

THE DoD HIGH PERFORMANCE COMPUTING MODERNIZATION PROGRAM IN 2002: MOVING DoD COMPUTATIONAL SCIENCE FORWARD

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The DoD High Performance Computing Modernization Program (HPCMP) has completed several significant changes in 2001. Several major acquisitions have now been concluded that will further improve the ability of the HPCMP to serve its DoD science and technology and test and evaluation user base. The results of these acquisitions are major additions of HPC hardware, software, and networking capabilities.

The HPCMP also continues its annual process to select and implement a set of mission-critical, computationally-intensive DoD Challenge Projects. These DoD Challenge Projects ensure that DoD's large, high-priority computational projects have access to HPC resources that are needed for timely progress in their support of DoD laboratories and test centers.

Computational chemistry and materials science (CCM) is one of the major computational technology areas (CTAs) that characterize the computational work of DoD's laboratories and test centers. An appreciable number of DoD's 4,000 laboratory and test center HPC users and an appreciable fraction of its total high performance computing requirements encompass CCM. Of the 41 active DoD Challenge Projects, several involve CCM. These CCM Challenge Projects have made substantial progress for the design of DoD materials.

NANOSCOPIC ORIGINS OF MATERIALS FAILURE

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Empirically, it is known that spray coating thin layers of ceramics onto metals can afford protection of the metal from both chemical corrosion and heat. For example, thin metal oxide coatings are used to protect Ni alloy components of gas turbine engines from the harsh operating conditions present during fuel combustion. The problem with current coating formulations is that they spall (chip off) after a number of heating and cooling cycles, which limits the practical lifetime of such ceramic coatings. The mechanisms of how the coatings fail remain less than clear. Experimental measurements of the intrinsic adhesion strengths of these coatings are difficult at best and tend to vary significantly due to the presence of defects, voids, etc., created upon sample preparation. It is virtually impossible to create an ideal interface and to reproducibly measure the work of separation of such an interface. Here is an arena where theory may play a constructive role, by systematically assessing the inherent stability of interfaces between materials. Therefore, we have carried out a series of studies utilizing density functional theory with periodic boundary conditions designed to characterize the adhesion and bonding at ideal interfaces between ceramics and metals. Our investigations of the electronic and mechanical properties of high temperature ceramics, such as alumina, zirconia, and silica, and their interactions with Ni and Ni-Al alloy surfaces reveal why certain thin films of ceramics do not adhere well to nickel and Ni-Al alloys, while others do. Insights from these simulations are used to suggest new designs for alloy bond coatings that should improve adhesion (and hence lifetime) of ceramic coatings on metals.

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SCALABLE ALGORITHMS AND PARALLEL COMPUTING FRAMEWORK FOR MULTISCALE MATERIALS SIMULATIONS BEYOND TERAFLOP

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Petaflop computers and a Grid of distributed supercomputers will offer tremendous opportunities for high-end computational materials research. To make applications scalable on such platforms, we are developing:

- Scalable linear-scaling algorithms based on space-time multiresolution schemes—clustering, hierarchical abstraction, and the analysis of asymptotic solution properties and error bound—for i) all-pairs function evaluation in the N -body problem, ii) dense linear system of equations in the variable N -charge problem, and iii) exhaustive combinatorial enumeration in the quantum N -body problem, which are common in many scientific/engineering applications;
- Multiscale simulation approach that seamlessly combines i) engineering mechanics calculation based on the finite element (FE) method, ii) atomistic simulation based on the molecular dynamics (MD) method, and iii) quantum mechanical (QM) calculation based on the density functional theory (DFT), so that expensive (often scalability-limiting) computations are performed only when and where they are needed.

The production-quality programs also feature wavelet-based computational-space decomposition for adaptive load balancing, spacefilling-curve-based adaptive data compression with user-defined error bound for scalable I/O, and parallel/distributed visibility culling for immersive and interactive visualization of massive simulation data.

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TERASCALE COMPUTING AT PSC

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I will discuss

- the architecture of the Terascale machine at the Pittsburgh Supercomputing Center,
- some challenges involved in working with a system this size,
- benchmarks of actual performance on user codes,
- examples of the groundbreaking science that has been done and will be done using these facilities,
- what the next generation of machines is likely to be

I will also describe how conference participants can get allocations on these and other NSF facilities.

