

The detailed mechanism of the local dynamics of polymer chains and the surface bound polymer chains have been investigated.
In the subsequent we assume to extend our simulation on polymer composite materials investigations.

BIOCKETCH

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CRITICAL PERIODIC IN THE NUCLEUS PROPERTIES AND PROBLEMS OF COMPOSITES CALCULATIONS

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There are two types of the periodical systems, one of them is the based on the properties of electrons, that were determined by periodic system, and another - on the nucleus properties. Periodic system is one projection of the whole periodic properties and another projection is periodical scale of the nucleus properties. Many facts, which can not be described by periodic system, may be seen in the natural systems (i.e. in geochemical structures).

On this base we realize new directions in the calculations of composites and quasinatural structures for the applications in electronics, high temperature superconductor, materials with extremal qualities.

BIOSKETCH

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COMPUTER SYNTHESIS OF FIBER ARCHITECTURE AND PROPERTIES OF TEXTILE STRUCTURAL COMPOSITES

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The design and fabrication of preforms for advanced composites have gained considerable attention in the light of the recently developed three-dimensional textile preforming techniques. Three-dimensional textile structural composites, based upon braiding, weaving, knitting and stitching, provide enhanced stiffness and strength in the thickness direction,improved damage tolerance, and most importantly, the potential of near-net-shape forming of components with complex surface contours. The ability in the integrated and system approach to textile structural composites from preform processing/manufacturing, matrix consolidation to composite characterization, and analytical modeling of composite performance has greatly broadened the potential of textile composites in primary structural applications.

Two aspects of the computer synthesis effort in the modeling of fiber architecture and performance of textile composites are outlined below. First in the area of process simulation, the development of a computer simulation of a general Cartesian braiding process has led to an understanding of process fundamentals. The simulation allows for the identification of individual yarn paths, number and location of yarn groups, and braid geometry. Innovative braid geometries were simulated and the preforms fabricated to demonstrate the feasibility of fabricating a wide range of preform architectures given an advanced braiding machine. Additionally, interesting distributions of yarn groups have been found which suggest an application to hybrid composites. These new and advanced braids, termed "multi-step" braids, are only possible with individual row/column control. The multi-step braiding process greatly extends the range of possible preform microstructures.

Next the thermal and mechanical property modeling and prediction follows a hierarchical approach which entails mechanical and geometric modeling of each fiber tow, followed by the identification of mechanical relationships between each of the tows, and the use of an assembly scheme to determine the thermo-elastic properties of the composite. The predicted stiffnesses for typical 3D architectures are then compared with the experimental data to validate the model predictions. Estimates for the strength of the textile composites along the principal material directions are obtained from the tow strength, the fiber volume distribution, and the parameters characterizing the tow undulation.

Through the analytical simulations and detailed parametric studies, a systematic approach has been accomplished to understand the relationships between key material and geometric parameters and the resultant composite properties.

BIOSKETCH

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Dr. Tsu-Wei Chou is the Jerzy L.Nowinski Professor of Mechanical Engineering of University of Delaware. Dr. Chou was educated at the National Taiwan University (B.S. in Civil Engineering, 1963), Northwestern University (M.S. in Materials Science, 1966) and Stanford University (Ph.D. in Materials Science, 1969). Dr. Chou was a post-doctor at the Materials Research Center of Allied Chemical Corporation before joining University of Delaware in 1969. Dr. Chou also has served as a visiting professor in the following institutes: Argonne National Laboratory, 1975-76; British Science Research Council, 1976; The University of Witerwatersrand, South Africa, 1977; National Commission for the Investigation of Space, Argentina, 1981; Germany Aerospace Research Establishment, 1982; London Branch office, Office of Naval Research, 1983; Tongji University, China, 1990; and Tokyo Science University, Japan (1990).

Dr. Chou's research interests are in materials science, applied mechanics and fiber composite materials and he has published more than 275 technical papers in these areas. Dr Chou is the co-author of the book, Composite Materials and Their Use in Structures, Elsevier - Applied Science, London (1975). He is also the editor of Textile Structural Composites, Elsevier Science publishers, Amsterdam (1988) and Structure and Properties of Composites in the Materials Science and Technology Series, VCH, Germany (under preparation). Dr. Chou is also the author of the new book, Microstructural Design of Fiber Composites, Cambridge University Press, England (1992).

Dr. Chou is the North American Editor of the international journal, Composites Science and Technology and serves on the International Editorial Advisory Board of ACTA Materiae Compositae Sinica and Encyclopedia of Composites (SAMPE).

ASYMPTOTIC METHODS FOR INVESTIGATION OF IMPACT– AND EXPLOSION– INDUCED WAVE PROCESSES

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INTRODUCTION

The study of nonstationary wave process in explosion or shock is of considerable interest for a multiplicity of uses. As a rule, the solving of such problems is associated with considerable mathematical and computing difficulties. This is particularly true in regard to the media with complex behavior under the high-speed loading. However, there exists class of problems when difficulties arise even in the case of simple media such as ideal gase.

Asymptotic methods are very useful in qualitative and quantitative analysis of complex wave processes.These methods are based on expansion of solution in asymptotic series over given small parameters set. However, direct expansion never leads to desired result, because of wave problems specificity. The reason is that, the validity domain of direct expansion in space of independent variables appears to be too small. The overcoming of this difficulty is possible by using of many-scales-method (MSM).This method was developed in 1970-s by the efforts of many investigators *(Cole, Kevorkian, Lick, Taniuti and Wei, and others)*. The contemporary form of MSM supposedly was suggested by Leibovich and Seebass, and Oikawa and Yajima.

In nonlinear wave theory, MSM is used to decompose initial complex system of equations. As a result, the independent system of equations for the functions, which are Riemann's invariants analogs has been derived. In first-order (nonuniformly valid) approximation these functions are constant along characteristic directions. Keeping an account of nonlinearity and kinetic processes leads to their slow variation. The necessary condition of MSM validity is weak nonlinearity, that is, insignificant variaiton of substance density in a wave or small ratio of pressure to bulk modulus. For the representative problems on impact– or explosion– induced deformation of metals, ceramics or composites, that condition is not too restrictive.

