Mini-Workshop on Theory & Computation of Nanomaterials Behavior
Center for Nanoscale Materials

May 3, 2001
8:20am - 12:30pm
APS 401 Rm A1100

8:20am -8:30am Opening remarks Wai Kwok

Chair: Mike Norman

8:30-9:00 DYNAMICS OF NANOSCALE SYSTEMS
Valerii Vinokur (MSD)

9:00-9:30 CURRENT-CONTROLLED SWITCHING BASED ON THE SPIN-TRANSFER EFFECT.
Yaroslaw Bazaliy (MSD)

9:30 - 10:00 PHASE AND CHARGE DYNAMICS IN SMALL-SIZE STACKS OF INTRINSIC JOSEPHSON JUNCTIONS
Alex Koshelev (MSD)

10:00 - 10:30 GRAIN GROWTH AND DEFORMATION OF NANOCRYSTALLINE MATERIALS
Dieter Wolf (MSD)

10:30 - 11:00 ELECTRONIC STRUCTURE STUDIES OF NANOSTRUCTURED MATERIALS
Larry Curtis s (CHM/MSD)

11:00 - 11:30 ATOMIC-LEVEL SIMULATION OF FERROELECTRICITY IN PEROVSKITES
Simon Phillpot (MSD)

11:30 - 12:00 THEORETICAL STUDIES OF ONE- AND TWO-COMPONENT METAL CLUSTERS AND CLUSTER-LIGAND SYSTEMS
Julius Jellinek (CHM)

12:00 - 12:30 ORDER PARAMETER DESCRIPTION OF DYNAMIC PHENOMENA IN MATERIALS SCIENCE
Igor Aranson (MSD)

DYNAMICS OF NANOSCALE SYSTEMS

V. Vinokur (MSD)

We review aspects of dynamics of nanoscale systems in relation with the research planned in the Center for Nanoscale Materials at ANL. We focus on the following directions: (i) Andreev reflection and related phenomena in nanoscale-size superconductors; (ii) Decoherence and noises in quantum devices; (iii) magnetization reversal and related processes in nanoscale magnets; and (iv) nanomechanics. Topic (i) includes theoretical analysis of phase transitions in nanoscale superconducting dots and constrictions and investigations of the structure of normal electronic excitations associated with vortex ensembles and their influence on transport properties of confined superconductors. Decoherence and noises (ii) are the main effects destroying *quantum interference*, the key phenomenon governing nanoscale physics, therefore understanding them is crucial for designing nanodevices. We focus on decoherence and noise in driven ballistic devices and discuss acoustically driven quantum channels, quantum point contacts between superconductors, and 2D electron gas. A progress in physics of relaxation processes in nanoscale magnets is central to engineering of the new generation of memory elements and recording devices (iii). We discuss a problem of magnetization reversal in a small magnetic grain and related effects. (iv) New field of nanomechanics covers the study of elastic and plastic phenomena in nanometer-scale materials. We touch upon the problem of self-assembly, friction in thin lubricating films, and the interplay between the electronic processes and micromechanics of small objects: as an exemplary example we discuss a superconducting grain moving between the two superconducting leads. We discuss other nanoscale electromechanical phenomena: instability of metallic nanoclusters and force oscillations in nanowires.

CURRENT-CONTROLLED SWITCHING BASED ON THE SPIN-TRANSFER EFFECT

Yaroslaw Bazaliy (MSD)

In a standard spin-valve structure two ferromagnetic layers separated by a normal spacer interact via an RKKY-like exchange interaction. Recently a lot of interest was shown to the situation when this system is driven out of equilibrium by pumping electric current perpendicular to the layers. It turns out that in this case magnetic interaction is changed in two ways. First, exchange coupling constant gets a correction proportional to the current. Second, a new term appears which does not conserve the total energy of the magnetic system and represents a possible influx of energy from the current source. This term was introduced by L.Berger and J.Slonczewski and got the name "spin-transfer". It was proposed that this term could be the cause of current-controlled switching between different (e.g. parallel and anti-parallel) magnetic configurations of the spin-valve. Several recent experimental studies have confirmed this possibility.

On the basis of equations proposed by J.Slonczewski for the case when magnetizations of the two ferromagnetic domains are uniform, we analyze the stability and switching for two types of magnetic and shape anisotropies of the layers. One case corresponds to the actual experimental situation and the other can be realized with different spin-valve preparation. We find qualitatively different behavior, including different shapes of bistable regions. Our study is analytic as opposed to recent numeric work and our predictions can be used to experimentally test the theory of spin-transfer torque. Such test would be especially interesting since alternative approaches are discussed in the literature.

