

Conference on

Emerging Issues in Mathematics and Computation from the Materials Sciences

April 18-20, 1994
Pittsburgh Vista Hotel
Pittsburgh, Pennsylvania

Conducted by
the Center for Nonlinear Analysis,
Carnegie Mellon University,
and SIAM

CONFERENCE THEMES

- Crystal Growth, Solidification,
and Interface Motion
- Effective and Optimal
Properties of Composite
Materials and Ceramics
- Liquid Crystals and other
Mesomorphic States of Matter
- Magnetic Materials
- Materials Issues in Nonlinear
Optics
- Material Microstructure and
Macroscopic Behavior
- Superconductivity and Its
Applications

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April 18 - 20, 1994

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D E A D L I N E D A T E S

Hotel Reservation
 Monday, March 28, 1994

 Conference Preregistration
 Monday, April 4, 1994

O R G A N I Z I N G C O M M I T T E E

- David Kinderlehrer, Chair**
 Department of Mathematics and Center for Nonlinear Analysis, Carnegie Mellon University
- John M. Ball**
 Department of Mathematics and International Centre for Mathematical Sciences, Heriot Watt University, Scotland
- Maria-Carme T. Calderer**
 Department of Mathematics, Pennsylvania State University
- Max D. Gunzburger**
 Department of Mathematics, Virginia Polytechnic Institute and State University
- Morton E. Gurtin**
 Department of Mathematics and Center for Nonlinear Analysis, Carnegie Mellon University
- Robert V. Kohn**
 Courant Institute of Mathematical Sciences, New York University
- Mitchell B. Luskin**
 School of Mathematics, University of Minnesota, Minneapolis
- Geoffrey B. McFadden**
 Computing and Applied Mathematics Laboratory, National Institute of Standards and Technology
- Jerome V. Moloney**
 Department of Mathematics, University of Arizona
- Peter Palffy-Muhoray**
 Liquid Crystal Institute, Kent State University

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P R O G R A M O V E R V I E W

Following are subject classifications for the sessions. The codes in parentheses designate session type and number. The session types are invited plenary presentations (IP), contributed presentations (CP), and minisymposia (MS). Some of the conference themes have been widely drawn. One may find concurrent sessions related to a particular theme. For the poster session, please refer to page 8 of the program.

Crystal Growth, Solidification, and Interface Motion

- Interfaces (IP3, page 5)
 Mathematical Perspectives in Diffusive Processes and Pattern Formation (MS1, page 4)
 Pattern Formation During the Motion of Phase Boundaries (IP5, page 7)
 A Phase-Field Diffuse Interface Solidification Model for Binary Alloys (IP4, page 7)
 Solidification Modeling and Computation — Parts 1 and 2 (MS8 and MS12, pages 7 and 8)
 Solidification and Phase Field Methods (CP2, page 6)
 Stability and Diffusion (CP5, page 8)
 Topological Transitions (MS16, page 9)

Effective and Optimal Properties of Composites

- Bounds and Optimization (CP4, page 7)
 Composite Materials and Structural Optimization (MS7, page 6)
 Computational Methods for Determining the Effective Properties of Composite Materials (MS22, page 11)
 Effective Moduli of Composites (MS2, page 4)
 Homogenization (CP6, page 8)
 Mathematical Perspectives on Composite Media (IP1, page 4)
 Percolation Problems in Materials Science (MS5, page 5)

Liquid Crystals and Other Mesophases of Matter

- Current Issues in Liquid Crystals — Parts 1 and 2 (MS14 and MS19, pages 9 and 10)
 Emerging Issues in Liquid Crystals (IP7, page 9)

Magnetic Materials

- Electromagnetic Fluids (MS10, page 7)
 Magnetic Materials (MS6, page 6)

Materials Issues in Nonlinear Optics

- Materials Issues in Nonlinear Optics (MS18, page 10)
 Nonlinear Optical Properties of Bulk, Quantum-Well, Quantum-Wire, and Quantum-Dot Semiconductors (IP9, page 10)

Microstructure and Macroscopic Properties of Materials

- Computation of Crystalline Microstructure (MS4 and MS9, pages 5 and 7)
 Dynamic Phase Transitions in Elastic Materials (MS21, page 11)
 Dynamics of Plasticity and Elasticity (CP3, page 6)
 Electronic Materials Processing: Modeling, Methodology and Challenges (MS17, page 10)
 Failure and Strength Mechanisms (CP7, page 10)
 Magnetic Materials (MS6, page 6)
 Mathematical Issues in Material Microstructure (MS13, page 8)
 Microstructure and Hysteresis (IP2, page 4)
 Some Statistical Issues in Materials Science (MS3, page 5)
 The Elastic Properties of Heterogeneous Materials (MS11, page 7)
 Variational Methods in Materials Sciences (IP6, page 8)
 Viscoelasticity and Cavitation (CP1, page 5)

Superconductivity

- Modeling, Analysis and Computation for Macroscopic Phenomena in Superconductors (IP8, page 9)
 Recent Trends and Developments in Superconductivity (MS15 and MS20, pages 9 and 11)

F U N D I N G A G E N C Y

This conference is conducted with the partial support of the National Science Foundation.

G E T - T O G E T H E R

Welcoming Reception
 Sunday, April 17, 1994
 6:00 PM - 8:00 PM
 Cambria Room
 Cash Bar and mini hors d'oeuvres.

