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Multiscale Phenomena in Materials

Author(s): * Alan R. Bishop, T-DO

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Jun Zang (City University of New York)
Tong Zhou (University of Chicago)
Shujia Zhou (Washington University)
I. Zubarev (CNLS,T-11)

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*Principal Investigator, e-mail: arb@lanl.gov

Abstract

This project developed and supported a technology base in nonequilibrium phenomena underpinning fundamental issues in condensed matter and materials science, and applied this technology to selected problems. In this way the increasingly sophisticated synthesis and characterization available for classes of complex electronic and structural materials provided a testbed for nonlinear science, while nonlinear and nonequilibrium techniques helped advance our understanding of the scientific principles underlying the control of material microstructures, their evolution, fundamental to macroscopic functionalities. The project focused on overlapping areas of emerging thrusts and programs in the Los Alamos materials community for which nonlinear and nonequilibrium approaches will have decisive roles and where productive teamwork among elements of modeling, simulations, synthesis, characterization and applications could be anticipated – particularly multiscale and nonequilibrium phenomena, and complex matter in and between fields of soft, hard and biomimetic materials. Principal topics were: (i) Complex organic and inorganic electronic materials, including hard, soft and biomimetic materials, self-assembly processes and photophysics; (ii) Microstructure and evolution in multiscale and hierarchical materials, including dynamic fracture and friction, dislocation and large-scale deformation, metastability, and inhomogeneity; and (iii) Equilibrium and nonequilibrium phases and phase transformations, emphasizing competing interactions, frustration, landscapes, glassy and stochastic dynamics, and energy focusing.

Background and Research Objectives

The notion of "spatiotemporal complexity" has emerged as an enduring and ubiquitous theme of nonlinear and nonequilibrium science built on the concepts of: (a) coherent space-time structures in strongly nonlinear classical and quantum systems and (b) the possibility of deterministic chaos even in low-dimensional nonlinear dynamical systems. Most importantly, the combination of these two concepts characterizes mesoscopic space-time complexity in which dominant lower-dimensional, collective patterns emerge and are embedded in high-dimensional spaces spanned by all microscopic degrees-of-freedom. Understanding and controlling the origin, structure and macroscopic consequences of these "mesoscales" represents a fundamental new field of nonlinear, nonequilibrium statistical mechanics – typically characterized by multiple relevant spatial scales (textures), and related multiple timescales (controlling "glassy" evolution and aging).

Our objective was to further develop and exploit these concepts for significant problems in condensed matter and materials science. In this way materials advances in synthesis and characterization of complex electronic and structural materials can motivate and validate approaches in nonlinear science, while nonlinear-nonequilibrium techniques can provide underpinnings to our understanding of microscopic processes controlling relevant structural and dynamic scales in classes of materials. This is a key element in establishing the "bridges" between microscopic, mesoscopic and macroscopic levels of modeling and control of materials – the predictive scientific principles for the nonlinear-nonequilibrium statistical mechanics of mesoscale complexity, which are necessary to provide a scientific basis for multiscale "synthesis-structure-property" relations in materials with rapidly increasing complexity and stringency of demands on functionality. This need for developing techniques to bridge between multiple scales is common to many disciplines, from biology to fluids to plasmas to astrophysics. In electronic and structural materials, experimental advances enable increasingly detailed resolution of microstructures and evolution, and this is matched by advances in simulation capacity. Their combined input must create the interpretative frameworks for multiscale phenomena necessary to guide next generation technology.

