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Nonlinearity in Structural and Electronic Materials

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Abstract

This is the final report of a three-year, Laboratory Directed Research and Development (LDRD) project at the Los Alamos National Laboratory (LANL). The project strengthens a nonlinear technology base relevant to a variety of problems arising in condensed matter and materials science, and applies this technology to those problems. In this way the controlled synthesis of, and experiments on, novel electronic and structural materials provide an important focus for nonlinear science, while nonlinear techniques help advance our understanding of the scientific principles underlying the control of microstructure and dynamics in complex materials. Our research is primarily focused on four topics: (1) materials microstructure: growth and evolution, and porous media; (2) textures in elastic/martensitic materials; (3) electro- and photo-active polymers; and (4) ultrafast photophysics in complex electronic materials. Accomplishments included the following: organization of a "Nonlinear Materials" seminar series and international conferences including "Fracture, Friction and Deformation," "Nonequilibrium Phase Transitions," and "Landscape Paradigms in Physics and Biology"; invited talks at international conferences on "Synthetic Metals," "Quantum Phase Transitions," "1996 CECAM Euroconference," and the 1995 Fall Meeting of the Materials Research Society; large-scale simulations and microscopic modeling of nonlinear coherent energy storage at crack tips and sliding interfaces; large-scale simulation and microscopic elasticity theory for precursor microstructure and dynamics at solid-solid diffusionless phase transformations; large-scale simulation of self-assembling organic thin films on inorganic substrates; analysis and simulation of smoothing of rough atomic surfaces; and modeling and analysis of flux pattern formation in equilibrium and nonequilibrium Josephson junction arrays and layered superconductors.

Background and Research Objectives

During the last 15 years nonlinear, nonequilibrium science has flourished, driven by a number of new concepts and techniques, including (i) coherent space-time structures in strongly nonlinear classical and quantum systems; (ii) deterministic chaos, even in low-dimensional nonlinear dynamical systems; and (iii) the coexistence of (i) and (ii), leading to a variety of "complex" phenomena.

Our objective is to strengthen these concepts and apply them to a variety of significant problems in condensed matter physics and materials science. In this way materials synthesis and controlled experiments can contribute directly to nonlinear science, while nonlinear techniques can advance our understanding of the microscopic processes determining the structure and dynamics of complex materials. This is a key element in establishing the mesoscopic "bridge" between microscopic and macroscopic modeling of

materials and providing predictive scientific principles underlying the nonlinear, nonequilibrium statistical mechanics of mesoscale complexity. There is a growing need to understand and control "texture" or "microstructure" of materials, particularly at mesoscopic scales, a need shared by many other disciplines, including biology, fluids, and astrophysics. Experimental advances enable us to image increasingly detailed microstructures and even begin following their dynamics. Interpretative frameworks are urgently needed. The scientific needs that will dictate technology in the next decade are (i) understanding the microscopic driving forces controlling microstructure — the *interrelation* of electronic, magnetic, optical, and structural degrees of freedom, and the effects of dimensionality and disorder (ultimately, this must underpin synthesis/processing control of microstructure); (ii) not only imaging microstructure at appropriate space and time scales, but learning how to quantify it—in ways which are relevant to specific macroscopic properties; and (iii) understanding how a specific measure of complex textures can be used to predict macroscopic properties, an understanding that will then provide constructive schemes for including microstructure in, e.g., constitutive relation phenomenologies.

Important developments from nonlinear science are the following:

1. The formation and dynamics of "collective" or "coherent" space-time structures is now regarded as the central issue in "extended dynamical systems." Coherent structures include dislocations, vortices, domain walls, twin boundaries, and clusters. Opportunities to use nonlinear and nonequilibrium techniques to understand the microscopic origin of these textures and quantify their collective behavior have advanced substantially.

2. The developments in Item 1 clearly reveal that competing length and/or frequency scales are the key mechanism determining mesoscopic patterns in space and/or time. Competition of length scales or symmetries typically leads to patterns ("textures") in space which can be constant, periodic, quasiperiodic or even totally irregular.

3. Recently we have begun to appreciate the intimate relationship between space and time noted in 2. Multiple-length-scale ground-state spatial structures lead directly to the multiple time scales (e.g., stretched exponential) observed as a system relaxes from nonequilibrium configurations and as it responds to external forces. Problems from condensed matter and materials clearly demonstrate this coupling of space and time in "1/f" noise, in intermittency, and in "hierarchical/glassy/hysteretic" dynamics.