PROGRAM-AT-A-GLANCE

SUNDAY, APRIL 17	MONDAY MORNING, APRIL 18	TUESDAY MORNING, APRIL 19	WEDNESDAY MORNING, APRIL 20
<p>6:00 PM-8:00 PM Registration opens <i>Allegheny Foyer</i></p> <p>6:00 PM-8:00 PM Welcoming Reception <i>Cambria Room</i></p>	<p>7:00 Registration opens <i>Allegheny Foyer</i></p> <p>7:45 Opening Remarks David Kinderlehrer <i>Allegheny Room</i></p> <p>7:55 Welcome Avner Friedman <i>Allegheny Room</i></p> <p>8:05 IP1 Mathematical Perspectives on Composite Media Graeme W. Milton <i>Allegheny Room</i></p> <p>8:45 IP2 Microstructure and Hysteresis Richard D. James <i>Allegheny Room</i></p> <p>9:30 Coffee <i>Allegheny Foyer</i></p> <hr/> <p>10:00 AM-12:00 PM Concurrent Sessions</p> <p>MS1 Mathematical Perspectives in Diffusive Processes and Pattern Formation Organizer: Gunduz Caginalp <i>Somerset Room</i></p> <p>MS2 Effective Moduli of Composites Organizers: Robert V. Kohn and Graeme W. Milton <i>Allegheny Room</i></p> <p>MS3 Some Statistical Issues in Materials Science Organizer: Alan F. Karr <i>Crawford Room</i></p> <p>MS4 Computation of Crystalline Microstructure — Part 1 of 2 Organizer: Mitchell B. Lusk <i>Cambria Room</i></p> <p>CP1 Viscoelasticity and Cavitation Chair: Michael Renardy <i>Butler Room</i></p>	<p>7:30 Registration opens <i>Allegheny Foyer</i></p> <p>8:00 IP4 A Phase-Field Diffuse Interface Solidification Model for Binary Alloys William J. Boettinger <i>Allegheny Room</i></p> <p>8:45 IP5 Pattern Formation During the Motion of Phase Boundaries Robert F. Sekerka <i>Allegheny Room</i></p> <p>9:30 Coffee <i>Allegheny Foyer</i></p> <hr/> <p>10:00 AM-12:00 PM Concurrent Sessions</p> <p>MS8 Solidification Modeling and Computation — Part 1 of 2 Organizer: Geoffrey B. McFadden <i>Allegheny Room</i></p> <p>MS9 Computation of Crystalline Microstructure — Part 2 of 2 Organizer: Mitchell B. Lusk <i>Crawford Room</i></p> <p>MS10 Electromagnetic Fluids Organizer: Michael J. Shelley <i>Cambria Room</i></p> <p>MS11 The Elastic Properties of Heterogeneous Materials Organizers: Graeme Milton and David Kinderlehrer <i>Somerset Room</i></p> <p>CP4 Bounds and Optimization Chair: Frank Morgan <i>Butler Room</i></p>	<p>7:30 Registration opens <i>Allegheny Foyer</i></p> <p>8:00 IP7 Emerging Issues in Liquid Crystals Peter Palfy-Muhoray <i>Allegheny Room</i></p> <p>8:45 IP8 Modeling, Analysis and Computation for Macroscopic Phenomena in Superconductors Max D. Gunzburger <i>Allegheny Room</i></p> <p>9:30 Coffee <i>Allegheny Foyer</i></p> <hr/> <p>10:00 AM-12:00 PM Concurrent Sessions</p> <p>MS14 Current Issues in Liquid Crystals — Part 1 of 2 Organizers: Maria-Carme T. Calderer, Eugene C. Gartland, Jr., Mitchell B. Lusk, and Peter Palfy-Muhoray <i>Somerset Room</i></p> <p>MS15 Recent Trends and Developments in Superconductivity — Part 1 of 2 Organizers: Qiang Du and S. Jonathan Chapman <i>Allegheny Room</i></p> <p>MS16 Topological Transitions Organizer: Robert V. Kohn <i>Crawford Room</i></p> <p>MS17 Electronic Materials Processing: Modeling, Methodology and Challenges Organizer: H. Thomas Banks <i>Cambria Room</i></p> <p>CP7 Failure and Strength Mechanisms Chair: Luke E.K. Achenie <i>Butler Room</i></p>
	<p>MONDAY AFTERNOON, APRIL 18</p> <p>12:00-1:30 Lunch</p> <p>1:30 IP3 Interfaces Joseph B. Keller <i>Allegheny Room</i></p> <p>2:15 Coffee <i>Allegheny Foyer</i></p> <hr/> <p>2:45-4:45 Concurrent Sessions</p> <p>MS5 Percolation Problems in Materials Science Organizer: Kenneth M. Golden <i>Crawford Room</i></p> <p>MS6 Magnetic Materials Organizers: David Kinderlehrer, Ling Ma, and Robert Rogers <i>Allegheny Room</i></p> <p>MS7 Composite Materials and Structural Optimization Organizer: Robert V. Kohn <i>Butler Room</i></p> <p>CP2 Solidification and Phase-Field Methods Chair: Eduardo Socolovsky <i>Somerset Room</i></p> <p>CP3 Dynamics of Plasticity and Elasticity Chair: Timothy J. Burns <i>Cambria Room</i></p>	<p>TUESDAY AFTERNOON, APRIL 19</p> <p>12:00-1:30 Lunch</p> <p>1:30 IP6 Variational Methods in Materials Sciences Irene Fonseca <i>Allegheny Room</i></p> <p>2:15 Coffee <i>Allegheny Foyer</i></p> <hr/> <p>2:45-4:45 Concurrent Sessions</p> <p>MS12 Solidification Modeling and Computation — Part 2 of 2 Organizer: Geoffrey B. McFadden <i>Allegheny Room</i></p> <p>MS13 Mathematical Issues in Material Microstructure Organizers: John Ball and Irene Fonseca <i>Cambria Room</i></p> <p>CP5 Stability and Diffusion Chair: Karl Gustafson <i>Somerset Room</i></p> <p>CP6 Homogenization Chair: Michel Artola <i>Crawford Room</i></p> <p>Poster Session <i>Butler Room</i></p>	<p>WEDNESDAY AFTERNOON, APRIL 20</p> <p>12:00-1:30 Lunch</p> <p>1:30 IP9 Nonlinear Optical Properties of Bulk, Quantum-Well, Quantum-Wire, and Quantum-Dot Semiconductors Stephan W. Koch <i>Allegheny Room</i></p> <p>2:15 Coffee <i>Allegheny Foyer</i></p> <hr/> <p>2:45-4:45 Concurrent Sessions</p> <p>MS18 Materials Issues in Nonlinear Optics Organizer: Jerome V. Moloney <i>Fayette Room</i></p> <p>MS19 Current Issues in Liquid Crystals — Part 2 of 2 Organizers: Maria-Carme T. Calderer, Eugene C. Gartland, Jr., Mitchell B. Lusk, and Peter Palfy-Muhoray <i>Butler Room</i></p> <p>MS20 Recent Trends and Developments in Superconductivity — Part 2 of 2 Organizers: Qiang Du and S. Jonathan Chapman <i>Crawford Room</i></p> <p>MS21 Dynamic Phase Transitions in Elastic Materials Organizer: Morton E. Gurtin <i>Cambria Room</i></p> <p>MS22 Computational Methods for Determining the Effective Properties of Composite Materials Organizer: Leslie F. Greengard <i>Somerset Room</i></p> <p>5:00 Conference adjourns</p>

CP = Contributed Presentations
IP = Invited Presentations
MS = Minisymposium

Contributed presentations are spaced twenty minutes apart, allowing each presenter fifteen minutes for presentation and five minutes for discussion. Minisymposium presentations are spaced thirty minutes apart, allowing each presenter twenty-five minutes for presentation and five minutes for discussion. Each plenary talk is forty-five minutes, including time for discussion.

MONDAY MORNING, APRIL 18

7:00/Allegheny Foyer
Registration opens

7:45/Allegheny Room
Opening Remarks

David Kinderlehrer, Carnegie Mellon University

7:55/Allegheny Room
Welcome

Avner Friedman, University of Minnesota, Minneapolis

8:05/Allegheny Room
 IP1/Chair: Robert V. Kohn, Courant Institute of Mathematical Sciences, New York University

Mathematical Perspectives on Composite Media

Colloidal suspensions, polycrystalline materials, porous rocks containing oil or salt water, fibrous materials, foams, slurries, bubbly fluids, cracked solids, granular aggregates, and ceramics are all examples of composites. They are inhomogeneous materials which have the same macroscopic response to applied thermal, electrical, magnetic, or elastic fields as homogeneous materials. The effective coefficients governing this response depend non-linearly on the moduli of the constituent materials and upon the geometry of the composite. Research in the field has been driven by two objectives: the estimation of the effective coefficients of a given material, such as a sample of rock extracted from the earth; and the quest for optimal microstructures that maximise, or come close to maximizing, a given combination of properties. The speaker will present a broad survey of some of the progress that has been made through the development of fast algorithms, application of novel variational techniques, analytic function theory, and Hilbert space methods. He will review the connection with non-convex energy minimization problems.

Graeme W. Milton
 Courant Institute of Mathematical Sciences, New York University

8:45/Allegheny Room
 IP2/Chair: David Kinderlehrer, Carnegie Mellon University

Microstructure and Hysteresis

The presence of hysteresis is often considered to be a defining characteristic of first order phase transformations. The hysteresis observed during heating and cooling can vary from hundreds of degrees centigrade to one or two degrees centigrade in apparently similar materials that undergo first order phase transformations, and the size of the hysteresis does not seem to correlate with any of the standard material properties that are commonly measured for transforming materials. Hence, there is a challenge to understand the origins of hysteresis based on sound mathematical models of transforming materials.

In recent years, there has been increasing interest among applied mathematicians in the prediction of hysteresis, based on direct modeling of the hysteresis loops. The speaker will advocate a different viewpoint, in which the emphasis is on accurate modeling of the material. This approach will be illustrated by a survey of recent research that highlights the importance of microstructure, metastability, relaxation and computational method.

Richard D. James
 Department of Aerospace Engineering and Mechanics, University of Minnesota, Minneapolis

9:30/Allegheny Foyer
Coffee

10:00 AM-12:00 PM
Concurrent Sessions

MS1/Somerset Room
Mathematical Perspectives in Diffusive Processes and Pattern Formation

The formation of patterns arising from diffusive processes and shocks has been under study from a number of perspectives. Sharp interface, phase field and statistical approaches are among the modeling techniques used in analytical and numerical study. This minisymposium focuses on the comparative insight and information that can be attained from different approaches.

Michael Cross will discuss coarsening and the persistent dynamics of domain structures. He will also consider reduced descriptions of chaos and compare equilibrium and non-equilibrium. Gunduz Caginalp will also discuss comparisons of static and dynamic as they arise in layer formation in alloys from a phase field perspective. John Chadam will present studies on the stability of the interface using a sharp interface model. John Grove will also discuss sharp interface models as they are used in the numerical computation of shocks.

Organizer: Gunduz Caginalp, University of Pittsburgh, Pittsburgh

10:00 Chaotic Domains and Domain Coarsening in Non-equilibrium Systems
 Michael Cross, California Institute of Technology

10:30 Solute Trapping in Binary Alloys
 Gunduz Caginalp, Organizer

11:00 Solidification Interface Instabilities
 John Chadam, McMaster University, Canada

11:30 A Quantitative Numerical Analysis of Shock Accelerated Fluid Interfaces
 John Grove, State University of New York, Stony Brook

MS2/Allegheny Room
Effective Moduli of Composites

(This session will run until 12:30 PM)

Composite materials arise in many areas of materials science, physics, and engineering. A fundamental issue is to understand the link between microstructure and macroscopic behavior. One type of problem involves microstructures that are either partially or completely known; then the goal is to estimate the effective behavior. A different type of problem is the design of microstructures whose effective behavior is in some sense extremal. A variety of mathematical methods are relevant, including variational principles, compensated compactness, and complex analysis.