In the problems on strong blast wave propogation in gases or in porous media (for example, in rocks), the situation is fundamentally new. At the initial stage of explosion in gases, the pressure in a shock wave extremely exceeds the initial pressure in a medium. In a porous media, the pressure is extremely higher than the compression strength limit, which leads to irreversible packing. In both cases, the nonlinearity is strong and MSM can not be used in the general formulation. The most effective method for qualitative study of this type of problems is the representation of these problems as of models with lumped parameters by using of asymptotic expansions. The fundamental results in this field have been obtained in 1950-60s. We can state with assurance that models with lumped parameters have lost popularity due to extension of computing potentialities. However, for the optimal control problems, these models appear to be the only avilable method of the sufficiently full qulitative study.

Here, we consider the possibilities and peculiarities of application of MSM and models with lumped parameters to studying nonstationary wave processes under shock and explosion. The examples of qualitative investigation and of solving of applied problems are discussed.

GENERAL PROCEDURE OF DECOMPOSITION

A host of models of continuous media results in system of equations of the type:

$$\frac{\partial u_i}{\partial t} + C_{ik}(\vec{u})\frac{\partial u_k}{\partial x} = \mu \hat{D}_i[\vec{u}], i = 1, ..., N \tag{1}$$

were $\vec{u}$ is the unknown vector-function, $C_{ik}(\vec{u})$ is NxN matrix, $\hat{D}_i[\vec{u}]$ - are certain operators, $\mu << 1$ is a small parameter. In particular, system (1) describes one-dimensional nonlinear waves in visco-elastic and elastoplastic media with intrinsic degree of freedom, in relaxating fluids and gases, membranes, etc.

The problems on shock and explosion–induced deformation of materials are usually stated as the boundary-value problems. However, it is more convinient to consider the general procedure of decomposition on the example of Cauchy problem. This allows to demonstrate that procedure in the most general form, while the extension of the result to the boundary-value problems presents no difficulties.

Let $\vec{u} = \vec{u}(0, x), -\infty < x < \infty$, be given at the initial moment t=0, with

$$||\vec{u}(0, x) - \vec{u}_c|| \sim \epsilon \ll 1, \tag{2}$$

where $\vec{u}_c$ is unperturbed homogeneous stationary state of the medium. It is reasonable to represent the solution of system (1) in the form of expansion near the homogeneous stationary state

$$\vec{u} = \vec{u}_c + \epsilon\vec{u}_1 + \epsilon^2\vec{u}_{2\epsilon} + \epsilon\mu\vec{u}_{2\mu} + ... \tag{3}$$

. It is supposed about $C_{ik}(\vec{u})$ and $\hat{D}_i[\vec{u}]$ that

$$\begin{gathered} C_{ik}(\vec{u}) = C_{ik}^{(o)}(\vec{u}_c) + \epsilon C_{ik}^{(1)}(\vec{u}_c, \vec{u}_1) + ... \\ \hat{D}_i[\vec{u}] = \epsilon \hat{D}_i^{(1)}[\vec{u}_c, \vec{u}_1] + ... \end{gathered} \tag{4}$$

By substituting the expansion (3),(4) in (1) we find the system of equations in u_{1i}.

The first step of decomposition procedure involves diagonalisation of that system. The possibility of diagonalisation is provided by the reality of the eigenvalues of matrix $C_{ik}^{(o)}(\vec{u}_c)$. To put it otherwise, to a first approximation, system (1) is supposed to be a hyperbolic one. Let us introduce the unitary matrix $T_{ji}(\vec{u}_c)$ and vector V_j so that $T_{ji}C_{ik}^{(\epsilon)}T_{kl}^{*} = \lambda_j(\vec{u}_c)\delta_{jl}, V_j = T_{ji}u_i$ where $\lambda_j(\vec{u}_c)$ are eigenvalues of matrix $C_{ik}(\vec{u}_c)$. The expansion of V_j over small parameters follows from (3), were all V_{1j} are constant along their characteristic directions. At the second step it should be adopted that all V_{1j} along their characteristics are slow functions of time, that is V_{1j} has a form $V_{1j} = V_{1j}(\xi_j, \tau_\epsilon, \tau_\mu)$ with $\xi_j = x - \lambda_j t, \tau_\epsilon = \epsilon t, \tau_\mu = \mu t$. Then, the equations for the second-order terms of expansion are the following:

$$\frac{\partial V_{2j}^{(\epsilon)}}{\partial t} = -T_{ji}C_{ik}^{(1)}(\vec{V}_1)T_{kl}^{*}\frac{\partial V_{1l}}{\partial \xi_j} - \frac{\partial V_{1j}}{\partial \tau_\epsilon}$$

$$\frac{\partial V_{2j}^{(\mu)}}{\partial t} = T_{ji}\hat{D}_i^{(1)}[\vec{V}_1] - \frac{\partial V_{1j}}{\partial \tau_\mu} \qquad (5)$$

The derivatives in the left parts of equations (5) are calculated with fixed $\xi_j, \tau_\epsilon, \tau_\mu$ while in the right parts $V_{1k} = V_{1k}(\xi_j + \Delta\lambda_{jk}t, \tau_\epsilon, \tau_\mu), \Delta\lambda_{jk} = \lambda_j - \lambda_k$.

Furthermore, when integrating (5), we must eliminate the terms which increase with the "fast" time t. This can be arranged by the selection of "slow" time-dependence (i. e., τ_ϵ, τ_μ − *dependence*) of functions V_{1j}. Thereby, the smallness of the second-order terms in comparison with first-order ones in expansion (3) can be extended to the asymptotically long time interval $t \leq O(\epsilon^{-1} + \mu^{-1})$

For the application of interest here, the most frequently used type of system (1) is that of real one, where $C_{ik}^{(1)}(\vec{u}_c, \vec{u}_1)$ are linear combinations of $\vec{u}_1$ components and $\hat{D}_i^{(1)}[\vec{u}]$ are linear operators. We assume these operators to preserve the order of function value.