4. The importance of "noise" and "disorder" has long been known in *linear* condensed matter and materials science. However, we have only recently gained enough insight into strongly nonlinear systems to appreciate that (classical and quantum) noise, disorder, and nonlinearity must often be incorporated *simultaneously*, leading to qualitatively new phenomena.

5. High-performance computational capabilities such as those at the Los Alamos Advanced Computing Laboratory (ACL) are now effective enough to share a synergistic relation with modeling and experiment. This is qualitatively advancing our understanding of materials. We have developed many advanced simulation and visualization tools and capabilities for meshing computing, analytic techniques, and physical phenomena in condensed matter and materials science.

In summary, this project strengthens a nonlinear technology base relevant to a variety of problems arising in condensed matter and materials science, and applies this technology to those problems. In this way the controlled synthesis of, and experiments on, novel electronic and structural materials provide a focus for nonlinear science, while nonlinear techniques guide our understanding of the scientific principles underlying the control of microstructure and dynamics in complex materials.

Importance to LANL's Science and Technology Base and National R&D Needs

The Nation's and Laboratory's materials science programs are rapidly recognizing the need for predictive control of materials—from synthesis and processing to microstructure, and from microstructure to macroscopic properties. Nonlinear and nonequilibrium issues dominate many of the phenomena at all scales—microscopic, mesoscopic, and macroscopic. These phenomena include coherent, self-organizing and hierarchical structures, complexity, multi-scale and glassy dynamics, chaos, self-trapping, and competing interactions. The role for theory and simulation, closely coupled to experimental validation, as a means of systematically describing these phenomena is now widely appreciated by the DOE-BES and the industrial-laboratory program development efforts, such as the Materials Modeling Program and the Center for Process Modeling. Precisely the same needs and strategies are apparent in weapons (science-based stockpile stewardship), military, and civilian programs.

The condensed matter and materials science investigations in this project closely complement the electronic and structural materials synthesis, characterization, and application programs around the Laboratory. These include low-dimensional electronic materials and ultrafast spectroscopy studied in the Laboratory's Center for Materials Studies (CMS), Materials Science and Technology (MST) Division, Chemical Science and Technology (CST) Division, and Superconductivity Technology Center (STC); device development in MST, CST, and STC; and surface and thin film growth studied in CMS, MST, and the Los Alamos Neutron Science Center (LANSCE). Microstructure and texture

is studied extensively in MST, CMS and the Materials Science Laboratory (MSL), while vortex structures and their dynamics play key roles in the flux flow in high-temperature superconductors. Incorporation of microstructural information in process models is being developed in programs with, e.g., the Laboratory's Engineering Sciences and Applications (ESA), Theoretical (T), Applied Theoretical and Computational Physics (X) and MST Divisions and the ACL. Flow through porous media is central to environmental restoration programs, petroleum industries, etc. This project has served as a bridge between the techniques of nonlinear science and the practice of condensed matter and materials science, emphasizing the integration of analytical techniques and advanced computing with materials and measurements. Thus, there are mutually beneficial associations with many of the Laboratory's Centers and technical Divisions.

Scientific Approach and Accomplishments

Our research focused principally on the four topics listed below. Through workshops, seminars, and an ad-hoc LANL advisory group, we seeded nonlinear activities in many *additional* nonlinear, nonequilibrium areas, including process modeling, solidification, fracture and crack propagation, complex fluids, flux flow in superconductors, high-magnetic field phenomena, magnetic films and surfaces, plasticity and elasto-plasticity, polymers and molecularly-engineered materials, composites, ceramics, and glasses.

The initial focuses complemented existing thrusts in the LANL materials community, and were chosen in areas where nonlinear approaches can play clear roles and where there is good teamwork with existing synthesis, characterization, and device development efforts. These focus areas were the following: (1) materials microstructure: growth and evolution, and porous media; (2) textures in elastic/martensitic materials; (3) electro-and photo-active polymers; and (4) ultrafast photophysics in complex electronic materials.

Several common techniques were exploited: (i) description of coherent structures as collective particle-like objects; (ii) derivation of effective (nonlinear and/or nonlocal) equations of motion and evolution equations in terms of these (interacting) coherent structures and statistical approaches; (iii) relating time scales observed in near-equilibrium and nonequilibrium conditions to underlying spatial textures, including hierarchical, glassy and hysteretic conditions; and (iv) integrating large scale simulations with analytical

approaches to study strongly quantum mechanical, nonlinear, and nonequilibrium processes.