Achieving these goals requires the adaptation and application of fundamental advances from the current era of nonlinear science, including: (1) The isolation of competing length and/or timescales at microscopic scales, which typically drive nonlinearity leading to space-time complexity at coarser scales: (2) Nonlinear mode-projection techniques to identify and follow coherent structures (dislocations, vortices, domain walls, etc.), which typically control lower-dimensional "essential-state" subspaces at mesoscales; (3) Techniques to study the interaction and ordering of the collective coherent structures, including effects of noise and disorder (from the slaved modes and other sources) as well as driving fields; (4) Understanding intimate relationships between spatial and temporal scales. Competing and/or frustration interactions can lead to spatial patterns on many scales and to a multiplicity of "landscapes" (ground or metastable states in configuration space.) These complex textures are related to multiple timescales (typically related to the motion of coherent structures) characterizing relaxation and aging from nonequilibrium configurations or response to external forces. Excellent examples are available from condensed matter (spin glasses, pinned charge-density-wave materials, incommensurate phase transitions, flux flow in superconductors, etc.) which can guide systematics in this field of glassy/stretched-exponential/hysteretic/intermittent dynamics, and the relationships to spatial complexity; (5) Combining effects of disorder, noise and nonlinearity is unavoidable in many physical situations, and can lead to qualitatively new phenomena (smoothing of basins of attraction, pinning or destruction of collective patterns, nonlinear averaging of disorder, linear localization, anomalous diffusion, etc.).

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

Predictive control of multiscale phenomena in complex electronic and structural materials has emerged as a dominant need in the national and laboratory science base – a scientific underpinning for synthesis-microstructure-property-processing relationships. Nonlinear and nonequilibrium issues dominate most of the phenomena at all scales – fundamental space-time complexity issues such as mesoscopic self-organization and pattern formation, and glassy evolution and aging. The role for theory and simulation, closely coupled with experimental validation, as means of systematically and predictively describing these phenomena is now widely appreciated by DOE and Los Alamos Program offices, including science-based-stockpile, military and civilian elements.

The topics in this project complemented and supported emerging LANL activities in electronic and structural materials synthesis, characterization, modeling and applications. These include: novel electronic materials; thin film growth; device-development; ultrafast spectroscopy. Microstructure and texture are studied experimentally in the Manual Lujan Neutron Scattering Center and various Laboratory Divisions, and are focuses of the Materials Process Modeling Center as well as ASCI Programs. Fracture and friction are key concerns to programs in both MST- and X- divisions. Flux flow in superconductors is studied in the STC and is a focus of the National High-Magnetic Field Laboratory at Los Alamos. There is close integration with the high-performance computing facilities at Los Alamos. Thus this project will benefit LANL "Centers" and many Divisions.

Scientific Approach and Accomplishments

The research focused principally on the following topics:

(i) Complex organic and inorganic electron materials, including hard, soft and biomimetric materials, self-assembly processes and photophysics;

(ii) Microstructure and evolution in multiscale and hierarchical materials, including dynamic fracture and friction, dislocations and large-scale deformation, metastability, and inhomogeneity; and

(iii) Equilibrium and nonequilibrium phases and phase transformations, emphasizing competing interactions, frustration, landscapes, glassy and stochastic dynamics, and energy focusing.

These topics complemented emerging thrusts in the LANL materials community (including strong experimental components), and were chosen as areas where an approach to materials science based on interdisciplinary, nonlinear and nonequilibrium concepts are likely to lead to significant contributions of a fundamental nature, as well as integrate unique and/or distinguishing LANL expertise in complex systems modeling, condensed matter and statistical physics, condensed phase chemistry, mathematics, and high-performance computing—including the potential to bridge to biological and bio-mimetic materials. Through workshops, seminars, postdoctoral/visitor programs, and an ad-hoc advisory group, we seeded nonlinear activity in additional areas as appropriate – e.g., complex fluids and polymers; process modeling; composites; glasses; flow through porous media; behavior at high magnetic fields; biomimetic and biological materials.