PHASE AND CHARGE DYNAMICS IN SMALL-SIZE STACKS OF INTRINSIC JOSEPHSON JUNCTIONS

Alex Koshelev (MSD)

Submicron-sized mesas, fabricated from $Bi_2Sr_2CaCu_2O_x$ whiskers, provide realization of stacks of intrinsic Josephson junctions with significant quantum phase fluctuations. I will review phenomena expected in such mesas. As the mesa size decreases, the role of quantum phase fluctuations becomes progressively important. The strength of the quantum fluctuations is governed by the relationship between three major parameters: Josephson coupling energy, charging energy and c-axis quasiparticle damping. The most dramatic effect driven by quantum fluctuations is the superconductor-insulator phase transition, which is expected when the lateral size becomes of the order of several hundred nanometers. In larger mesas this transition can be driven by an external magnetic field. I will discuss transport properties in the vicinity of the transition.

GRAIN GROWTH AND DEFORMATION OF NANOCRYSTALLINE MATERIALS

Dieter Wolf (MSD)

Nanocrystalline materials are polycrystals with a grain size in the nanometer range. It has been suggested that because of the large volume fraction of grain boundaries in these materials, their physical behavior may differ fundamentally from that of course-grained polycrystals. During recent years we have performed extensive atomic-level simulations of the structure and thermo-mechanical properties of these materials, elucidating the manner in which they differ from coarse-grained polycrystals. For example, in conventional polycrystals grain growth results solely from the migration of grain boundaries in response to the driving force associated with the grain-boundary curvature. By contrast, in a nanocrystalline microstructure grain rotations and the subsequent coalescence of neighboring grains play an equally important role. Similarly, the interplay between dislocation and grain-boundary based mechanisms in plastic deformation differs fundamentally from that in coarse-grained materials.

ELECTRONIC STRUCTURE STUDIES OF NANOSTRUCTURED MATERIALS

Larry Curtiss (CHM/MSD)

We are using electronic structure methods including *ab initio* molecular orbital theory, density functional theory, and density functional based tight-binding molecular dynamics to investigate the chemical and physical properties of nanostructured materials. Some recent results on nanocrystalline diamond, molecular sieve materials, layered organic conductors, and titanium oxide nanoparticles will be reviewed. Future expected advances in computer technology and theoretical methodology will greatly enhance the insights that can be provided by electronic structure computations into the properties of nanostructured materials. The prospects for future computations will be discussed.

ATOMIC-LEVEL SIMNULAITON OF FERROELECTRICITY IN PEROVSKITES

Simon Phillpot (MSD)

We have recently succeeded in constructing the first atomic-level description of any perovskite that can both describe the full phase diagram and can be used for the simulation of ferroelectricity in interfacial and defected systems. This model, which combines a Buckingham potential with an isotropic shell model, provides a good description of the ferroelectric phase behavior of $KNbO_3$, reproducing the experimentally observed sequence of phases on heating: rhombohedral, orthorhombic, tetragonal and finally cubic, with transition temperatures very close to the experimental values. Furthermore, the lattice parameters in the four phases agree with experimental values to better than 1%, and the calculated polarization in the tetragonal phase is only about 20% larger than the experimental value.

We have also constructed a potential that describes the incipient ferroelectric behavior of $KTaO_3$; this has allowed us to simulate the ferroelectric properties of $KTa_xNb_{1-x}O_3$ solid solutions and $KNbO_3/KTaO_3$ superlattices. In each case, the atomic-level information provided by the simulations has allowed us to elucidate the intimate coupling of the ferroelectric behavior of the $KNbO_3$ and $KTaO_3$ components and the coupling between ferroelectricity and elastic strain.

THEORETICAL STUDIES OF ONE- AND TWO-COMPONENT METAL CLUSTERS AND CLUSTER-LIGAND SYSTEMS

Julius Jellinek (CHM)

I will review our studies of structural, electronic, thermal, phase and phase change properties of one- and two-component (alloy) metal clusters, and interactions of metal clusters with molecules.

ORDER PARAMETER DESCRIPTION OF DYNAMIC PHENOMENA IN MATERIALS SCIENCE

Igor Aranson (MSD)

We consider application of continuum order parameter theory to two problems of materials science: crack propagation in brittle materials and friction in ultra-thin liquid films.

We develop a continuum field model for crack propagation in brittle amorphous solids. The model is represented by the equations for elastic displacements combined with the order parameter equation which accounts for the dynamics of defects. This model captures all the important phenomenology of crack propagation: crack initiation, propagation, dynamic fracture instability, sound emission, crack branching and fragmentation.

We develop the theory for stick-slip motion in ultra-thin liquid films confined between two moving atomically-flat surfaces. Our model is based on the hydrodynamic equation for flow coupled to the dynamic order parameter field describing the "shear melting and freezing" of the confined fluid. This model successfully accounts for the observed phenomenology of friction in ultra-thin films, including periodic and chaotic sequences of slips and transitions from stick-slip motion to steady sliding.