Feasibility of decomposition is determined by the character of phase velocities spectrum $\{\lambda_j(\vec{u}_c)\}$. Let us suppose that there are no closely-spaced eigenvalues in the spectrum of phase velocities; that is the condition $|\Delta\lambda_{jk}| >> max\{\epsilon, \mu\}$ should be met for any $j \neq k$. Uniformity requirement for the first terms of expansion (3) can be satisfied if the initial disturbance is restricted , for example, by the condition

$$\sum_{i=1}^{N}\left|\int_{x_1}^{x_2} dx[u_i(0,x) - u_{ci}]\right| \leq \epsilon \qquad (6)$$

for any $x_1, x_2 \in (-\infty, \infty)$. As the consequence of (5) and (6), the following estimates can be obtained:

$$|V_{2j}^{(\epsilon)}|, |V_{2j}^{(\mu)}| \leq \sum_{l \neq j}\frac{Q_l}{|\lambda_j - \lambda_l|}$$

Here Q_l are nonnegative constants, $Q_l << min\{\epsilon^{-1}, \mu^{-1}\}$. In this case the general form of the equations for the first-order approximation (uniformly valid at the asymptotically large time interval) to the solution is

$$\frac{\partial V_{1j}}{\partial t} + \epsilon\alpha_j V_{1j}\frac{\partial V_{1j}}{\partial \xi_j} = \mu\hat{R}_j[V_{1j}], \quad j = 1, ..., N \qquad (7)$$

Here the derivatives with respect to time t are calculated with fixed phase variables ξ_j. The term in the right side of equation (7) is the summand of linear combination $T_{ji}\hat{D}_i^{(1)}[\vec{V}_1]$ which does not depend on the "fast" time.

The extension of outlined procedure to the case of closely-spaced eigenvalues presence is not difficult. Let only two eigenvalues λ_k *and* λ_m are close to each other. Let us introduce one further "slow" time $\tau_\lambda = \Delta\lambda_{km}t$. Then $V_{1m}(\xi_k + \tau_\lambda, \tau_\epsilon, \tau_\mu)$ and secular terms elimination leads to the coupling equations for V_{1k} *and* V_{1m}. The other (N-2) equations of the form (7) remain unchanged.

Modification to the case of boundary-value problem also leads to the equations of the form (7). The minor distinction consists in using the transformation $t \rightarrow x$ *and* $\xi_j \rightarrow -\xi_j$ in (7).

The consideration carried out here refers only to unidimensional problems. However, there is a host of interesting multi-dimensional problems. The impact-induced deformation wave propagation in solids is an example. Within the limits of MSM, the natural way to consider multi-dimensional effects is the using of so-called Leontovich parabolic approximation. To our knowledge this approximation was first applied to nonlinear problems by Zabolotskaya and Hohlov, and Kadomtzev and Petviashvili.

DEFORMATION WAVES IN THE ELASTOPLASTIC MEDIA : "INTERNAL" SMALL PARAMETERS

Elastoplastic behavior is a characteristic one for solids in impact and explosion - induced deformation. In the range of insignificant shear stresses, the material undergoes elastic deformation, while under the exceeding of certain threshold stresses the material flows. In such a situation, the application of MSM to description of deformation waves has certain peculiarities. These peculiarities are caused by strong dependence of medium kinetic characteristics on stresses (and temperature) in the domain of elastic-to-plastic transition. This is a handicap to the expansion of the kinetic functions into the series over the small parameter ϵ.

Let us accept the initial unidimensional equations of Maxwell elastoplasticity in the form proposed by Godunov and Romenskii. Deformation kinetics in this model is determined by a single scalar function of stress tensor invariants, namely, by the shear stresses relaxation time.

At first the initial system of equation must be represented in the dimensionless form. The resulting set of small parameters may be written as:

$$\epsilon = -\frac{\sigma_1^*}{K_0} \sim \frac{\Delta\rho}{\rho_0}, \quad \mu_1 = \frac{3\zeta + 4\eta}{3K_0\tau_0}$$

$$\mu_2 = \frac{\kappa}{c_v K_0 \tau_0}, \quad \nu = \frac{c_l^2 - c_0^2}{2c_0^2}$$

Here K_0 *and* ρ_0 are respectively bulk modulus and solid density, ζ, η *and* κ are internal friction and heat transfer coefficients, c_l is phase velociy of longitudinal elastic waves, $c_0 = \sqrt{K_0/\rho_0}$, σ_1^* *and* τ_0 are characteristic values of stress and time from the boundary condition.

One further small parameter δ defines the width of elastic-to-plastic transition domain in the relation between relaxation time and dominant shear stress. The substitution of new small parameter δ provides the agreement between the calculated deformation wave structure and its experimentally observed splitting into elastic and plastic waves. It is apparent that the expansion of the relaxation equations over the ϵ/δ ratio makes no sense when $\delta \leq \epsilon$. Hence, the initial form of relaxation equations must be preserved. The decomposition procedure therewith reproduces the discussed above one, exept that the new restriction is substituded to provide the validity at the lenth range $x \leq O(\epsilon^{-1} + \mu^{-1})$

It is of interest to compare the results of numerical solution of initial elastoplastic equations and MSM ones. Such comparision was performed for the explosion–induced deformation wave in iron. The results of numerical calculations was found to be in a good agreement.

IMPULSE PROCESSES IN THE ELASTIC LIQUID-FILLED PIPES

Additional examples of MSM efficiency are the nonlinear problems on wave processes in a simple hydro-elastic systems. Here we shall consider nonlinear waves induced by a local build up of pressure in the liquid-filled elastic pipe. Liquid is presumed to be an ideal compressible one.

On the assumption that the shell deformations are insignificant, the hydraulic approximation for the liquid in motion can be used. The equation for the relative variation of pipe cross section under the effect of angle-independent loading may be written as

$$\frac{\partial^2 S}{\partial t^2} = -\frac{E_s h^2}{12\rho_s(1-\nu^2)}\frac{\partial^4 S}{\partial x^4} - \frac{E_s}{\rho_s a^2}S + \frac{2\Delta P(x,t)}{\rho_s a h} \tag{8}$$

Here E_s, ρ_s, ν - are Young modulus, density and Poisson ratio of shell material respectively, a is radius and h is thickness of the shell.

The possibility of MSM application is based on the presence of two small parameters. The first is the ratio of characteristic pressure to the bulk modulus of liquid $\epsilon = \Delta P_* / \rho_0 c_0^2$ and the second is liquid-shell interaction parameter $\mu = 2\rho_0 c_0^2 a / E_s h$.