HIGH PERFORMANCE COMPUTING, COMPUTATIONAL GRID, AND NUMERICAL LIBRARIES

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In this talk we will look at how High Performance computing has changed over the last 10-years and look toward the future in terms of trends. In addition, we advocate the 'Computational Grids' to support 'large-scale' applications. These must provide transparent access to the complex mix of resources - computational, networking, and storage - that can be provided through aggregation of resources. The vision is of uniform, location independent, and transient access to the

Computational
Catalogued data
Instrument system
Human collaborator

resources of contemporary research activity in order to facilitate the solution of large-scale, complex, multi-institutional/multidisciplinary data and computational based problems. It envisages these resources being accessible through a Problem Solving Environment appropriate to the target community.

TERASCALE OPTIMAL PDE SOLVERS

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Computational performance on full-scale scientific applications, as tracked by the Gordon Bell prize, has increased by four orders of magnitude since the prize was first awarded in 1988 --- twenty-five times greater than can be accounted for by Moore's Law alone. The extra factor comes from process concurrency, which is as much as 8,192-fold on the \$100M "ASCI White" machine at Lawrence Livermore, currently ranked as the world's most powerful. Though architectural concurrency is easy to achieve, algorithmic concurrency to match is less so in scientific codes. Intuitively, this is due to global domains of influence in many problems presented to the computer as implicitly discretized operator equations --- implicitness being all but legislated for multiscale systems, in which dynamics fast relative to dynamics of interest must be "stepped over."

For many years, we have been pursuing optimal parallel algorithms for PDE simulations in the Newton-Krylov methodology, preconditioned with Schur and Schwarz decompositions, including multilevel generalizations of the latter. A characteristic of this family of algorithms is multiple discrete representations of the underlying continuous operators --- high fidelity on the right-hand side and various shortcuts on the left-hand side, including physics-based operator-splitting. Simultaneous advances in object-oriented software engineering have enabled the construction of complex software systems in which these algorithmic elements can be combined modularly, recursively, and relatively efficiently in parallel. Recently, we have helped show how large-scale PDE-constrained optimization (e.g., design, control, parameter identification --- usually the ultimate practical problem behind the proximate PDE) can be placed into the same algorithmic framework.

In this talk, we first focus on basic algorithmic methodology, we illustrate with a university-NASA-DOE collaboration that led to a recent Gordon Bell prize, and finally we describe major goals of a five-year, nine-institution project, "Terascale Optimal PDE Simulations," which is one of the seven "Integrated Software Infrastructure Centers" of the DOE's new "Scientific Discovery through Advanced Computing" initiative whose aim is to package several existing license-free DOE software toolkits -- including Argonne's PETSc and Livermore's HYPRE -- for wider community use.

AIR FORCE RESEARCH IN NANOENERGETICS – POTENTIAL ADVANTAGES AND CHALLENGES

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The Advanced Energetics group at the AFRL Munitions Directorate is developing new, emerging types of energetic materials. The broad goal is to exploit new types of energetic materials to improve conventional munitions performance or capabilities. One class of these alternative materials is based upon intermolecular reactions in materials that have greater chemical energy per unit volume than conventional high explosives. These materials have potential to provide very high temperature, high heat, and tunable partitioning of energy into blast and metal acceleration. However, reaction and energy release rates in micron-sized materials of this type, such as traditional pyrotechnic materials, are too slow to achieve the power needed for conventional weapons effects. One approach we are now pursuing is to promote very high-rate reaction in mixtures of nano-scale fuels and oxidizers. Nanometric fuel-oxidizer systems that release energy at power levels comparable to that of conventional uni-molecular HCNO-explosives are being studied for munitions and propulsion applications. Reaction rates are accelerated by reducing particle size to nanometric scale, increasing surface area for a given mass, and reducing diffusion path lengths.