We briefly summarize activity in the above focal areas.

1. Materials microstructure: growth and evolution

We have worked closely with the LANL Materials Modeling and Process Modeling Centers in CMS and associated structural materials modeling thrusts in T and MST Divisions. We have focused on the growth and evolution of mesoscopic structures in materials, emphasizing surface and thin film growth, solidification, and grain growth. These phenomena have many mathematical aspects in common, including multiple length and time scales, and are of great importance in numerous technologies. We have modeled microscopic driving forces, using reduced (nonlinear mode) models for mesoscale structures and their dynamics, and developed simulation strategies and quantitative measures of "complexity" (e.g., statistical, mode-reduction, pattern recognition, nonlinear imaging, wavelets). Principal applications are to (i) grain growth, including solidification, casting, crystallization, and sintering; (ii) surface and thin film growth — interface dynamics, epitaxial growth, nucleative, dendritic and columnar growth, and nonlinear reaction-diffusion effects in models of, e.g., MBE processes; and (iii) magnetic, ferroelectric, and superconducting films.

For example, the nonlinear community has long been interested in solidification, with most research being focused on individual dendritic trees. Of greater interest to practical materials science is the solidification of fluids with a large number of nucleating sites, the consequent development of grains of different orientation, and the evolution of this initial microstructure over time. Being able to couple these phenomena promises to greatly improve our ability to predict final microstructures (and thus materials properties) of complex processing methods, such as casting and welding. Nonlinear science can help by studying the underlying driving forces, providing quantitative measures of complexity, and determining how this complexity affects the macroscopic materials properties. This understanding will then feed directly into many new fields where a microscopic understanding of "polarizability" from the coupling of ionic and electronic degrees of freedom is critical -- including biosciences and nanostructured electronic materials.

The scientific issues of flow through porous media are also rapidly increasing in economic significance and involve intrinsically nonlinear, nonequilibrium phenomena. The rate and direction of oil, water or chemicals in underground flows are governed by fine-scale heterogeneities in the subsurface formation. Mathematical models, based on coupled systems of nonlinear partial differential equations, are used to predict these flows in

petroleum reservoirs and predict the extent of contamination and environmental danger posed by flows from hazardous waste sites. Even though the material properties of the subsurface formation may be characterized on a fine scale, because of the limitations of our computers, the model must be simulated on a coarser scale. The goal of this research has been to develop and analyze new mathematical models that incorporate fine-scale detail into the coarse-scale computer representation of these flows by deriving new averaged equations (using homogenization theory) and numerical methods (based on multigrid and upscaling techniques that accurately capture the average effective properties of the medium). This research will lead to significant improvements in upscaling homogenization and mesoscale modeling of porous media flows, and will provide new tools for more accurate and realistic simulations of underground aquifers and reservoirs.

2. Textures in elastic/martensitic materials

We have worked closely with our experimental colleagues in CMS and MST Division and with Krumhansl (U. Mass.), Lookman (Western Ontario, Canada), and Shenoy (ICTP, Trieste, Italy). The metallurgical and solid state/condensed matter communities have been brought together recently by the increasingly refined imaging of textures in elastic and martensitic materials (e.g., using STM or Newton scattering). This has focused attention on aspects of structural phase transitions that do not display "universal criticality" in the sense of critical exponents, but are nevertheless now understood to be "generic" and of great practical importance. These transitions include improper and proper ferroelastic transitions in perovskite-structured compounds and defect-mediated heterogeneous martensitic (diffusionless) transformations. Phenomena include formation of collective space-time structures (antiphase and twin boundaries, heterophase fluctuations, pretransitional discommensuration textures like tweed, ...) which control textures, responses, nucleation, and transition rates. We have developed a microscopic description for these aspects of phase transitions by combining simulation and statistical mechanical analysis of nonlinear lattice dynamics. We can now study thermal and mechanical twin and tweed formation, structure and hysteretic dynamics, the role of precursor textures in incomplete first-order phase transitions, and the role of defects and heterophase fluctuations as nucleation events for a martensitic cooling transformation. The physics here is also characteristic of many weapons materials.