Organizers: Robert V. Kohn and Graeme W. Milton
 Courant Institute of Mathematical Sciences, New York University

10:00 Optimal Bounds Correlating Electric, Magnetic, and Thermal Properties of Two-Phase, Two-Dimensional Composites
 Karen Clark, Stevens Institute of Technology, and Graeme W. Milton, Organizer

10:30 Viscoelastic Composites: Bounds and Realizable Models
 James Berryman, Lawrence Livermore National Laboratory; Leonid Gibiansky, Princeton University; and Graeme W. Milton, Organizer

11:00 Perturbation Methods in the Study of the Overall Behavior of Composite Materials
 Oscar Bruno, Georgia Institute of Technology

11:30 Nonlinear Homogenization: Application to Metal-Matrix Composites and Polycrystals
 Pedro Ponte-Castaneda, University of Pennsylvania

12:00 An Optimal Lower Bound on the Elastic Energy of a Composite Made from Two Non Well-Ordered Isotropic Materials
 Gregoire Allaire, Commissariat à l'Energie Atomique, France; and Robert V. Kohn, Organizer

10:00 AM-12:00 PM

Concurrent Sessions

MS3/Crawford Room

Some Statistical Issues in Materials Science

The minisymposium will focus on issues in materials science with important statistical content, on which progress is possible by means of collaboration between materials and statistical scientists. The speakers will focus on materials microstructure and microstructure - property relations. They will discuss important materials issues driven by considerations of data, mathematical modeling and simulation, and with substantive mathematical and computational content.

The minisymposium builds on workshops held at the Catholic University of America in June, 1993, and the National Institute of Standards and Technology in July, 1993, in identifying promising directions of collaborative research between materials scientists and statisticians.

Organizer: Alan F. Karr, National Institute of Statistical Sciences

10:00 Mechanical Properties of Strongly Nonhomogeneous Systems
Stewart K. Kurtz, Pennsylvania State University

10:30 Scalings and Distributions in Lattice Models for Material Failure
S. Leigh Phoenix, Cornell University

11:00 Some Statistical Issues in Materials Science Related to the Evolution and Inhomogeneity of Microstructure
Owen Richmond, Alcoa Technical Center, Pittsburgh

11:30 Macroscopic Behavior of Random Media from the Microstructure
Salvatore Torquato, Princeton University

MS4/Cambria Room

Computation of Crystalline Microstructure (Part 1 of 2)

The computation of material microstructure is important to the development and control of new materials such as shape memory materials, martensitic crystals, and magnetostrictive crystals. Effective computational methods are essential for comparing the results of new theories and models with experiment.

Material microstructure occurs when twinning occurs on a fine scale or when the deformation gradient oscillates on a fine scale. Theories have been developed which treat this phenomena on an atomic as well as on a continuum scale. This minisymposium will feature some of the important advances which have been made during the past several years in the computation of solutions to these models.

Organizer: Mitchell B. Luskin, University of Minnesota, Minneapolis

10:00 Atomistic Structure and Dynamics of a Displacive Transformation Interface
Philip C. Clapp and Shuangjian Chen, University of Connecticut, Storrs

10:30 Adaptive Finite Element Analysis of Crystalline Microstructures
Ellad Tadmor, Rob Phillips and Michael Ortiz, Brown University

11:00 Computational Modeling of the Martensitic Transformation
Mitchell Luskin, Organizer and Petr Klouček, University of Minnesota, Minneapolis

11:30 Tweed Precursors in Martensitic Transformations
Sivan Kartha, Institute for Advanced Study; James P. Sethna and James A. Krumhansl, Cornell University

CPI/Butler Room

Viscoelasticity and Cavitation

Chair: Michael Renardy, Virginia Polytechnic Institute and State University

10:00 Linear Stability of Hyperbolic PDEs and Viscoelastic Flows
Michael Renardy, Virginia Polytechnic Institute and State University

10:20 About Mathematical Models for Anisotropic n -dimensional Viscoelastic Materials
Jaime E. Munoz Rivera, Laboratorio Nacional de Computacao Cientifica, Brasil

10:40 Spurt and Instability in a Two-Layer Johnson-Segalman Liquid
Yuriko Yamamuro Renardy, Virginia Polytechnic Institute and State University

11:00 Effects of Material Anisotropy and Inhomogeneity on Cavitation for Composite Incompressible Anisotropic Nonlinearly Elastic Spheres
Debra A. Polignone, Carnegie Mellon University, and Cornelius O. Horgan, University of Virginia

11:20 Numerical Simulation of the Deformation of Viscoelastic Solids
S. Shaw, M.K. Warby, and John R. Whiteman, Brunel University, United Kingdom

11:40 An Algebraic Criteria for Cavitation
Pablo V. Negron, University of Puerto Rico, Rio Piedras

12:00-1:30

Lunch

1:30/Allegheny Room

IP3/Chair: Avner Friedman, University of Minnesota, Minneapolis

Interfaces

Interfaces between materials are usually rough or irregular on a microscopic scale, and sometimes they are even rough on a macroscopic scale. Consequently the boundary or interface conditions satisfied by fields (elastic, electro-magnetic, acoustic, thermal, etc.) at such interfaces are complicated. Various methods have been employed to simplify them in order to facilitate their use in analytical and numerical studies of fields. The speaker will review some of these methods, which are based upon the assumed smallness of the height of the roughness elements. He will then present a new method, valid for roughness of any height. This new method is based upon the assumed smallness of the "wavelength" of the roughness.

Joseph B. Keller

Departments of Mathematics and Mechanical Engineering, Stanford University

2:15/Allegheny Foyer

Coffee

2:45-4:45

Concurrent Sessions

MSS/Crawford Room

Percolation Problems in Materials Science

The physical properties of many inhomogeneous materials with highly contrasting phases depend strongly on whether or not one phase "percolates", or forms a connected matrix which spans a sample. Percolation effects on atomic and macroscopic scales dominate the behavior of a broad range of materials, such as semiconductors, cermets, piezoresistors, and porous media. In recent years, there have been a number of mathematical advances in both the pure theory of percolation and in the analysis of discrete and continuous models of transport in percolating systems. However, these advances fall short of providing a comprehensive foundation for understanding the properties of the above rather complex materials. In this minisymposium, the speakers will describe recent mathematical developments, and a number of actual percolation problems arising in the analysis of materials.

Organizer: Kenneth M. Golden, University of Utah

2:45 Percolation Problems Arising in the Analysis of Inhomogeneous Materials
Kenneth M. Golden, Organizer

3:15 How to Use Percolation Theory for PDE's Describing Transport Through Inhomogeneous Media
Serguei M. Kozlov, Université de Provence Aix-Marseille 1, France

3:45 Applications of Percolation Theory to Experimental Measurements of the Electrical Properties of Some Binary Media
David S. McLachlan, University of Witwatersrand, South Africa

4:15 Percolation and Conductivity in Magnetized Heterogeneous Media
Michael B. Isichenko, University of Texas, Austin and Kurchatov Institute of Atomic Engineering, Russia

2:45-4:45

Concurrent Sessions

MS6/Allegheny Room

Magnetic Materials*(This session will run until 5:15 PM)*

Magnetic materials have a long and distinguished history and, since the early days of electromagnetic theory, an important technological role. What are the contemporary issues and potential applications associated with these materials? Two areas of rapid progress in recent times are magnetic recording and highly magnetostrictive materials. They will be highlighted here. Moreover, promising new analytical methods are under development. This is an opportune moment to assess the promise of applied mathematics and interdisciplinary research in this agenda.

Organizers: David Kinderlehrer, Carnegie Mellon University Ling Ma, Carnegie Mellon University and Institute for Advanced Study and Robert Rogers, Virginia Polytechnic Institute and State University

- 2:45 Modeling in Magnetic Recording**
Stanley H. Charap, Carnegie Mellon University
- 3:15 On the Macroscopic Response of Magnetostrictive Materials**
Antonio De Simone, Carnegie Mellon University and Università di Roma "Tor Vergata", Italy
- 3:45 The Computation of Magnetic Materials: The Thin Film Case**
Ling Ma, Organizer
- 4:15 New Mathematical Tools for Studying Microstructures**
Luc Tartar, Carnegie Mellon University
- 4:45 Giant Magnetostrictions and High Power Magnetostrictive Devices**
Joseph P. Teter, Naval Surface Warfare Center

MS7/Butler Room

Composite Materials and Structural Optimization*(This session will run until 5:15 PM)*

The goal of structural optimization is to choose the shape or composition of a structure so as to optimize some aspect of its response. This problem has traditionally been approached by methods based on "front-tracking". In recent years a new approach has emerged, based on the use of composite materials as structural components. As numerical experience has been gained in applying this new approach, many questions have arisen: what types of discretizations avoid undesired instabilities? Is it better to use simple composites, optimal ones, or maybe even "fictitious" ones? Can one design a numerical method that prefers "classical" designs over relaxed ones, other things being equal?

