

A Division of The American Physical Society

August 1996

DMP Focus Sessions for the 1997 APS March Meeting

15(a) Materials Theory:

Computer Simulation of Dynamical Phenomena

15(b)Materials Theory:

Electronic and Atomic Structure

15(c) Fullerenes, Carbon Nanotubes,

and Related Materials

15(d) Granular Materials, Avalanches,

Fracture, and Related Instabilities

15(e) Critical Currents in High Temperature

Superconductors

15(f) Coercivity in Rare-Earth Magnets:

Theory and Practice

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Call for Input in Recommending Invited Speakers

DMP Focused Sessions typically include an invited speaker and contributed talks. DMP General sessions consist solely of contributed talks. Focused Sessions organizers are empowered to recommend invitees to the DMP Executive Committee for approval. All official invitations for the entire March Meeting are issued uniformly by the APS Executive Officer and no one else. If you would like input into the process, send your

suggestions to the appropriate Focused Session organizers listed in the Call for Abstracts elsewhere in this issue.

The format you use is free-style, but please include a title, a brief descriptive paragraph, and the name, address, telephone and FAX number of both the proposed speaker and the nominator.

Methods to Access the DMP Call for Abstracts

- 1. Check your personal paper version of the DMP August 1996 Newsletter.
- 2. Check your personal e-mail version of the August Newsletter.
- 3. Check the Oct. or Nov. 1996 issue of the APS Meeting News.
- 4. Check the DMP Homepage: /units/dmp/

Dates To Remember...

Aug. 15: Deadline for submitting suggestions for invited speakers to focused-session organizers.

Dec. 6: Deadline for all March Meeting abstracts (contributed and invited) due at APS. Sending an extra copy to your focused session organizers is highly recommended.

Feb. 15: Deadline for DMP Fellowship Nominations due at APS Headquarters.

March 17-21, 1997: APS March Meeting, Kansas City, MO

DMP HomePage Debuts

We invite you to visit the DMP Homepage at /units/dmp/. If you do so, here is a glimpse of the beginning of it. Help us improve it with your suggestions and contributions to a new 'Images of Materials' section.

Call for Abstracts for 1997 APS March Meeting DMP FOCUSED SESSIONS:

15(a) Materials Theory: Computer Simulation of Dynamical Phenomena

Abstracts are solicited in the areas of computer simulation of dynamical and/or kinetic phenomena in condensed matter. Topics include, but are not limited to, diffusion, interface roughening, defect (dislocation, grain boundary, etc.) migration, growth phenomena (vapor phase film growth, solidification, solid state reactions, etc.), fracture, and microstructural evolution (grain growth, crystallographic texture development, void

formation, etc.). Papers based upon atomistic (classical or quantum-based forces), microstructural and/or continuum modeling are encouraged. New developments in computer simulation of dynamical phenomena in condensed matter will be emphasized.

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15(b) Materials Theory: Electronic and Atomic Structure

This session will focus on the application of quantum theoretical methods to materials. Specifically, submissions which involve electronic structure methods to predict structural and electronic properties of materials are encouraged. Typical topics to be covered within this session will include materials-related applications of large-N systems, pseudopotentials, quantum Monte Carlo methods, methods for 'quantum' molecular dynamics, basis sets methods, real space methods, parallel computing, and density functional theory.

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15(c) Fullerenes, Carbon Nanotubes, and Related Materials

These sessions will focus on experimental and theoretical research involving fullerenes, carbon nanotubes, and related materials such as organic derivatives or inorganic compounds with similar topologies. Representative topics include electronic structure and transport, superconductivity, high pressure effects, formation and reaction mechanisms, photochemical, magnetic, vibrational, thermal and mechanical properties.

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15(d) Granular Materials, Avalanches, Fracture, and Related Instabilities

The goal is to explore the relationships between these topics as applied to wide range of materials and length scales, from macroscopic processes in granular materials to mesoscopic instabilities in electronic transport or magnetic flux bundle arrangements. The recognition of such relationships has led to some very exciting interdisciplinary research in recent years. Abstracts on all aspects of granular materials, avalanches, and dynamical phase transitions from asolid-like to a fluid-like phase in materials are solicited. We intend to provide a stimulating atmosphere, characterized by an unusually wide point of view and perspective, in which all aspects of the fundamentals of these complex materials problems can be discussed. We plan to highlight recent progress on the dynamics of granular materials, which is a subject of great interest to many disciplines in science and engineering. The unusual properties of granular materials (e.g., segregation, arching, bistability, onset of collective motion) are currently under intense scrutiny using a variety of methods, including novel imaging techniques. We also plan to highlight recent progress on dynamical instabilities in magnetic, superconducting, or semiconducting systems. Here, avalanching or breakdown are found on mesoscopic length scales, and, again, many novel observation techniques have recently been developed. We envision to devote a special session to recent results on dynamical phase transitions in these systems, emphasizing the interplay between plastic and elastic deformations. A session devoted to fracture is anticipated as well.