With microscopic predictability of textures such as tweed, we are now in a position to model "shape-memory" effects observed in several classes of martensitic materials (e.g. NiTi, FePd, InTi, CuZnAl alloys). Tweed and twins of various length scales are observed experimentally by high-resolution electron microscopy at the MSL and elsewhere. A basic

understanding of transformation microstructures is essential to fully realize the potential of shape-memory materials in applications such as storage devices, strain tunable lasers, dampers, and prosthetic devices. From a nonlinear perspective shape-memory is an exciting example of emergent structures through hierarchical ordering, information imprinting, and information retrieval. The hierarchy also drives a correlation with time scales, producing non-exponential (multi-timescale) decay.

3. Electro- and photo-active polymers.

Novel, low-dimensional electronic materials are recognized as an area where nonlinear effects are critical to both basic science and device applications. Los Alamos has developed expertise in this area, due to its extensive research on, e.g., conducting polymers, organic superconductors, mixed-valence solids, quantum Hall effect systems, high-temperature superconductors, and buckminsterfullerenes. These materials are all characterized by (a) reduced dimensionality and/or restricted geometry and (b) strongly coupled electronic and lattice degrees of freedom. The coupled fields lead to nonlinear equations with competitions (enhanced by dimensionality and disorder) for broken-symmetry ground states—charge-density wave, spin-density wave, spin-Peierls, ferroelectric, superconducting, etc. Excitations from these stoichiometric ground states are fundamentally “soliton” like—polarons, bipolarons, excitons, domain walls, vortices—and directly control the electronic and lattice dynamic properties that are critical to the applications.

We have worked closely with Smith et al. (MST), McBranch et al. (CST) and Heeger (UCSB) in the context of polymer light-emitting diodes, which are being developed for electroluminescence applications in displays and optical interconnects. Polymer light emitting diodes consist of a thin polymer film sandwiched between two metals with different workfunctions. When a voltage is applied, electrons and holes are injected from the low and high workfunction contacts, respectively. The electrons and holes recombine in the polymer film emitting light.

We have provided nonlinear infrastructure in two ways: (a) microscopic modeling of charge carriers (especially polarons) and luminescence centers (especially excitons) in conjugated polymeric materials (here we have combined state-of-the-art electronic structure techniques with the effects of electron-electron, electron-lattice, disorder, and dimensionality to understand how these influence photo- and electro-excitation and decay); and (b) analysis of device models under equilibrium and nonequilibrium conditions, so that we can compare predictions with capacitance and I-V curve measurements and determine the factors controlling model parameters in terms of the charge carriers in (a).

4. *Ultrafast photophysics in complex electronic materials*

We have provided theoretical and modeling guidance for the ultrafast spectroscopy capability at the MSL, focusing on thin films of complex, strongly correlated electronic materials. We have collaborated with the Optical Sciences Center (U. of Arizona), White (UCI), Wudl (UCSB), and McBranch (CST) and Taylor (MST). Guiding applications include charge transfer and photoinduced charge transfer in systems such as conducting polymer or fluorescent films, blends and heterostructures, which are being developed as molecularly engineered materials for applications in microelectronics, photonics, energy-storage, and sensors.

We have developed new theoretical techniques for this area by combining approaches from chemistry and solid-state—quantum-chemical, mean-field, RG, molecular dynamics, etc.—taking full advantage of the massively parallel computation capability of the ACL. Such techniques will be increasingly critical to interpret and motivate experiments at the MSL, where we must describe nonlinear, nonadiabatic, nonequilibrium effects in time-resolved photo excitation and decay including solid-state and macromolecular charge transfer and separation. These are issues closely related to those faced in bioscience and biomimetic materials. We need new fundamental understanding to model femtosecond optical spectroscopy (absorption, luminescence...) and picosecond vibrational (infrared, Raman) spectroscopy. We have also begun to apply statistical and large-scale computing techniques to model the mesoscopic structure and formation kinetics of organic thin film growth, crucial to optimal macroscopic functionality.

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Figure 1. Simulation of a ductile material with 35 million atoms with an embedded atom potential. An elliptical crack (center of figure) in a 0.1-mm-thick copper sheet is placed under tension in the vertical direction. As the crack attempts to propagate horizontally, it emits clouds of dislocations (white dots), some of which have collided directly above the crack. Only the atoms at the surface of the crack, or within the cores of the dislocations, are depicted.