Organizer: Robert V. Kohn, Courant Institute of Mathematical Sciences, New York University

- 2:45 Proposal for an Integrated Design System Involving Concurrent Design and Manufacturing**
Noboru Kikuchi, University of Michigan, Ann Arbor
- 3:15 Optimal Design of Material Properties and Material Distribution for Single and Multiple Loading Conditions**
Martin Bendsoe, Technical University of Denmark, Denmark
- 3:45 Relaxation of Optimal Design Problems: Reduction to the Minimization of a Sum of Energy Densities**
Andrei Cherkov, University of Utah
- 4:15 Materials with Prescribed Constitutive Parameters: An Inverse Homogenization Problem**
Ole Sigmund, Technical University of Denmark, Denmark
- 4:45 An Algorithm for Three-Dimensional Shape Optimization**
Gilles Francfort, Carnegie Mellon University

CP2/Somerset Room

Solidification and Phase Field Methods*(This session will run until 5:05 PM)*

Chair: Eduardo A. Socolovsky, Hampton University

- 2:45 Phase Field Computational Approaches to Crystal Growth and Propagating Fronts**
Eduardo A. Socolovsky, Hampton University
- 3:05 Rigorous Asymptotics for a Fully Nonlinear Phase-Field Equation**
Robert Jerrard, University of California, Berkeley
- 3:25 Cahn-Hilliard Simulations of Ternary Alloy Separation**
David J. Eyre, University of Minnesota, Minneapolis
- 3:45 Banded Microstructures in Rapid Solidification**
Douglas A. Huntley, University of Minnesota, Minneapolis; and Stephen H. Davis, Northwestern University
- 4:05 Tight-Binding Molecular Dynamics Simulations of Liquid Gallium Arsenide**
Rebecca Mih, University of California, Berkeley; R. Virkkunen, and R. Nieminen, Helsinki University of Technology, Finland
- 4:25 Oscillatory Instabilities in Directionally Solidified Eutectics**
Brenda A. Diesslin and William T. Grayhack, Iowa State University

CP3/Cambria Room

Dynamics of Plasticity and Elasticity*(This session will run until 5:05 PM)*

Chair: Timothy J. Burns, National Institute of Standards and Technology

- 2:45 Singular Poincaré-Andronov-Hopf Bifurcation in a Model of "Discontinuous" Plastic Deformation**
Timothy J. Burns, National Institute of Standards and Technology
- 3:05 Granular Flow with a Hypoplastic Constitutive Relation**
E. Bruce Pitman, State University of New York, Buffalo
- 3:25 A Traveling-Wave Analysis in Uniaxial Plastic Flows and Application to Longitudinal Impacts**
Feng Wang, State University of New York, Stony Brook
- 3:45 Perturbed Scale-Invariant Initial Value Problems in One-Dimensional Dynamic Elastoplasticity**
Michael S. Gordon, North Carolina State University
- 4:05 Wave Propagation and Internal Pressure in Liquid-Filled Elastomeric Composite Tubes**
C.R. MacCluer, and C.J. Radcliffe, Michigan State University; A.J. Hull, Naval Undersea Warfare Center; and T.L. Scofield, Michigan State University
- 4:25 Phase Boundary Motion in Elastic Materials: Kinetically Governed Approach to Equilibrium**
Thomas J. Pence, Michigan State University
- 4:45 Hyperbolic Equations of Inelastic Media and Their Symmetric Form**
E.I. Romensky, Institute of Mathematics, Russia

7:30/Allegheny Foyer
Registration opens

8:00/Allegheny Room
 IP4/Chair: Geoffrey B. McFadden, National Institute of Standards and Technology
A Phase-field Diffuse Interface Solidification Model for Binary Alloys

The phase-field method was previously developed for pure materials to treat solid-liquid interface motion with complex (dendritic) shapes. A field variable describes the state (solid or liquid) at different points in the material and the dynamics of this field are governed by the Cahn-Allen equation. The speaker will discuss present work that extends the method to binary alloys using a single free energy function to couple this equation to the Cahn-Hilliard equation. This second equation describes the evolution of the composition field. Physical effects such as capillarity, nonequilibrium interface kinetics and solute trapping are naturally included. Composition segregation patterns that remain after dendritic solidification have been obtained.

William J. Boettinger
 Metallurgy Division, Materials Science and Engineering Laboratory, National Institute of Standards and Technology

8:45/Allegheny Room
 IP5/Chair: Morton E. Gurtin, Carnegie Mellon University
Pattern Formation During the Motion of Phase Boundaries

The boundaries that separate phases during a first order phase transformation, such as crystallization, can have morphologies that are quite complex. This is due to morphological instabilities, but also to anisotropic capillarity and interface attachment kinetics. Examples are cells and dendrites. The governing free boundary problems are difficult to solve except in special cases.

The speaker will discuss a phase field model in which two coupled PDEs are solved numerically in order to eliminate boundary tracking. He will present results for solution of the phase field model in the context of dendritic growth at high undercoolings and compare dendrite tip radii and growth speeds with the predictions of theoretical principles such as marginal stability, microscopic solvability, and optimum stability. (This work is supported by the National Science Foundation under grant DMR 9211276).

Robert F. Sekerka
 University Professor of Mathematics and Physics, Carnegie Mellon University

9:30/Allegheny Foyer
Coffee

10:00 AM-12:00 PM
Concurrent Sessions

MS8/Allegheny Room
Solidification Modeling and Computation (Part 1 of 2)

The behavior of interfaces separating different phases of a material is a subject of scientific and technological importance, involving interdisciplinary contributions from pure and applied mathematicians, physicists, and materials scientists. Current work in this area includes the derivation and analysis of models of the creation, thickness, stability, shape, and motion of phase boundaries. The speakers will describe problems in solidification and other types of phase transitions and discuss treatments of both sharp and diffuse interfaces will be discussed.

Organizer: Geoffrey B. McFadden, National Institute of Standards and Technology

- 10:00 **Computation of Laplacian Dendrites**
 Robert Almgren, University of Chicago
- 10:30 **Computational Crystal Growth Using Fully Faceted Interfaces**
 A. Roosen, National Institute of Standards and Technology
- 11:00 **Studies of Pattern Formation in a Binary Alloy Using a Phase-Field Model**
 James A. Warren, National Institute of Standards and Technology
- 11:30 **Monte Carlo Simulation of Growth Patterns in Eutectic Systems**
 J. Iwan D. Alexander, Rong-Fu Xiao, and Franz Rosenberger, University of Alabama, Huntsville

MS9/Crawford Room
Computation of Crystalline Microstructure (Part 2 of 2)

For description, see MS4 on page 5

Organizer: Mitchell B. Luskin, University of Minnesota, Minneapolis

- 10:00 **Computations of Twinning in the Two-Well Problem**
 Charles R. Collins, University of Tennessee, Knoxville

- 10:30 **Oscillation Problems in the Calculus of Variations**
 Michel Chipot, Université de Metz, France
- 11:00 **Algorithms for the Computation of Microstructure**
 Noel J. Walkington, Carnegie Mellon University
- 11:30 **The Effects of Mesh Orientation on Computed Microstructures**
 Han Wang and R. A. Nicolaides, Carnegie Mellon University

MS10/Cambria Room
Electromagnetic Fluids

Electro-magnetic (EM) fluids are candidates as "Smart Fluids" that can respond to applied electromagnetic fields with changes in their basic fluid rheology and stability properties. Their application to control of fluid flows and devices, or to understanding dipolar fluidic systems, are active areas of research in the engineering and physics communities. EM fluids have a rich phenomenology whose study lies between the fields of materials science and fluid mechanics. Basic questions of such as microscopic and macroscopic formulation, stability, and phase transition, are being pursued. The speakers in this minisymposium will discuss the current state of experimental, theoretical, and computational work.

Organizer: Michael J. Shelley, Courant Institute of Mathematical Sciences, New York University

- 10:00 **Rheological Properties of Ferrofluid Composites**
 Ronald Rosensweig and J. Popplewell, Exxon Research and Engineering, Annandale, NJ
- 10:30 **Ferrofluid Labyrinths: Theory and Experiment**
 Raymond Goldstein, Princeton University
- 11:00 **Do Spontaneously Magnetized Liquids Exist?**
 Mike Widom, Carnegie Mellon University
- 11:30 **The Leaky Dielectric Model of Electrohydrodynamics**
 Dudley Saville, Princeton University

MS11/Somerset Room
The Elastic Properties of Heterogeneous Materials

(This session will run until 12:30 PM)

Heterogeneous solids exhibit a wide range of elastic behaviours, influenced by variations in material moduli, the presence of cracks, internal stresses arising from the formation of precipitates, or other mechanisms such as ductile fracture. The talks in this minisymposia provide a sampling of problems in this field.