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15(e) <u>Critical Currents in High Temperature Superconductors</u>

We will focus on recent developments in our understanding of the physics and materials science of enhanced critical currents in high temperature superconducting materials. Abstracts are solicited on techniques to enhance vortex pinning and the connectivity of polycrystals, and on physical measurements and theory which are relevant to these phenomena. Some areas which could be emphasized are bulk pinning in single crystals, in ceramics, and thin and thick films, particularly biaxially textured thick films, experimental and numerical studies of pinning and vortex dynamics in the presence of well characterized defects such as damage tracks produced by high energy heavy ion

bombardment and splayed configurations of columnar disorder. The strong correlation between material anisotropy and the position of the irreversibility line makes studies of alterations to anisotropy by chemistry and by correlated defect structures also of interest. This includes studies of the effect of correlated defects on the dimensionality of the vortex system. We welcome abstracts on vortex and flux imaging experiments and computer simulations of vortex dynamics in the presence of various pinning defect structures. Attempts to understand all the effects controlling the critical current density of high temperature superconductors are encouraged, including appropriate experiments on low temperature superconductors.

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15(f) Coercivity in Rare-Earth Magnets: Theory and Practice

Experimental and theoretical or modeling abstracts are solicited for this session which will deal with increasing the coercivity of permanent magnet materials. There is widespread interest today in the physics of the magnetization process in magnetic materials, which provides the means for understanding and developing new magnetic materials with improved properties such as enhanced coercivity and maximum energy product. Pushing magnetic materials towards the theoretical limit of a maximum energy product is a major challenge. Further progress can only be achieved now through a more thorough understanding of the fundamental magnetization mechanisms. The session will include abstracts discussing the origins of coercivity in magnetic materials, and the effects of various factors such as magnetocrystalline anisotropy and domain wall pinning on coercivity of magnetic materials. In addition abstracts on recent developments in the

use of computer modelling and simulation methods for predicting magnetic properties are sought. Abstracts are also solicited on recent progress in permanent magnets which can operate at higher temperatures, through increase in the Curie temperatures of known hard magnet materials such as samarium-cobalt or neodymium-iron-boron; or by discovery of new hard magnetic materials. This Focus Session is jointly sponsored by DMP and TGMAG.

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15(g) Magnetic Nanostructures and Heterostructures

These focused sessions will emphasize experimental and theoretical advances in novel and artificial magnetic structures whose properties are controlled by limited dimensions at the nanometer length scale. Surface and interface phenomena in ultrathin films, superlattices, nanocrystalline and granular films, nanocomposites, heterostructures and dots are of interest. Emphasis will be placed on growth and fabrication of nanostructures including atomic-scale control and characterization of interfaces, element-sensitive methods to probe magnetic properties, and novel deposition techniques to create magnetic features with nano-scale lateral dimensions. Abstracts that address topics such as low-dimensional phenomena, interlayer exchange coupling and quantum confinement, intermetallic compound and alloy thin films, effects of disorder on magnetic anisotropy and coupling, and magneto-transport phenomena including spin-polarized tunneling and spin-valve structures are also most welcome.

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15(h) Magnetoresistive Oxides

Abstracts are solicited on the properties of conducting magnetic oxides that exhibit unusual magnetoresistive properties. While the doped manganite perovskites are prototypical materials, other compounds such as pyrochlores are appropriate for inclusion in the session. Experimental and theoretical results on the nature of the electronic, magnetic, and structural properties, the effects of substitutions and doping, the role of microstructure and lattice distortions, the behavior of thermodynamic properties, and the presence of field-induced phase transitions are all appropriate to this session. Reports of new magnetoresistive materials and oxide-based heterostructures that have potential applications are also welcomed.

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15(i) Silica Waveguides and Fibers

Silica fibers and planar waveguides are playing an increasingly important role in

communications technologies, not only as passive transmissive elements, but increasingly as active sources and amplifiers, modulators, switches, and optical pulseformers. This session will focus on the materials physics of guided-wave and fiber silica optical elements.