Decomposition of the initial system results in two independent Witham - type equations for the Riemann's invariants $V_\pm = (u \pm \Delta p/\rho_0 c_0)/c_0 \epsilon$.

$$\frac{\partial V_\pm}{\partial \tau} \pm V_\pm \frac{\partial V_\pm}{\partial \xi_\pm} = \alpha \frac{\partial}{\partial \xi_\pm} \int_{-\infty}^{\infty} d\xi' R(\xi_\pm - \xi') V_\pm(\xi', \tau) \tag{9}$$

where $\tau = 4\epsilon\omega_0 t/(1+n), \xi_{\pm} = \omega_0(t \mp x/c_0), \omega_0 = \sqrt{E_s/\rho_s a^2}, \alpha = \mu/(1+n)\epsilon, n$ - is politropic exponent for liquid or gas. In equation (9), the integral operator kernel is defined by its Fourier tranfsorm

$$\bar{R}(\omega) = \frac{1}{1 - \omega^2 + D^2\omega^4} \tag{10}$$

for

$$D^2 = \frac{E_s^2 h^2}{12(1-\nu^2)\rho_s^2 a^2 c_0^4}$$

The equation (9), in view of (10), are conservative and can be found from the well-known variational principle for Witham's equations. It follows that equation (9) has three polynomial conservation laws and the conservation law, which contains the independent variables in an explicit form.

In the long-wave limit, equation (10) may be rearranged into the well-studied KdV-equation. The usual scenario of initial disturbance evolution for non-local generalisations of KdV-equation is disturbance decomposition into the soliton - like solutions and damping background. In this connection, the localised steady-state solutions of equation (9) are of importance. These solutions depend only on variable $y = \xi + \alpha\lambda\tau$, where λ is some arbitrary constant.

In $D \to 0$ limit, the stationary solutions can be found without difficulties. It turns out that localised soliton-like solutions exist only in the range $0 < \lambda < 1$; there exist two different kinds of localised solutions: the smooth ones and the singular ones. The smooth solutions (solitons) are characterized by positive pressure in pulse while the singular ones (we call them cavitons) differ in that they have a negative pulse pressure and two points with infinite derivatives. The computer simulation has showed that (with D = 0) the initial disturbance evolution really shows up as decomposition into sequence of solitons and cavitons and fast-damping background.

With $D \neq 0$, the localised solutions have been studied both by numerical and asymptotical (with $D << 1$) methods. The main result is that the spectrum of eigenvalues λ for solitons and cavitons becomes discrete and consisits of the finite number of points in the range from 0 to 1. With small D, "the quantisation rules" are obtained for the spectrum calculation in the first order in D.

The continuous spectrum decomposition is accompanied by the appearance of combined states and weak stationary chaos. The combined states may be treated as "molecules" composed of finite number of solitons and cavitons. Stationary chaos is defined as a series of randomly positioned solitons and cavitons. Thus we call it "soliton glass".

In adddition, with $D \neq 0$ there appears a new set of localised solutions with oscillating asymptotics with $|y| \to \infty$. The spectrum of eigenvalues λ of this set is continuous. With $D^2 < 1/4$ it fills the interval $(-4D^2/1 - 4D^2, 0)$; otherwise it fills semiaxes $\lambda < 0$ and $\lambda > 4D^2/(4D^2 - 1)$.

THE APPLICATION OF LUMPED PARAMETERS MODELS TO THE OPTIMAL CONTROL PROBLEMS OF STRONG BLAST WAVES

Optimal control problems of explosion-induced shock waves consist in search for optimal kinetics of energy discharge, which provides the "best" characteristics of the shock wave at given energy and certain restrictions of the energy discharge rate. The general formulation of these problems is extremely complicated both for blast waves in porous elastoplastic media and gases. Here, we shall restrict our consideration to the most simple case of strong explosion in an ideal gas.

A significant simplification of the problem may be achieved due to application of the method proposed by G. G. Chernyi. The essence of that method lies in the uniformly valid expansion of gas dynamic functions in series over small parameter $(\gamma - 1)/(\gamma + 1)$, where γ - is isentropic exponent. However, the first-order equations may be obtained in simple qualitative reasons.

The model is based on the fact that almost all gas mass behind the strong blast wave front is concentrated in the thin layer adjacent to the front.The mass velocity V varies insignificantly over the layer thickness and coincidence with the mass velocity on the shock, while the internal domain pressure P_c is leveled off and depends only on time. If the layer thickness to be neglected, the system of ordinary differential equations for P_c and front parameters can be obtained from the integral conservation laws:

$$\frac{dmV}{dt} = 4\pi R^2 P_c, m = \frac{4}{3}\pi R^3$$

$$\frac{4}{3}\pi R^3 \frac{P_c}{\gamma - 1} + \frac{mV^2}{2} = E(t); V = \frac{2}{(\gamma + 1)}\dot{R} \tag{11}$$

Here ρ_0 is undisturbed gas density, R(t) is front radius of blast wave, $E(t) \equiv E[R(t)]$ is the total energy value.

Furthermore, we can apply the set of equations (11) to give the first-order equation for the value $u_1 = R^3 \dot{R}^2$ ($\dot{R}$ is shock front velocity):

$$R\frac{du_1}{dR} + \frac{3(3\gamma - 1)}{\gamma + 1}u_1 = \frac{9(\gamma^2 - 1)}{4\pi P_0}E(R) \tag{12}$$

Equation (12) enables one to determine shock front parameters and integral values of thermal and kinetic gas energy for the arbitrary control function E(R). The evident boundary condition for equation (12) is the boundedness of u_1 with $R \to 0$.

An extraordinary simplicity of equation (12) makes it possible to reveal the main qualitative peculiarities of optimal control problems. In particular, the controllability of blast wave parameters under the given restrictions to kinetics may be easily evaluated in that model. The possibility of kinetics restoration by measuring of shock front parameters follows directly from equation (12).

The use of Pontryagin's maximum principle allows qualitative investigation of applied problems. For example, there has been performed the investigation of the problem on the most uniform heating of finfite gas mass by the blast wave. It is of interest to compare the results obtained within the context of gas dynamics equations with that of model under discussion. Such comparison was conducted by the example of the problem of thermal energy maximization. It has been detected that the results are in a good agreement between each other, though, in this case, the optimal kinetics is outside the formal limits of the model applicability.

CONCLUSION

Here, the object was to demonstrate the potentialities and peculiarities of asymptotic methods utilisation for qualitative and quantitative analysis of impact- and explosion-induced wave processes. The problems discussed above should be treated as the examples. An important point is that methods under consideration may be effective in solving of applied problems.

BIOSKETCH

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(see page 27)

EXPERIMENTATION AND MODELING OF COMPOSITE MATERIALS

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The discussion will be focused on dynamic behavior of continuous fiber reinforced polymeric composite materials. Experimental techniques using ultrasonic measurements, plate impact and high loading rate pneumatic test machine to characterize composite materials will be briefly discussed.
The test results of a S-2 glass reinforced plastic laminate obtained with the aforementioned testing techniques will be presented. A simple mechanical response material model will be formulated based on the test results, and be implemented into a hydrodynamic computer program for simulating a particular impact experiment. Technical issues related to the simulation and material modeling will be discussed.