Organizers: Graeme Milton, Courant Institute of Mathematical Sciences, New York University and David Kinderlehrer, Center for Nonlinear Analysis and Department of Mathematics, Carnegie Mellon University

- 10:00 **Small-contrast Perturbation Expansions for the Effective Properties of Nonlinear Composites**
 Pierre M. Suquet, LMA/CNRS, France; and Pedro Ponte-Castaneda, University of Pennsylvania
- 10:30 **Frobenius Series Solutions for Materials with Radially-Varying Elastic Moduli**
 Melanie P. Lutz and Mauro Ferrari, University of California, Berkeley
- 11:00 **Elastic Equilibrium of Heterophase Solids**
 A.L. Roytburd, University of Maryland, College Park
- 11:30 **Issues Concerning Ductile Fracture of Materials**
 Warren M. Garrison, Jr., Carnegie Mellon University
- 12:00 **The Energy Balance Relations for a Small Crack in a Solid with a Nonlinear Displacement Field**
 Alexander Movchan, University of Bath, United Kingdom

CP4/Butler Room
Bounds and Optimization

Chair: Frank Morgan, Williams College

- 10:00 **Clusters Minimizing Energy of Interfaces and Singular Curves**
 Frank Morgan, Williams College
- 10:20 **Extremal Microstructure for Two Isotropic Phases with Distinct Stress-free Strains in Two Space Dimensions**
 Robert V. Kohn, Courant Institute of Mathematical Sciences, New York University; and Jiangbo Lu, Carnegie Mellon University
- 10:40 **Explicit Optimality Conditions for Elastic Energy in a Two Phase Composite with Anisotropic Component Materials in Two Space Dimensions**
 Yury Grabovsky, Courant Institute of Mathematical Sciences, New York University
- 11:00 **Composite Plates of Extremal Rigidity**
 Andrei Cherkov, University of Utah; and Leonid Gibiansky, Princeton University
- 11:20 **Accurate Phenomenological Models that Agree with Experiments for Ferroelectric-Ferroelastic Crystals: A Semi-infinite Optimization Formulation**
 L. Vu-Quoc and V. Srinivas, University of Florida; and J. Cross, Digital Equipment Corporation
- 11:40 **Optimal Control of Phase Transitions**
 Matthias Heinkenschloss, Virginia Polytechnic Institute and State University

12:00-1:30

Lunch

1:30/Allegheny Room

IP6/Chair: John Ball, Heriot-Watt University, Scotland

Variational Methods in Materials Sciences

The speaker will discuss the study of material instabilities such as phase transitions and the formation of defects and microstructure in crystalline materials from the point of view of the calculus of variations.

She will discuss new mathematical techniques that have been introduced for the treatment of equilibria for nonconvex problems and for models involving interfacial energy contributions and will consider the formation of microstructure and oscillatory behavior using the notion of generalized solutions such as Young measures, H-measures and varifolds.

Irene Fonseca

Department of Mathematics, Carnegie Mellon University

2:15/Allegheny Foyer

Coffee

2:45-4:45

Concurrent Sessions

MS12/Allegheny Room

Solidification Modeling and Computation (Part 2 of 2)

(For description, see MS8 on page 7)

Organizer: Geoffrey B. McFadden, National Institute of Standards and Technology

2:45 **Phase-field Model of Eutectic Growth**

Alain S. Karma, Northeastern University

3:15 **Stochastic Eutectic Growth**

Martin Grant, McGill University, Canada

3:45 **Diffuse-Interface Modeling of Phase Transitions of a Binary Alloy with FCC Crystal Structure**

Richard J. Braun, William J. Boettinger, John W. Cahn, and Geoffrey B. McFadden, National Institute of Standards and Technology, and Adam A. Wheeler, National Institute of Standards and Technology and University of Bristol, United Kingdom

4:15 **Phase-field Modeling with Nonlocal Free-energies**

Kirk Brattkus, Southern Methodist University

MS13/Cambria Room

Mathematical Issues in Material Microstructure

(This session will run until 5:15 PM)

In recent years there has been a remarkable progress in the mathematical understanding of the formation of microstructure in crystalline materials. The successful exploitation of smart materials is among its many applications in materials sciences. As older techniques fail to apply, new mathematical tools have been introduced in the theory of partial differential equations and in the calculus of variations. They rely on the concept of generalized solutions and require the handling of new homogenization problems.

This session is directed to applied mathematicians and materials scientists and the agreement between theory and experiments will be discussed.

Organizers: John Ball, Heriot-Watt University, Scotland and Irene Fonseca, Carnegie Mellon University

2:45 **The Behavior of Polycrystalline Shape-Memory Materials**

Kaushik Bhattacharya, California Institute of Technology and Robert V. Kohn, Courant Institute of Mathematical Sciences, New York University

3:15 **Transition Between Martensitic Variants Under Biaxial Stress**

Chun-hwa Chu and Richard D. James, University of Minnesota, Minneapolis

3:45 **Stress-induced Microstructures in Crystals, and a Necessary and Sufficient Condition for Attainment in the Scalar Calculus of Variations**

Gero Friesecke, Carnegie Mellon University

4:15 **A Model for Twinning in BCC Crystals**

Phoebus Rosakis and Hungyu Tsai, Cornell University

4:45 **Phases and Phase Stability in the Cu-Al-Zn System**

Marc De Graef, Carnegie Mellon University

CP5/Somerset Room

Stability and Diffusion

Chair: Karl Gustafson, University of Colorado, Boulder

2:45 **Bistability and Multistability**

Karl Gustafson, University of Colorado, Boulder

3:05 **Stability of Cylindrical Bodies in the Theory of Surface Diffusion**

Bernard D. Coleman, Richard S. Falk, and Maher Moakher, Rutgers University

3:25 **Modeling and Simulation of Reaction and Diffusion in a Corrosion Cell**

Jeffrey H. Dunn, Naval Research Laboratory

3:45 **Nonlinear Diffusion from a Lattice-Gas Model**

William T. Grayhack and James W. Evans, Iowa State University

4:05 **An Advanced Model for Dopant Diffusion in Polysilicon**

Helmut Puchner and Siegfried Selberherr, Technical University of Vienna, Austria

CP6/Crawford Room

Homogenization

(This session will run until 5:05 PM)

Chair: Michel Artola, Université Bordeaux I, France

2:45 **Wave Propagation in Some Chiral Composite Materials**

Michel Artola, Université Bordeaux I, France; and Michel Cessenat, CEA - Centre d'Etudes de Limeil, France

3:05 **Wave Propagation Along Grain Boundaries**

Elliott S. Alber, Courant Institute of Mathematical Sciences, New York University; and J.L. Bassani, University of Pennsylvania

3:25 **Effective Moduli and Quasi-Regular Mappings**

Vincenzo Nesi, University of L'Aquila, Italy

3:45 **A Homogenized Model for a Molten Carbonate Fuel Cell**

Joseph D. Fehribach, Worcester Polytechnic Institute

4:05 **Homogenization of Two Phase Emulsions with Surface Tension Effects**

Robert Lipton and Bogdan Vernescu, Worcester Polytechnic Institute

4:25 **Two-point Padé Approximants for Effective Transport Coefficients**

Stanislaw Tokarzowski and Jerzy Blawoziewicz, Institute of Fundamental Technological Research, Poland; and Igor Andrianov, Civil Engineering Institute, Ukraine

4:45 **Flow of Conductive Fluids in Porous Media**

A. Galka, J.J. Telega and Richard Wojnar, IPPT of Polish Academy of Sciences, Poland

Butler Room

Poster Session

Ab-initio Total-energy Calculations: Ground State Instability of the Uniform Electron Gas

Yefim Levin, C.D. Wu and Y. Bar-Yam, Boston University

An Algebraic Grid Generation Technique for Tracking Interface Motion

Bonita V. Saunders, National Institute of Standards and Technology

Electronic Structure Calculations for Organic Superconductors on High-Performance Architectures

A. Smith, University of Washington; Michael Minkoff and R. Benedek, Argonne National Laboratory; and L.H. Yang, Lawrence Livermore National Laboratory

Propose of Basic Idea for Mathematically Composing and Simple Calculations for Liquid-Glass- Encapsulation Growth GaAs Crystal Stoichiometric Deviations

Yasuyuki Saito, Toshiba Corporation, Japan

Coupled Fields in Heterogeneous Solids and Homogenization

S. Bytner, B. Gambin, A. Galka, J.J. Telega, and Richard Wojnar, IPPT of Polish Academy of Sciences, Poland

7:30/Allegheny Foyer
Registration opens

8:00/Allegheny Room
 IP7/Chair: Maria-Carme T. Calderer, Pennsylvania State University
Emerging Issues in Liquid Crystals

Liquid crystalline materials play key technological roles in information display and structural applications. Many recent advances in modeling their behavior are the result of relaxing restrictive assumptions of earlier descriptions. Characterizing orientational order by a tensor rather than a vector field, for example, has led to qualitatively new features in both static configurations and in dynamic response, in agreement with experimental observations. The increased complexity of the models gives rise to challenging mathematical and numerical problems. The speaker will present some illustrative examples, involving equilibrium structures, steady state configurations in the presence of shear and other fields, and interfacial instabilities.