Specific areas covered include: fundamental limits: Rayleigh scattering limits to propagation loss, effects of waveguide bends and micro-roughness, dispersion control, compositional effects, defect physics and chemistry; extrinsic effects: photosensitivity, hydrogen loading, Bragg gratings, poling for second-order nonlinearities; intrinsic optical nonlinearities: four-wave mixing, self-phase modulation, soliton formation and propagation; and rare-earth doped structures: gain, amplification and lasers.

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15(j) Phase Transformations

Phase transformations has always been an intriguing area of research in materials physics and has received increasing attention in recent years. Materials frequently exhibit novel and critical behavior in the vicinity of a phase transition, and can be strongly influenced by complex long- lived morphologies that often emerge during the kinetics of phase transformations. The focus of this session will be on experimental, analytical and numerical approaches to understanding various nontraditional and novel aspects of phase transformations. A wide range of topics will be considered: equilibrium and dynamic properties, metastable phases, diffusional and diffusionless transformations, transitions at surfaces and interfaces, melting, amorphization, interfacial motion, order/disorder transitions, phase separation, critical phenomena and dynamical scaling behavior.

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15(k) Wide-Band-Gap Semiconductors

This session will focus on the materials physics of wide-band-gap semiconductors used for short-wavelength optoelectronics and high-temperature or high-power applications. Experimental and theoretical abstracts are solicited in the field of III-V nitrides, wide-gap II-VI compounds, and SiC. All aspects of this very active and growing field will be covered, including epitaxial growth, role of point defects and extended defects, impurity incorporation and doping, heterojunctions, surface physics, optical properties, degradation mechanisms, metal contacts, and oxidation of SiC.

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15(l) Nanometer-scale Morphology of Surfaces and Interfaces

In recent years, significant advances have been made in the synthesis of nanometer-scale morphologies using self-organized epitaxial growth and the direct fabrication of small structures using scanning probes. These sessions will focus on two primary issues: (1) the scientific understanding needed to control the production of nanometer-scale epitaxial morphologies and fabricated nanostructures, and (2) the unique physical properties of these nanostructured materials and their promise for improved electronic, magnetic, and optoelectronic devices.

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15(m) Novel Scattering Techniques Applied to Materials

This session will focus on the application of novel electron, x-ray and neutron scattering techniques to determine the structure and dynamics of materials. Topics to be covered within this session will include the production and utilization of spatially limited beams, as used to scan selective regions of materials or in speckle holography when the incident beam can be made partially coherent. Abstracts are encouraged that deal with the "phase problem" and propose new solutions. Experimental innovation may include holography with a reference scatterer internal or external to the sample. New methodological or theoretical approaches to convert the information from reciprocal to direct space are also encouraged.

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15(n) Applications of Positrons to Materials Physics

These sessions will focus on areas where positrons are making unique contributions to the measurement of the electronic, surface and defect structures of solids, including polymers, pure metals, alloys, semiconductors, and composites. Topics will include Fermi surfaces, surface characterization by positron diffraction and positron annihilation induced Auger emission, electromigration in Al(Cu) interconnects in microelectronics and the identification and quantification of particular defects such as voids in polymers

and epoxies, He clusters and defects in metals, EL2 and DX centers in GaAs, H in SiO2 on Si, epitaxial growth in ion implanted semiconductors, and structural defects at interfaces. New areas such as positron re-emission microscopy and positron diffraction holography.

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15(o) Laser Ablation and Low-Energy Beam-Assisted Film Growth

The physical processes governing film growth by laser ablation and low-energy beams has become increasingly important in recent years. In addition to their use in depositing "conventional" oxides, semiconductors and metals, laser ablation and low-energy beams have proven useful in the formation of a wide variety of novel thin-film materials, including metastable phases, multilayers, and nanocrystallites, as well as to induce crystallographic texture in polycrystalline films. However, many fundamental issues remain unresolved, including the role of energetic species in laser ablation, the formation of particulates in the ablation plume, and the mechanism(s) by which low energy beams induce biaxial texture in polycrystalline films. Developing a fundamental understanding of these and related effects in the formation of thin-film phases, defect structures, and crystallographic textures, is important to the development of this field.

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15(p) Battery Materials: Structural and Interfacial Aspects

Modern batteries present many challenging problems related to physics. These sessions will focus on the structural and interfacial aspects of battery materials with emphasis on lithium and metal hydride batteries. The scope of the sessions includes theoretical studies of hydrogen insertion and intercalation compounds, the synthesis of new materials, the application of in-situ spectroscopies in electrochemical cells to the study of electrode reactions, interfacial processes and degradation mechanisms. Abstracts on fundamental studies of the electrode/electrolyte interface on model systems such as single crystals are also solicited.