BIOSKETCH

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SOME APPROACHES TO MODELING OF COMPOSITES MECHANICAL PROPERTIES WITH EMPLOYMENT OF GRAPHS THEORY.

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1. The character of arrangement of composite`s structure elements and their transference has big meaning for mechanical properties of materials. Hence the problem of structural analysis together with the problem of structure modeling acquire the paramount meaning when the substance synthesis, properties and behavior under the external influence are investigated. Designing the model by direct or indirect methods it is possible to predict the material structure and its manufacturing. Perhaps the only possible and obligatory condition in this case is the geometrical equivalence between the unit model`s element and the full material`s structure. It is considered that the medium structure units, including liquid haves character volume, spatial disposition and preferable distance between each other.

The analysis of literature on the composites modeling allows to select three main groups, namely:

-The modeling using molecular view on structure. Further development of this approach is nano-scale of structure.

-Rather large group of models with mechano-mathematical approaches for description of the structure and properties.Some attempts on using stochastic apparatus for description of composite`s behavior mechanism was done.

-Phenomenological approaches have especially large application. Structure-phenomenological modeling have the greatest development. In this case the structure of composite is described by two type of models:

-type A - the set of components without consideration of interphase processes;

-type B - the same with type A ,but with interphase. For example, model A - two component system without interphase, model B - three component system with interphase.

All variety of structure-phenomenological models is based on four concepts of connecting model`s elements:

1-successive;
2-parallel;
3-by combination successive and parallel;
4-using power function in the model.

Out off all proposed for today models which contain mentioned above principles it is possible to highlight the following:

A. The models with hard particles in the soft matrix;
B.The models with hard particles in the rigid matrix;
C.The models with interphase;

D.Another ones.

In this paper according to the graphs theory positions the analysis of some approaches to composite's modeling described in literature for practically all known phenomenological structure models was done. The results were compared with our own geometrical approach of modeling the elastic-strain properties of composites.

The principles of this geometrical approach has been presented below.

2. Proceeding from the supposition about the base impact of the fiber-matrix interphase and surface processes on the composite's structure and properties the agreed-upon model of compounded polymer, but taken as composites bit ("combit") - one-dimensional part of composite material has been considered below. Combit is separated to parts proportionally with content by volume of composite compounds and the elastic-strain problem is solved.

By analogy with Om's laws for circuit the problem is reduced to the calculation of graphs with the help of the generalized Kirgoph's laws and the concept of bar's rigidity is introduced.

$$G_c = \sum E_i /(1-\mu_2) \times S_i /l_i \qquad (1)$$

where E - modulus of elasticity, μ - Poisson's coefficient, S - cross section, l - length, i - combit's parts.

3. Assuming the hipothesis of interphase existense in composites and supporting the elastic-strain properties continuous from fiber to matrix using of the small parametr's method the formula for calculation the rigidity of interphase was founded as

$$G_{ph} = G_m * 3l_m/\delta \times E_f / (E_m + 2E_f) \qquad (2)$$

where G_m - the rigidity of matrix, E_m and E_f - matrix and fiber moduls, l_m - matrix length, δ - interphase thickness.

4.The variant of model with the normal force on the layer components of combit (x-direction) was investigated. The graph of this model was drawn and Kirgoph's and Guk's laws were applied to it.

From (1) and (2) x-model's rigidity equals

$$G_x = [(1/G_m) + (1 + \alpha_f) / G_f]\text{-}1 \qquad (3)$$

In the case of the action of force along the layer's compcnents of combat (y-direction) the formula for y-model's rigidity is equal to

$$G_y = G_f + (1 + \alpha_f) G_m \qquad (4)$$

where $\alpha = \delta/3l_m \times (2 + E_m/E_f)$.

By the action of the force in 0x-direction under some angle the formula is following:

$$G(\Theta\cdot) = G_x G_y / \sqrt{(} G_x^2 \cos 2\Theta + G_y^2 \sin 2\Theta) \qquad (5)$$

5. It is proposed to consider the matrix or compounded polymer structure as the set of combits consisting of segments, for example as triangles. In this segment strain was counted by approximate method where the rigidity G is described according to (1).

In the case of homogeneous-polymer matrix medium it is supposed that the sides of triangular segment have equal properties. For heterogeneous medium the triangular segment is designed from combits with parameters of components from this medium.

Finite element method was applied for calculation the triangular segment's strain-stress state using polynomial functions for the description of deformation. Rigdities between points are described by following equations:

$$G_i = E_i /(1 - \mu_i^2) \times 1/4A \times [B_{1,2,3} + C_{1,2,3} \times (1 - \mu_i) / 2 \qquad (6)$$

where $B_{1,2,3}$ and $C_{1,2,3}$ - elements of gradients matrix, A - area of a triangle.

Using graphs theory the corresponding graph is constructed and its calculation with the help of Kirgoph's generalized laws leads to receiving the equation for the rigidity of triangular segment:

$$G_c = G_1 + G_2 G_3 /(G_3 + G_2) \qquad (7)$$

where digits check with the numbers of triangular segments sides or with the composites components.

In this paper the results of calculation was compared with the experimental results. The difference between them is about 2-16%.

6.The analysis of the results of calculation and specifically the experimental data allows to support that the "ideality" of the composite's model is necessary to approach to the "reality" of material. The further search will be directed to the development of the model insertion-block for the general composite model with accounting a disparity between "ideality" and "reality".

BIOSKETCH

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ON THE ENTROPY DAMAGE ACCUMULATION MODEL OF COMPOSITE MATERIALS

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INTRODUCTION

The micromechanical model of the accumulated disperse damages for composites is presented. As a measure of the damage effect the increment of entropic density is proposed. The entropic formulation allows to account the mechanical and non-mechanical factors of failure process.

The formulation of the problem, the basic difficulties and some approaches of modelling and the bulk of experimental data are given in the papers[1-7].

Here the measure of local microdefect is assumed to be the associated increment of the local entropic density. The generation and growth of defects is modelled in real time t. The variable t may be the number of loading cycles, length of loading arc.

The increase of entropic density is supposed to be process accounting the microdefect eneration and growth, viscous resistance, diffusion, chemical reactions.