Peter Palffy-Muhoray
 Liquid Crystal Institute and Department of Physics, Kent State University

8:45/Allegheny Room
 IP8/Chair: Mitchell B. Lusk, University of Minnesota, Minneapolis
Modeling, Analysis and Computation for Macroscopic Phenomena in Superconductors

Superconductivity has become of subject of renewed interest since the recent discovery of materials that retain superconductive properties at temperatures above the boiling point of nitrogen. A brief history of superconductivity will be presented, along with a brief description of some applications in which superconducting materials are used. Various mathematical models for superconductivity will be discussed, including some that are thought to apply to the "high critical temperature" materials. A sample of the analyses and computations that have been performed based on these models is then presented. The speaker will close with a brief discussion of the possible roles that mathematicians can play in the further development of the science and technology of superconductivity.

Max D. Gunzburger
 Department of Mathematics and Interdisciplinary Center for Applied Mathematics, Virginia Polytechnic Institute and State University

9:30/Allegheny Foyer
Coffee

10:00 AM-12:00 PM
Concurrent Sessions

MS14/Somerset Room
Current Issues in Liquid Crystals (Part 1 of 2)

Liquid crystals are orientationally ordered fluids with anisotropic bulk properties. The speakers will discuss problems in pure liquid crystals and liquid crystal composites which are materials with great promise for information displays; orientational order also plays a key role in polymers in structural applications, the understanding of equilibrium configurations, the response to applied fields, and instabilities in non-equilibrium situations. They will consider the description and determination of equilibrium configurations, the dynamics of the approach to equilibrium, hydrodynamics, convective and interfacial instabilities, and intensity dependent optical nonlinearities.

Organizers: Maria-Carme T. Calderer, Pennsylvania State University, University Park, Eugene C. Gartland Jr., Kent State University, Mitchell Lusk, University of Minnesota, Minneapolis, and Peter Palffy-Muhoray, Kent State University

- 10:00 **On the Topology of Defects in Nematics and the Changes of Defect Structures at Uniaxial-Biaxial Phase Transitions**
 Alfred Saue, Max-Planck-Gesellschaft, Germany
- 10:30 **Numerical Minimization of a Landau-deGennes Free Energy for Liquid Crystals**
 Eugene C. Gartland Jr., Timothy A. Davis, and Peter Palffy-Muhoray, Kent State University
- 11:00 **Defect Structures in Nematic Solutions of a Rodlike Polymer**
 Guy C. Berry, Carnegie Mellon University
- 11:30 **Flow Instabilities and Dynamics of Defects in Liquid Crystals**
 Maria-Carme T. Calderer, Pennsylvania State University

MS15/Allegheny Room
Recent Trends and Developments in Superconductivity (Part 1 of 2)
 The theory of Type-II superconductors is a rapidly changing and exciting area, which has a key role in the continuing development of high-Tc materials. Of particular importance is the understanding of the so-called "vortices" which are characteristic of Type-II superconductors.

There are two sessions, which have been designed to highlight the mathematical stimulation that has resulted from some complementary theoretical and computational approaches to vortex modeling.

The talks in the first session will feature (i) a rigorous mathematical analysis of a certain boundary-value problem, which sheds light on the problem of vortex nucleation, (ii) more formal methods of matched asymptotic expansions that are needed to understand vortex dynamics, the key mechanism for losses in superconducting materials, and (iii) formal averaging to produce a model for the vortex density analogous to the Euler equations for an inviscid rotational fluid.

The talks in the second session will feature (i) discussions of simplified dynamical equations for vortices, vortex liquids and vortex lattices, (ii) analytical and computational studies of vortex motion and vortex pinning, simulations in various geometrical regions, analysis of different discretization techniques.

Organizers: Qiang Du, Michigan State University and S. Jonathan Chapman, University of Oxford, United Kingdom

- 10:00 **Creation, Motion and Homogenization of Vortices in Type-II Superconductor**
 S. Jonathan Chapman, Organizer
- 10:30 **A Semi-Elliptic System for a Superconductor Model**
 Henri Berestycki, Université Pierre et Marie Curie, France; Alexis Bonnet, CERMICS, ENPC and École Normale Supérieure (DMI), France; and S. Jonathan Chapman, Organizer
- 11:00 **Magnetic Flux Dynamics in Superconductors**
 Alan T. Dorsey, University of Virginia
- 11:30 **Vortex Dynamics in Superconductors**
 Jacob Rubinstein, Indiana University, Bloomington

MS16/Crawford Room
Topological Transitions

This minisymposium brings together two related themes: (i) Weak solutions of interface motion laws, even after singularity formation or change of topological type; these are so far understood primarily for "local" models of interface motion. (ii) Problems in which diffusion plays an essential role, for example Hele-Shaw flow, which represents a quasistatic limit of solidification dynamics; here singularities can form, but there is not yet much theory for what happens afterward. The hope, of course, is that by focusing on both themes at once we might discover some points in common.

Organizer: Robert V. Kohn, Courant Institute of Mathematical Sciences, New York University

- 10:00 **Singularity Formation in Hele-Shaw Flow and in the Motion of Vortex Sheets**
 Michael Shelley, Courant Institute of Mathematical Sciences, New York University
- 10:30 **Interface Motion with Triple Junctions**
 H. Mete Soner, Carnegie Mellon University
- 11:00 **Interface Evolutions with Boundary Conditions**
 Yoshikazu Giga, Hokkaido University, Japan
- 11:30 **Topological Transitions and Singularities in Nonlinear Diffusion Equations**
 Andrea Bertozzi, Michael Brenner, Leo Kadanoff and Todd Dupont, University of Chicago

10:00 AM-12:00 PM
Concurrent Sessions

MS17/Cambria Room

Electronic Materials Processing: Modeling, Methodology and Challenges

In recent years, the modeling of fluid flow and mass transport processes in physical vapor transport and chemical vapor deposition reactors has provided significant insights into the phenomena controlling the performance of the processes such as reactor geometry, flow patterns, and temperature.

This minisymposium will focus on the modeling and control of transport phenomena in crystal growth processes. The speakers will describe mathematical models that can be used to predict and control the process outcome and their influence on the experimental implementation of these processes. They will also discuss computational issues related to flow simulations and validation of the mathematical models. The multidisciplinary scope of both experimental design and mathematical modeling will be emphasized in order to stimulate exchange of ideas.

Organizer: H. Thomas Banks, Center for Research in Scientific Computation, North Carolina State University

- 10:00 **Modeling of Transport in Crystallization from Vapors**
Franz Rosenberger, University of Alabama, Huntsville
- 10:30 **Thermal Diffusion Effects in Chemical Vapor Deposition**
Ivan O. Clark, NASA Langley Research Center
- 11:00 **Modeling and Optimal Control of Transport Process in High Pressure Vapor Deposition of Optoelectronic Devices**
Klaus J. Bachmann, H. Thomas Banks, Kuzufumi Ito, Hien T. Tran, and Jeffrey S. Scroggs, North Carolina State University
- 11:30 **Effect of Radiation Heat Transfer on the CVD Process for Materials**
Mohammed Kassemi and S.A. Gokoglu, NASA Lewis Research Center

CP7/Butler Room

Failure and Strength Mechanisms

(This session will run until 12:20 PM)

Chair: Luke E.K. Achenie, University of Connecticut

- 10:00 **Thermomechanical Behavior of a Porous Material and its Failure During Combustion**
N.J. Salamon and Sun-pyo Lee, Pennsylvania State University, University Park
- 10:20 **Interface Failure Analysis of Multilayered Ceramic Composites**
Jose F. Magalhaes and Ashley F. Emery, University of Washington
- 10:40 **Computational Analysis of Failure Mechanisms in Synthetic Membrane Laminates**
Luke E.K. Achenie and Robert J. Fisher, University of Connecticut
- 11:00 **Stress-Strength Reliability for Braced Systems**
Hossein Arsham, University of Baltimore; Darush Davani, Towson State University; and Arthur B. Kahn, University of Baltimore
- 11:20 **Long Time Behaviour of an Evolutionary Ginzberg-Landau System**
Q. Tang, University of Sussex, United Kingdom
- 11:40 **Discontinuous Deformation Gradients and the Onset of Fracture in Nonlinear Elasticity**
Salim M. Haidar, Grand Valley State University
- 12:00 **A Quasi-Steady Approximation to an Integro-Differential Model of Interface Motion**
Piotr Rybka, Warsaw University, Poland

12:00-1:30

Lunch

1:30/Allegheny Room

IP9/Chair: Jerome V. Moloney, University of Arizona

Nonlinear Optical Properties of Bulk, Quantum-Well, Quantum-Wire, and Quantum-Dot Semiconductors

Strong optical excitation may change the insulating characteristics of semiconductors all the way to quasi-metallic behavior. These changes are the source of large optical nonlinearities which are interesting not only because of their intrinsic quantum mechanical nature, physical complexity, and richness of dynamic phenomena, but also because of their substantial device application potential. The nonlinear optical response can be manipulated by material design, e.g. by changing the effective dimensionality of the structure from three-dimensional bulk material to quasi-two-dimensional quantum wells, to quasi-one-dimensional quantum wires, or to quasi-zero-dimensional quantum dots. The speaker will review the mathematical modeling of light-matter interaction effects in semiconductor media. He will discuss important physical mechanisms underlying the nonlinear optical response and provide examples of results for different systems.