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15(q) Novel Materials for Thermoelectrics

Sessions will be focused on recent advances in materials physics of both traditional thermoelectrics and new materials including Bi compounds, superlattice structures, organic polymers and skutterudites. Abstracts are solicited in areas of experimental synthesis, physical characterization, and fundamental measurements such as energy gaps and optical properties. Theoretical studies of electronic structure, phonon modes and other properties important for improving thermoelectric applications will be included. We are particularly interested in new approaches to defining structure-property relationships that will lead to improved control and synthesis of novel thermoelectric materials.

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15(r) Clusters and Small Systems

Studies of clusters focus on size-evolutionary patterns of physical and chemical properties of materials systems. The focused sessions on "Clusters and Small Systems" will include experimental and theoretical investigations of: atomic and molecular clusters in various states and environments (gas, liquid, solid); collisions of clusters with solid and liquid surfaces; structure and dynamics of clusters on surfaces; supported clusters and small materials structures, such as nanowires and dots; passivated clusters and their

assemblies; nano-crystals and their structural, mechanical and electronic properties; physical properties of colloidal systems, and the physics of fine powders and granular materials.

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15(s) Nucleation and Crystallization

This focused session concentrates of nucleation and crystallization phenomena in the most general sense. Abstracts on the very initial stages of semiconductor epitaxy are welcome, but contributions that concern quite different material systems are solicited most particularly. Included papers will emphasize recent work made possible by new experimental techniques (STM, AFM, LEEM, grazing incidence x-ray scattering, etc.), novel physical simulations, and more powerful computational methods. Controlled crystallization for a wide range of materials yields tailored properties, e.g. semicrystalline polymers, metals, semiconductors, photographic film and even some foods such as chocolate. In other situations, suppression of crystallization is desired. This is the case for glass formation and for gas hydrates and waxes in the petroleum industry. This session is intended to bring together workers with very different backgrounds who find themselves confronted with the problem of understanding and controlling nucleation and crystallization. The organizers solicit contributions from diverse areas to fully illustrate the broad range of subject matter germane to these areas.

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15(t) Nanoscale Tribology

The interplay between the atomic-scale structure of surfaces and their tribological properties is the subject of this focused session. Nanoscale tribology is a relatively new area in materials sciences that is experiencing great development thanks to the advent of scanning force microscopy probes, the surface forces apparatus, the quartz microbalance and their combinations with a variety of spectroscopic tools. With these tools the forces of friction, viscosity and adhesion can be measured with near atomic-scale resolution. These developments are paralleled by advances in the theory and in the computational modeling and simulations.

Abstracts are solicited that emphasize atomistic aspects of tribology, both in the experimental and the theoretical areas, stick-slip behavior, energy dissipation, role of adsorbed atoms and molecules etc.

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15(u) Intelligent Materials and Systems

Intelligent materials and systems have received increasing attention during the last years. These materials have the ability to perform both sensing and actuating functions.

Passively intelligent materials respond to changes in the environment in a useful manner without assistance, whereas, actively intelligent materials have the ability to learn from the environment and hence to optimize their functions. Experimental and theoretical papers on all aspects of intelligent materials and systems are solicited. Possible topics include piezoelectric and electrostrictive ceramics, electrorheological fluids, magnetorheological fluids, shape memory materials, intelligent optics, intelligent gels, and other adaptive materials. The focused session will provide a broad forum on recent advances in physical mechanism, technology, properties, structure, and applications of intelligent materials and systems.

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15(v) Dislocations in Deformed Metals and Semiconductor Thin Films and Multilayers

Abstracts are sought in theory and experiments associated with two general subjects: (1) Formation of partially ordered dislocation structures in deformed metals and the work hardening associated with these structures. (2) Dislocation processes in semiconductor thin films or multilayers, including dislocation generation from sources and misfit dislocation formation during and after growth.

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For dislocations in metals: Lyle Levine Washington State University Mailing address: Metallurgy Division Room B261 Matls. Bldg. **NIST**

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GENERAL SESSIONS:

- 16(a) Hydrogen in Metals
- 16(b) Radiation Effects
- 16(c) Defect Structure
- 16(d) Mechanical Behavior
- 16(e) Diffusion in Solids
- 16(f) Amorphous and nanocrystalline materials
- 16(g) Materials research at high pressure
- 16(h) Conducting polymers
- 16(i) Other

EXECUTIVE COMMITTEE

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