Several common techniques were exploited, including: Analytical and numerical procedures to extract and project into essential, collective nonlinear modes and derive effective (nonlinear and/or nonlocal) equations of motion for the essential modes and their interactions (e.g., projecting particial differential equations (pde's) into noisy lower-dimensional pde's); Image-processing and statistical measures for complex patterns (bayesian, fractal, wavelets, nonlinear optimization, etc.); Course-graining techniques (time-scale separation, homogenization, Landau-Ginzburg, renormalization group, path-integration, Fokker-Planck) and self-consistent treatment of (colored) additive and muliplicative noise baths; Relating multiple time-scales under nonequilibrium conditions to underlying spatial textures; including glassy and hysteretic situations; numerical, multiscaling and memory-function analysis of coupled-fields (electron-lattice, reaction-diffusion, etc.) in classical and quantum-mechanical contexts.

Principal accomplishments:

Substantial research progress was made on several fronts, including:

- Large-scale molecular dynamics and Monte Carlo simulation and visualization of 3-dimensitional fracture and friction in metals and amorphous solids. These gave quantitative mesoscale information on dislocation dynamics and plastic deformation mechanisms, which are now being fed into more traditional continuum (macroscopic) models.
- Development and application of new numerical algorithms to understand and model long-range interactions in condensed matter systems. These new approaches have now revealed the origins and multiple length scales of mesoscopic pattern formation in superconductors (the organization and flow of flux structure induced by external magnetic fields), hard materials (charge ordering and dynamics in transition metal oxides and charge-density-wave materials), and soft matter (polyectrolytes adhesion

and aggregation, organization of biomacromolecules on surfaces, multilayer organic films).

- Development of new models and techniques for "landscapes" and associated multi-timescale ("glass"), nonequilibrium dynamics in complex materials, including: hierarchical elastic materials and solid-solid phase transformations in martenstic materials; thin-film morphology and evolution, and semiconductor quantum dots; and vortex dynamics in magnetic materials and layered superconductors. In all these cases, the interplay of long-range and short-range interactions, disorder, dimensionality and entropy were the driving forces for complex, multiscale structure and dynamics. These behaviors and associated metastable states will be key to understanding and controlling phenomena in the emerging fields of biological structure and function, and nonoscale science.
- Modeling of the origins, control and experimental signatures of energy/charge localization and transduction in electronic and structural materials. In particular, we demonstrated that the <u>combination</u> of nonlinearity and discreteness (typical of most real materials) leads in very general circumstances to intrinsic localization (so-called "intrinsic local modes"), non-thermal distributions of mesoscopic structures, anomalously long lifetimes, and novel coherent, collective transport mechanisms. We applied this undertaking to several classical and quantum systems, including: refinement processes at crack tips and sliding interfaces: arrays of Josephson junctions and coupled Josephson transmission lines; localization in polarizable electronic materials in which there is strong electon-elastic coupling. Controlling the formation, manipulation and properties of patterns of such intrinsic local modes is proving to be an exciting new direction in nanoscience international attention.
- Simulation and modeling of new experimental probes of multiscale (space and time) probes in organic, inorganic and biomimetric materials. We particularly emphasized situations (e.g. strongly coupled matter, active interfaces) where nonlinear, nonadiabatic and nonequilibrium issues render traditional protocols for data interpretation very dubious. Examples studied included pair-distribution function neutron scatteries, extended x-ray fine structure, ultrafast pump-probe optical spectroscopy, and tunneling microscopies. The <u>interpretation</u> of this new array of experimental probes to study functional length and time scales will be critical to enabling a new era of understanding and using "complex matter" (hard, soft, biological) for key present and future technologies.

We leveraged our work with the "Frontiers in Materials" program, involving UC Campuses (funded by the UCDRD Program). This provides a principal mechanism for developing, guiding and facilitating research in materials complexity at Los Alamos. A major result has been the creation of a thrust in "Complex Adaptive Matter" at Los Alamos and the beginnings of a national Institute for Complex Matter with distributed Centers.

Our LDRD project was benefited through the recruitment of graduate students, postdoctoral fellows and visitors to work with Laboratory staff in the project (see author/publication list).

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If you would like figures, please contact Alan R. Bishop (7-6491).