THE MODEL FORMULATION

The velocity of entropic density generation defined by mechanical and non-mechanical factors is written based on the Coury principle and Honsager relations .The first invariant of the deformation rates, the gradient of the temperature,deviator of the greep deformation velocities and so on are thermodynamical forces of various nature (scalar, two-rank tensor etc.). The associated thermodynamical flows are of the independent factors of the same nature.

For modelling of the processes it may be written the system of the government equations (Honsager relations) that are connected thermodynamical forces to flows. Taking into account the heat conductivity coefficient, concentration of the given element for diffusion, the deviators of the creep deformations and stresses the increment of entropic density defined by viscous resistance and diffusion are written .

The one of the entropic models may be formulated with the aid of the energy balance equation, where member with of the free energy density accounts the entropy increasing based on the microdefect generation and growth. The distribution of stiffness E defined by microdefects as a function of time is to be known from experimental data.

However the other model is formulated which possess the advantages of the micromechanical approach and based on the use the micromechanical parameters. The number of these parameters may be defined directly in experiment and show the clear physical interpretation.

Let the variable s(t,r) is a function of local microdefect is defined by vector r. Based on local measure it may introduce the vector (for plate cracks) and the tensor (for pores) parameters of the defects. The local measure of the damage may be formulated as a symmetrical micromechanical two-rank tensor s. It accounts the value of the elementary microdefect and orientation of the defect. The microparameter p can introduce as averaging of the tensor s over the accounted volume. This value is described also the irreversible process and s function of increasing of local entropic density. The trace of the tensor p describes the change of the material volume.

For the plate microcrack system the local measure of microdefect is vector directed across the crack plane and it length defined the microcrack length.

The increment of the entropic density S in accounted volume is defined by the defect growth and the generation of the new ones. Using of the microparameter s and macroparameter S we can introduce value of defects density.

Let P is density of defects (a number of defects). Then we can define the rate of the new microdefects generation. As a result the equation for macroparameter S of damage accumulation is written.

The value s and the rate of the new microdefect generation may be considered accordingly as a thermodynamical force and a thermodynamical flux. The value s is the measure of the damage effect (the entropy increment) depended on the microdefect initiated at time t.

The equation for S may be written in the statistical form if P is presented as the random variable of the Poisson process. For example, in the case of function s(r,t) =qexp[-a(t-r)]. The equation for S may be written in the form of the Langeven stochastic equation [8] with the fluctuation member qv.

The accumulation of damages including the heat conductivity, viscous deformations and ets. is modelled with the aid of kinetic equation for the rate of the entropy density increment S.

It may be pointed out the two basic micromechanical parameters of the entropy density ncrement: the microdefect density P (the rate of the microdefect nucleation v(t,S) and the damage factor due to the microdefect s(t).

In generally s is the tensor object. Therefore P is the tensor of the same rank and accounts the defects and its orientation.

The types of defects are depended from the loading direction with respect to fires, the strength of resin, fibres and strength of bonds between fibres and resin. To describe these items the kinetic equations for microparameters s and P are written.

Thus we can write complete system of kinetic equations for the model.

The two form of CDS for the layered composites are considered The first form is depended on the propagations of transversal cracks in the matrix, and the second one is depended on the microdamages in the reinforced elements (fiber crushing). There are another forms of the microdamages, for example, the fiber breaking is initiated the cracks in matrix which under propagation are delayered the matrix along fibers and then are initiated macrocracks.

It was found based on the experiments that the polynomial and exponent functions are appropriate approximations for the distribution of the macrodefect density for different stages of accumulation process.

The degradation of transversal cracks under quasistatic and cyclic loading is developed with deacceleration and strength stabilization. For the second stage of the characteristic damage states the microdefect density is increased with acceleration. The transformation to the second stage is depended on the stress level of the actual damage status. To describe his stage we used more complicate form of approximation for microdefects density.

The composite structure is accounted in the form of the stress reanalysis according the layered material.

The analysis of this model have led to the following conclusions.

1. The distribution of the damage status for the time is S- ype.
2. The stage of the low growth of the damage effect is smaller for the case of the microcracks in matrix directed in fibres and transversal cracks than for the case of delamination from broken fibres.
3. Under the fatigue loading the damage accumulation isn't controlled by the delayering process .
4. The heating of composite is important factor of the defect development process and is stimulated essentially the second stage of the damage accumulation process.
5. As a result of the thermocycle loading and multisection process analysis was found that the linear summation hypothesis may be incorrect.

The two-stage approach of development of the microdefects is allowed to model satisfactorily the processes of the stiffness degradation and residual strength.

The model of the stiffness degradation is based on the local equilibrium hypothesis and balance energy equations for thermodynamical potential. According to the formulation of the model the variation of the residual strength with the damage status growth is approximated well (in qualitative form) the experimental data.

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BIOSKETCH

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CONCURRENT ENGINEERING

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Efficient application of composites calls for a concurrent analysis of materials selection, design and manufacturability. The need for such concurrent engineering is more imperative for composites than for conventional materials because, for the latter, product geometry and materials selection dictate the manufacturing processes that can be used.

In the present paper we describe a concurrent engineering strategy for composites. We identify relational databases that are needed and survey some of the available process simulation models that can be used to interrogate manufacturability during design phase. A unified model is then proposed for simulation of fiber compaction and resin flow.

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PROGRESS IN COMPUTATIONAL MODEL BY FINITE ELEMENT METHOD OF VISCOELASTIC HETEROGENEOUS CONTINUA PROPERTIES. OBJECT-ORIENTED FINITE ELEMENT PROGRAMMING FOR RESEARCH OF COMPOSITE MATERIALS.

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Finite element method (FEM) is very widely used in practice for numerical calculation of strength-stress states and mechanical behavior of materials and constructions.

Distinctive feature of the new program complex "UNIVERS" from traditional finite element programs, which have been usualy written on procedure languages (such as ALGOL, FORTRAN, PL1 and etc.), is its object-oriented nature. All algorithms, functions and methods of the program are constracted pursuant to the laws of mathematical abstraction (mathematical laws of transformation of objects). Hierarchy of objects and laws of their interaction was developed too. It allows, particulary, to expediently use of vectoral and tensoral nature of displacements, strains and stresses, for solution of the continuous media and composite materials, mechanics and the geomechanics problems.