Stephan W. Koch
Fachbereich Physik, Philipps Universität, Germany

2:15/Allegheny Foyer

Coffee

2:45-4:45

Concurrent Sessions

MS18/Fayette Room

Materials Issues in Nonlinear Optics

The search for suitable materials with large nonlinear optical coefficients is of paramount importance in telecommunications and industrial applications. There is a critical need for all-optical, ultrafast large bandwidth network switches which circumvent the speed limitations of currently used electronic systems. The current state of materials research in nonlinear optics provides great scope for innovative ideas on mathematical modeling and the exploration of scaling laws for nonlinear optical coefficients.

In discussing materials issues in nonlinear optics, the focus is usually on determining the nonlinear optical response for the material in question. This reflects the fact the electromagnetic wave and material property are inseparable entities. A proper description of the optical response function is extremely complicated, requiring full scale microscopic quantum mechanical calculations. Perhaps the greatest limitation to date in the technological implementation of a host of nonlinear optical effects, is the lack of suitable materials. The speakers in this minisymposium will highlight a subset of problems relating to materials that show most promise, namely semiconductors, organics and photorefractives.

Organizer: Jerome V. Moloney, University of Arizona

- 2:45 **Nonlinear Optical Response of Semiconductors**
John E. Sipe, University of Toronto, and Ontario Laser and Lightwave Research Center, Canada
- 3:15 **Optics of Fractals**
Mark I. Stockman, Washington State University
- 3:45 **Anharmonic Oscillator Modeling of Nonlinear Susceptibilities in Molecular Nanostructures and Conjugated Polyenes**
Shaul Mukamel, Akira Takahashi and Michael Hartmann, University of Rochester
- 4:15 **Photorefractive Nonlinear Optics**
Alex Zozulya and Dana Z. Anderson, University of Colorado, Boulder

MS19/Butler Room

Current Issues in Liquid Crystals (Part 2 of 2)

(For description, see MS14 on page 9)

Organizers: Maria-Carme T. Calderer, Pennsylvania State University, University Park
Eugene C. Gartland Jr., Kent State University, Mitchell Luskin, University of Minnesota, Minneapolis, and Peter Palffy-Muhoray, Kent State University

- 2:45 **Filamentation and Undulation of a Self-Focused Laser Beam in a Nematic Liquid Crystal**
Luc P. Faucheux, Princeton University
- 3:15 **Light Interacting with Liquid Crystals**
David W. McLaughlin, Princeton University
- 3:45 **Convection Instabilities in Liquid Crystals**
Lorenz Kramer and Werner Pesch, Universität Bayreuth, Germany

- 4:15 **Pattern Formation at Travelling Chiral Liquid Crystal Phase Boundaries**
Patricia E. Cladis, AT&T Bell Laboratories, H.R. Brand University of Bayreuth, Germany, and *J.T. Gleeson*, University of Calgary, Canada, and *P.L. Finn*, AT&T Bell Laboratories

MS20/Crawford Room

Recent Trends and Developments in Superconductivity (Part 2 of 2)

(For description, see MS15 on page 9)

Organizers: Qiang Du, Michigan State University and S. Jonathan Chapman, University of Oxford, United Kingdom

- 2:45 **Analyses and Simulations of Ginzburg-Landau Type Equations**
 Qiang Du, Organizer
- 3:15 **Dynamics of Vortices in Ginzburg-Landau Theories with Application to Superconductivity**
 Weinan E, Institute for Advanced Study
- 3:45 **Title to be determined**
 Karl-Heinz Hoffmann, Technische Universität Munich, Germany
- 4:15 **Numerical Simulation of the Time Dependent GL Equations**
 Man Kam Kwong, Argonne National Laboratory

MS21/Cambria Room

Dynamic Phase Transitions in Elastic Materials

For a large class of two-phase problems discussed by materials scientists the material is presumed to be *rigid*, but there are situations in which deformation is important. The speakers in this minisymposium will address four areas of current research in dynamic phase transitions in elastic materials: highly nonequilibrium phase transitions with interface kinetics; dynamic phase transitions in elastic materials with phase characterized by an order parameter, emphasizing the modeling of nucleation; dynamical balance laws for magnetostrictive solids; computational solutions for the dynamics and energetics of particle evolution in stressed elastic solids.

Organizer: Morton E. Gurtin, Carnegie Mellon University

- 2:45 **Dynamics of Phase Transitions in Thermoelastic Solids**
 James K. Knowles, Massachusetts Institute of Technology
- 3:15 **The Dynamics and Energetics of Particle Evolution in Elastically Stressed Solids**
 C.H. Su, M.E. Thompson, and *Peter W. Voorhees*, Northwestern University
- 3:45 **Nucleation and Growth in the Solid State**
 Eliot Fried, Pennsylvania State University
- 4:15 **On the Dynamics of Magnetostrictive Solids**
 A. DeSimone and *P. Podio-Guidugli*, Università di Roma "Tor Vergata", Italy

MS22/Somerset Room

Computational Methods for Determining the Effective Properties of Composite Materials

(This session will run until 5:15 PM)

The focus of this minisymposium is on recently developed numerical methods for the solution of partial differential equations in heterogeneous media and for the determination of the effective properties of such materials. The speakers will discuss finite element and integral equation approaches to the solution of the governing equations, from which the effective properties can be computed, as well as variational methods for the calculation of bounds on the effective properties. The first class of methods yields more information than the second but requires more computational effort. The speakers will also discuss future directions for research.

Organizer: Leslie F. Greengard, Courant Institute of Mathematical Sciences, New York University

- 2:45 **Unified Methodology to Characterize the Microstructure and Properties of Composite Media**
 Salvatore Torquato, Princeton University
- 3:15 **A Study of the Singularity Structure of the Conductivity of a Sheet with Polygonal Inclusions**
 J.H. Hetherington and *M. F. Thorpe*, Michigan State University
- 3:45 **Fast Computation of Structural Parameters**
 Leslie F. Greengard, Organizer and *J. Helsing*, Courant Institute of Mathematical Sciences, New York University
- 4:15 **A Voronoi Cell Finite Element Model for Microstructural Analysis of Random Heterogeneous Media**
 Somnath Ghosh, Ohio State University
- 4:45 **On the Evaluation of Electrostatic Fields in Composite Media**
 Leslie F. Greengard, Organizer and *M. Moura*, Instituto Superior Tecnico, Portugal

5:00

Conference Adjourns

SIAM Conferences, Meetings, Symposia, Tutorials, and Workshops

Sponsored by the Society for Industrial and Applied Mathematics

1994

June 15-18, 1994

Fifth SIAM Conference on Applied Linear Algebra

Snowbird Ski and Summer Resort, Snowbird, Utah

Sponsored by SIAM Activity Group on Linear Algebra

Organizer: Beresford N. Parlett, University of California, Berkeley

June 22-25, 1994

Seventh SIAM Conference on Discrete Mathematics

Ramada Classic Hotel, Albuquerque, NM

Sponsored by SIAM Activity Group on Discrete Mathematics

Organizer: William T. Trotter, Bellcore

July 22-23, 1994

Symposium on Control Problems in Industry

Holiday Inn on the Bay, San Diego, CA

Conducted with the cooperation of INRIA

Organizers: Irena Lasiecka, University of Virginia, Blaise Morton, Honeywell Corporation, and Jacques Henry, INRIA