Programs constructed on the base of traditional finite elements method are characterized by a lot of calculations, unsufficient reliability of a programm code at large volumes the initial text. Such kind of programs, written on procedure algorithm languages are very hardly madified and adapted for other conditions (programming environments, computing systems etc.).

Above indicated problems could be avoided by using of the object-oriented approach in programming. Such approach allows to create of the high level, large reliability, easily adapting to different systems programm product. Taking into account above said, algorithm language C ++, as the most suitable was accepted for development of a programm complex.

The newest lexical opportunities of the language C++ are used in the program . In particular, finite elements tamplates, principles of inheritance in hierarchy of data classes vectoral representation for storage base of multy dimensional arrays was employed.

The program complex is intended for the decision of the stress-strain state, stability and strength problems :

- continuous media and composite materials;
- geomechanics;
- truss constructions.

The finite element formulation for continuous medium is realized isoparametric. The library of finite elements includes:

1. One-dimensial isoparametric element.

2. Two-dimensial isoparametric elements with quantity of node points from 4 up to 8, which describe following conditions stress-strain state:
- plane-straine state;
- plane-stress state;
- axisymmetric state.

3. Solid elements with quantity of node points from 8 up to 21.

For finite elements continuous media simulation the number of mathematical models, allowing to simulate the nonlinear features deformation of natural and constructional materials was provided. Following models in the program complex are realized:

1. Isotropic material.
2. Unisotropic material.
3. Nonlinear-elastic material.
4. Incremental model of defomability type.
5. Model of elastic-plastic current with criterium of plasticity:
   - Fon-Mises;
   - Drucker-Prager.
6. Viscoelastic material.

As a whole the program permits:
- elastic and nonlinear-elastic accounts;
- to use in accounts simultaneously some materials with various characteristics;
- to use in accounts simultaneously some materials with various models;

Using of the "UNIVERS" program the elastic- plastic calculations by one-axes compression and extension and pure shear for the cell of periodicity of filled fibrous composite with interphase layers vere made.

BIOSKETCH

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Alex N.Vlasov is a Associate Professor of Moscow Civil Engineering University and senior Scientific Researcher of Institute of Applied Mechanics of Russian Academy ofSciences. He graduated from Mechanics and Mathematics Department of Moscow State University (1978). From 1979 to 1984 he worked at Military Scietific Research Institute and from 1984 up to now at the Moscow Civil Engineering University. He received his Ph.D.degree in 1990 from above University. He is the author of more than 20 scientific articles.

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RECENT ADVANCES IN MECHANICS OF COMPOSITES

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Research in mechanics of composites dealing with physically based theories for the deformation, damage initiation, damage growth and failure of polymer matrix composite materials, subjected to complex stress states and severe environments will be discussed. Recent accomplishments in the Mechanics of Composites research thrust at the Office of Naval Research will be described. Accomplishments in the following areas will be summarized: micromechanics based three-dimensional constitutive theories for laminated composites; local-global approaches for the analysis of thick laminates; microbuckling theories for unidirectional composites; models for compression failure; delamination growth models; impact damage models; moisture absorption and moisture-induced damage in composites; and the effect of defects on mechanical response and failure.

BIOSKETCH

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Dr. Yapa D.S. Rajapakse manages research in Mechanics of Composite Materials, Fracture Mechanics, Quantitative Non-destructive Evaluation and Ice Mechanics in the Ship Structures Division at the Office of Naval Research, Arlington, VA., U.S.A.

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He is on the editorial boards of six technical journals (J. Composite Materials, Intl. J.Composites Engineering, J. Reinforced Plastics and Composites, Intl.J.Plasticity, Engineering Fracture Mechanics, J. Computational Mechanics). He is very active in several technical societies. He has organized Symposia on Mechanics of Thick Composites, Impact Response of Composites, and Ultrasonic Characterization and Mechanics of Interfaces for the American Society of Engineering Science (SES). He was elected Vice-President of SES for 1994 and President of SES for 1995.

THE NEW CONSTITUTIVE EQUATION FOR SHAPE MEMORY MATERIALS END SHAPE MEMORY COMPOSITES

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The shape memory material (SMM) show the cosiderable promise for the creation new structures and advanced technology. These materials utilize in deployable structures, demountable tight joints, adaptive sistems, geometry changing surfaces, active elements with high power or (and) high accuracy and so on. The most promissing for such structures are the composites with shape memory filaments or plies and flexible matrix (SMC). One of the number adventures of such composites is the opportunity of the structural two way shape memory effect [1,2].

The broad introduction of SMM and SMC is restrained because of lack of the constitutive equations such a materials that would can describe the whole set of its unique mechanical properties. The known phenomenological constitutive equation for SMM [3,4] is onedimensional. The equations based on the structural-analitical approach [5] and known micromechanical approaches [6,7] are too complex for practical purposes in solution two- or threedimensional problems.

It is known that the reason of the unusual behavior of SMM are the termoelastic martensitic transformations prosiding in such materials under changes of temperature or (and) stresses. This process comprises the nucleation (dissapearance) and drowing (degradation) the martensitic crystals in austenitic matrix.

Formerly the new micromechanical approach was elaborated to formulate the constitutive equations for solids of complex structure the changing of state of witch is connected with nucleation and growth some microcarriers [8,9]. Previously this method was applied in continuous damage mechanics where microdefects play the role of microcariers. The damage accumulation equations was derived for damage tensor in the case of metall working process and for damage axial vector in the case of low-cycle fatigue theory [8].

In the case of SMM the role of microcariers play the crystals of martensite. The models are formulate for nucleation, disappearance and development these crystals during forward and reverse martensitic transformation.

In the framework of nucleation model the contribution B_{ij} to the increment of phase deformation due to this process is calculated from equation

$$B_{ij} = \beta\delta_{ij} + C_0\sigma'_{ij}$$

where δij is the unit tensor, $\sigma' ij$ - deviator of stress, β, C_0 parameters of material. In the model of disapearance of the martensite crystals during reverse transformation tensor B_{ij} consists of two terms coresponding to the reverse B_{1ij} and monotonic B_{2ij} shape memory effect. The unified model is formulate for microcariers development just as for forward so for reverse transformation. For this model the increment of microphase deformation because of development of single crystal is proportional to the current value of this deformation.