July 25-29, 1994

1994 SIAM Annual Meeting

Sheraton Harbor Island East, San Diego, CA

Organizer: Barbara L. Keyfitz, University of Houston

December 12-14, 1994

Symposium on Inverse Problems: Geophysical Applications

Tenaya Lodge at Yosemite, Fish Camp, CA

Sponsored by GMM and SIAM

Abstract deadline: 4/25/94

Organizer: William Rundell, Texas A&M University, College Station

1995

January 22-24, 1995

Sixth ACM/SIAM Symposium on Discrete Algorithms

The Nikko Hotel, San Francisco, CA

Sponsored by ACM Special Interest Group on Automata and Compatibility Theory and

SIAM Activity Group on Discrete Mathematics

Abstract deadline: 7/5/94

February 8-10, 1995

SIAM Conference on Geosciences

San Antonio, TX

Sponsored by SIAM Activity Group on Geosciences

Abstract Deadline: 8/8/94

February 15-17, 1995

Seventh SIAM Conference on Parallel Processing for Scientific Computing

The Nikko Hotel, San Francisco, CA

Sponsored by SIAM Activity Group on Supercomputing

Abstract Deadline: 5/16/94

Organizer: Robert S. Schreiber, RIACS, NASA, Ames Research Center

April 27-29, 1995

Third SIAM Conference on Control and Its Applications

Adams Mark Hotel, St. Louis, MO

Sponsored by SIAM Activity Group on Control and Systems Theory

Abstract Deadline: 10/7/94

Organizer: John E. Lagnese, Georgetown University

October 16-19, 1995

1995 SIAM Annual Meeting

The Galt House Hotel, Louisville, KY

Abstract Deadline: 4/24/95

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Berry, G.C.	MS14	Wed 11:00	9	McLachlan, D.S.	MS5	Mon 3:45	6
Berryman, J.	MS2	Mon 10:30	4	McLaughlin, D.W.	MS19	Wed 3:15	10
Bertozzi, A.	MS16	Wed 11:30	9	Mih, R.	CP2	Mon 4:05	6
Bhattacharya, K.	MS13	Tue 2:45	8	Milton, G.W.	IP1	Mon 8:00	4
Boettinger, W.J.	IP4	Tue 8:00	7	Minkoff, M.	Poster	Tue 2:45	8
Bonnet, S.	MS15	Wed 10:30	9	Morgan, E.	CP4	Tue 10:00	7
Brattkus, K.	MS12	Tue 4:15	8	Moura, M.	MS22	Wed 4:45	11
Braun, R.J.	MS12	Tue 3:45	8	Movehan, A.	MS11	Tue 12:00	7
Bruno, O.	MS2	Mon 11:00	4	Mukamel, S.	MS18	Wed 3:45	10
Burns, T.J.	CP3	Mon 2:45	6	Munoz-Rivera, J.	CP1	Mon 10:20	5
Caginalp, G.	MS1	Mon 10:30	4	Negron, P.V.	CP1	Mon 11:40	5
Calderer, M.-C.T.	MS14	Wed 11:30	9	Nesi, V.	CP6	Tue 3:25	8
Chadam, J.	MS1	Mon 11:00	4	Ortiz, M.	MS4	Mon 10:30	5
Chapman, S.J.	MS15	Wed 10:00	9	Paffly-Muhoray, P.	IP7	Wed 8:00	9
Charap, S.H.	MS6	Mon 2:45	6	Pence, T.J.	CP3	Mon 4:25	6
Cherkaev, A.	MS7	Mon 3:45	6	Pesch, W.	MS19	Wed 3:45	10
Chipot, M.	MS9	Tue 10:30	7	Phoenix, S.L.	MS3	Mon 10:30	5
Chu, C-H.	MS13	Tue 3:15	8	Pitman, E.B.	CP3	Mon 3:05	6
Cladis, P.E.	MS19	Wed 4:15	10	Podio-Guidugli, P.	MS21	Wed 4:15	11
Clapp, P.C.	MS4	Mon 10:00	5	Polignone, D.A.	CP1	Mon 11:00	5
Clark, I.O.	MS17	Wed 10:30	10	Ponte-Castaneda, P.	MS2	Mon 11:30	4
Clark, K.	MS2	Mon 10:00	4	Puchner, H.	CP5	Tue 4:05	8
Coleman, B.D.	CP5	Tue 3:05	8	Renardy, M.	CP1	Mon 10:00	5
Collins, C.R.	MS9	Tue 10:00	7	Renardy, Y.Y.	CP1	Mon 10:40	5
Cross, M.	MS1	Mon 10:00	4	Richmond, O.	MS3	Mon 11:00	5
De Graef, M.	MS13	Tue 4:45	8	Romerfsky, E.I.	CP3	Mon 4:45	6
De Simone, A.	MS6	Mon 3:15	6	Roosen, A.	MS8	Tue 10:30	7
Diesslin, B.A.	CP2	Mon 4:25	6	Rosakis, P.	MS13	Tue 4:15	8
Dorsey, A.T.	MS15	Wed 11:00	9	Rosenberger, F.	MS17	Wed 10:00	10
Du, Q.	MS20	Wed 2:45	11	Rosensweig, R.	MS10	Tue 10:00	7
Dunn, J.H.	CP5	Tue 3:25	8	Roytburd, A.L.	MS11	Tue 11:00	7
Eyre, D.J.	CP2	Mon 3:25	6	Rubinstein, J.	MS15	Wed 11:30	9
Fauchoux, L.P.	MS19	Wed 2:45	11	Rybka, P.	CP7	Wed 12:00	10
Fehribach, J.D.	CP6	Tue 3:45	8	Saito, Y.	Poster	Tue 2:45	8
Fonseca, I.	IP6	Tue 1:30	8	Salamon, N.J.	CP7	Wed 10:00	10
Francfort, G.	MS7	Mon 4:45	6	Saunders, B.V.	Poster	Tue 2:45	8
Fried, E.	MS21	Wed 3:45	11	Saupe, A.	MS14	Wed 10:00	9
Friesecke, G.	MS13	Tue 3:45	8	Saville, D.	MS10	Tue 11:30	7
Garrison, W.M.	MS11	Tue 11:30	7	Scroggs, J.S.	MS17	Wed 11:00	10
Garland, E.G.	MS14	Wed 10:30	9	Serkerka, R.F.	IP5	Tue 8:45	7
Ghosh, S.	MS22	Wed 4:15	11	Shelley, M.	MS16	Wed 10:00	9
Gibiansky, L.	CP4	Tue 11:00	7	Sigmund, O.	MS7	Mon 4:15	6
Giga, Y.	MS16	Wed 11:00	9	Sipe, J.E.	MS18	Wed 2:45	10
Golden, K.M.	MS5	Mon 2:45	5	Socolovsky, E.A.	CP2	Mon 2:45	6
Goldstein, R.	MS10	Tue 10:30	7	Soner, H.M.	MS16	Wed 10:30	9
Gordon, M.S.	CP3	Mon 3:45	6	Stockman, M.I.	MS18	Wed 3:15	10
Grabovsky, Y.	CP4	Tue 10:40	7	Suquet, P.M.	MS11	Tue 10:00	7
Grant, M.	MS12	Tue 3:15	8	Tang, Q.	CP7	Wed 11:20	10
Grayhack, W.T.	CP5	Tue 3:45	8	Tartar, L.	MS6	Mon 4:15	6
Grove, J.	MS1	Mon 11:30	4	Teter, J.P.	MS6	Mon 4:45	6
Gutzburger, M.D.	IP8	Wed 8:45	9	Thorpe, M.F.	MS22	Wed 3:15	11
Gustafson, K.	CP5	Tue 2:45	8	Tokarzewski, S.	CP6	Tue 4:25	8
Haidar, S.M.	CP7	Wed 11:40	10	Torquato, S.	MS3	Mon 11:30	5
Heinkenschloss, M.	CP4	Tue 11:40	7	Torquato, S.	MS22	Wed 2:45	11
Helsing, J.	MS22	Wed 3:45	11	Voorhees, P.W.	MS21	Wed 3:15	11
Hoffmann, K.-H.	MS20	Wed 3:45	11	Vu-Quoc, L.	CP4	Tue 11:20	7
Huntley, D.A.	CP2	Mon 3:45	6	Walkington, N.J.	MS9	Tue 11:00	7
Isichenko, M.B.	MS5	Mon 4:15	5	Wang, F.	CP3	Mon 3:25	6
James, R.D.	IP2	Mon 8:45	4	Wang, H.	MS9	Tue 11:30	7
Jerrard, R.	CP2	Mon 3:05	6	Warren, J.A.	MS8	Tue 11:00	7
Karma, A.S.	MS12	Tue 2:45	8	Weinan E	MS20	Wed 3:15	11
Kartha, S.	MS4	Mon 11:30	5	Whiteman, J.R.	CP1	Mon 11:20	5
Kassem, M.	MS17	Wed 11:30	10	Widom, M.	MS10	Tue 11:00	7
Keller, J.B.	IP3	Mon 1:30	5	Wojnar, R.	CP6	Tue 4:45	8
Kikuchi, N.	MS7	Mon 2:45	6	Wojnar, R.	Poster	Tue 2:45	8
Knowles, J.K.	MS21	Wed 2:45	11	Zozulya, A.	MS18	Wed 4:15	10
Koch, S.W.	IP9	Wed 1:30	10				
Kozlov, S.M.	MS5	Mon 3:15	5				
Kramer, L.	MS19	Wed 3:45	10				
Kurtz, S.K.	MS3	Mon 10:00	5				
Kwong, M.	MS20	Wed 4:15	11				