On the foundation of these micromodeles one can deduce with aid of micromechanical procedure [8,9] the constitutive equations for phase deformation tensor ε_{ij}^F in SMM:

$$d\varepsilon_{ij}^F/dq = B_{ij} + \alpha_0\varepsilon_{ij}^F \qquad (1)$$

where q is the volume part of martensite,

$$B_{ij} = \begin{cases} \beta\delta_{ij} + C_0\sigma'_{ij} & \text{if} \quad dq>0 \\ \lambda B_{1ij} + (1-\lambda)B_{2ij} & \text{if} \quad dq<0 \end{cases}$$

α_0, C_0, β, λ is the material parameters.

Besides of equation (1) it is used the equations for elastic deformation and termal expansion. In these equations it takes into account the difference between the values of elastic modulus and termal expansion coefficient for martensite and austenite states.

Unlike the known proposals, this model descripts the most broad set of properties of SMM namely:

- forward martensitic transformation with constant or;
- variable stress, includind complex stress state;
- oriented martensitic transformation;
- shape memory including reverse and two way shape memory effects;
- martensitic inelastisity;
- pseudoelastisity and so on.

The constitutive equations is formulated for finite phase deformation using Jaumann derivatives for Henky tensor of deformation and Cauchy stress tensor.

In the simplest case this nonlinear problem for two - or three dimensional body can be solved analytically with aid of Laplas transformation. For more complicated problem will be create the finite element computer program.

This constitutive equation for SMM was used for investigation of the behavior of composites, containing filaments or plies from SMM and flexible matrix. Two example of such composites are considered in thise work. The thirst is onedirectional composite beam with filaments from SMM. The filaments in austenitic phase state are loaded of constant tensile stress and cool through the iterval of forward martensite transformation temperature. These filaments elongate ap to the deformation of 8%-10%. Then the filaments are embedded into the flexible matrix such as silicone, polyurethane or diflone. If the temperature of filaments in such a composite increase (for example due to current) within the interval of reverse transformation they shorten because of shape memory effect. The lenght of beam decrease. In this state matrix have some compressive stress, filaments have some tensile one. Then if the temperature of filaments decrease, the filaments elongate because of forward martensitic transformation in the presence of tensile stress. By this means structural two way shape memory effect is relevant for such a composite. But the tensile stress in filaments have to be suffisient to restitute the original size of composite. The condition of closed two way shape memory effect is derived for such composite beam:

$$z \leq e^{\alpha_0(1-1/z)}$$

where

$$z = [\alpha_0/C_0E_f](1+([1-\mu]/\mu)(E_f/E_m))$$

E_f, E_m is the elastic modulus of filament and matrix, μ - volume fraction of filaments. As well are found the relations between useful load, temperature and displasement, stresses and strains in such a composit. Similarly was considered composites beam with two outer thin shape memory plies and flexible thick middle layer. This beam is able to twist if the temperature in outer plies changes.

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BIOSKETCH

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ELASTICALLY TAILORED COMPOSITES: ANALYSIS AND TESTING

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Elastically tailored composite designs are being used to achieve favorable deformation modes under a given loading environment. Coupling between deformation modes such as extension-twist or bending-twist is created by an appropriate selection of fiber orientation, stacking sequence and blend of materials.

Two main challenges are associated with the implementation of elastically tailored composites. The first, is concerned with the development of a reliable analytical model which accounts for the influence of the material's anisotropy. The second, is the design of test methods which can accurately measure the various coupling associated with a given loading.

From the analytical standpoint, the fundamental mechanism producing elastic failoring in advanced composites is a result of their anisotropy. A review of the analytical methods developed for elastically tailored composites is presented. A theory based on a variational asymptotical analysis of 2D shell theory is proposed in order to assess the accuracy of predictions from previously developed theories.

A number of methods for testing extension-twist coupling in elastically tailored composites are discussed. The benefits and limitations of each of the methods are highlighted. Quantitative results for each of the testing methods using a standard specimen are shown and compared to determine the applicability and suitability of each of the methods.

A comparison of results with previously developed theories, Finite Element simulations and test data will be presented. Two demonstration tests featuring bending-twist and extension-twist coupling will be conducted in order to illustrate the physical mechanisms which induce coupling.

BIOSKETCH

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His areas of expertise include the analysis and design of advanced composite structures, failure characterization and damage modeling of laminated composites, computational solid mechanics and elastic tailoring of composites. He has published over 50 articles in refereed journals, conference proceedings and parts of books. He edited a book on Interlaminar Fracture of Composites and is presently working on a follow up volume on Fracture of Composites.

He received a number of awards including the 1985 Sigma Xi Award for Outstanding Ph.D. Thesis in Engineering, the 1989 ASTM Best Paper Award, the 1990 ASCE Outstanding Paper Award and the 1991 Sigma Xi Ph.D. Thesis Advisor Award for Outstanding Ph.D. Thesis in Engineering.

He is an Associate Fellow of AIAA, member of several professional societies and their technical committees. He is the editor of Key Engineering Materials, published by Trans Tech Publications and member of the editorial board for the Journal of Composites Technology and Research published by ASTM.

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INSTITUTE OF APPLIED MECHANICS
OF RUSSIAN ACADEMY OF SCIENCES
(IAM RAS)

IAM RAS was organized in 1989 for promotion of three very important fundamental scientific directions on theoretical and applied mechanics, namely: i) mechanics of composites and constructions; ii) mechanics of structured and heterogeneous continua; iii) physico-chemical mechanics.

There are close connection between IAM RAS and many scientific and industrial institutions and companies. The applications of scientific achievements and treatments and inculcations them to industry are so very important part of IAM RAS activity.

Many outstanding scientists have been working here among them are: active member of Russian Academy of Sciences academician, Doctor of Sciences (Dr.Sc.) Ivan F. Obraztsov, Director of IAM RAS; active member of Russian Academy of Engineering, professor, Dr.Sc. Alex I.El'kin; active member of New York Academy of Sciences, professor, Dr.Sc. Yuri G. Yanovsky, Deputy Director; professor, Dr.Sc.Andrey A.Movchan, Head of Department; Doctor Alex I.Malkin, Head of Department; Doctor Yuri A. Basistov and Nikolai V. Nikitin, leading scientific associates etc.

IAM RAS is organizer of International Symposia on Rheology and "Advances in Structured and Heterogeneous Continua".

More than twenty articles have been published in International Scientific Journals yearly. Three monographs and few books of collected articles have been printed for the last three years too.

The main interests area of IAM RAS are: theoretical and applied mechanics problems, fluid dynamics, rheology, mechanics of composites, new computational methods in mechanics and applied mathematics, computer mechanics and nanotechnology.