One disadvantage in reduction to nanometric scale is that inert surface layers become a significant proportion of total mass. Processing disadvantages are also encountered. Nano-particles tend to agglomerate, making it difficult to mix and homogeneously distribute the material. Viscosity of mixes is significantly increased due to high specific surface area. To minimize these practical difficulties, we have been studying the use coatings to reduce surface tension and tendency to agglomerate. Techniques are being developed for direct polymer encapsulation of nano-particles. Nano-thin layers of other types of energetic materials, such as conventional explosives, coated onto the nanometric metal fuel particles have also been developed as part of this work. Small-scale safety tests of these coated energetic composites surprisingly have indicated that their safety properties materials may be superior to that of conventional micron-sized explosive particles.

STRENGTH AND PLASTICITY IN NANOCRYSTALLINE CU AND NI -ATOMIC SCALE SIMULATIONS AND EXPERIMENTAL OBSERVATIONS

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We present atomistic simulations of nanocrystalline materials under deformation. These large-scale molecular dynamics simulations are performed in parallel computers such as the ASCI machines at Lawrence Livermore National Laboratory, that allow for systems containing several millions of atoms. We study mainly two metals, copper and nickel, using the modified embedded atom model. Our simulations start with a Gaussian distribution of grain sizes, with average grain sizes up to 30nm in order to mimic the distributions observed experimentally. The construction of the grains is such that the orientation of the grain boundaries can be selected. Previous simulations with mainly high angle grain boundaries have shown that deformation at grain sizes between 12 and 20nm is driven by intra-grain dislocation activity [1]. Recent experiments by Lu et al. reported high ductility for electrodeposited nanocrystalline Cu at room temperature. An important characteristic of this material is the presence of high concentration of low angle grain boundaries. In order to address this problem, we compare the results of simulations with random grain boundaries to those with texture, low angle grain boundaries, identifying the deformation mechanisms. Our simulations show higher dislocation activity for the case of low angle grain boundaries, with partial dislocations traveling across grains. The results of these simulations are compared to experimental observations of electrodeposited nanocrystalline nickel .

Some experiments have also shown a dependence of ductility on strain rate. High strain rates can be achieved using laser driven experiments. We will present the evolution of a nanocrystalline material under laser driven shocks in the particular case of converging shocks, and compare the results with simulations in single crystals. These simulations show the importance of anisotropies due to crystal orientation and grain boundaries in the shock induced damage, such as void nucleation and growth.

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ATOMISTIC SIMULATIONS OF THE PLASTICITY BEHAVIOR OF SINGLE CRYSTAL AND POLYCRYSTALLINE METALS

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We examine the effects of deformation on single crystal and polycrystalline FCC metals. We perform simple shear molecular dynamics simulations using the Embedded Atom Method (EAM) on nickel samples ranging from 100 atoms to 100 million atoms to study yield and work hardening. It is found that the deformation is always inhomogeneous when a free surface or grain boundary is present. The results of the single crystal simulations are compared to data from nano-indentation experiments, micro-indentation experiments, and small scale torsion experiments. This comparison shows that the yield stress varies as $L^{-0.4}$ over five orders of magnitude in which a length scale parameter, L , is defined by the ratio of volume to surface area. The atomistic simulations reveal that dislocations nucleating at free surfaces and grain boundaries are critical to causing yielding in pristine material as observed in experiment [1, 2].

Detailed investigation shows that the grain boundaries are significantly weaker than the bulk material and yield at a lower stress. Even so, the yield stress of the polycrystalline samples with both low angle and high angle grain boundaries are found to be similar and only slightly lower than the yield stress of single crystals with the same characteristic dimensions. Reduction of geometric constraint in the calculations results in a significant lowering of the yield stress.

The atomistic simulations and experimental data show that differences in applied strain rate, temperature, stacking faults (several FCC materials have been examined), deformation mode, and crystal orientation on yield and plasticity are small compared to the size scale effect.

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INORGANIC NANOCRYSTALS AND NANORODS: SYNTHESIS AND BIOLOGICAL APPLICATIONS

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In semiconductor nanocrystals, due to confinement of the charge carriers, analogous to a particle-in-a-box model, the band gap is size-dependent. Therefore the wavelength of emission following photoexcitation can be tuned by the size of the nanocrystals. Recent advances in the synthesis of colloidal CdSe and Co nanocrystals have been made allowing for shape control. Nanocrystal bio-polymer conjugates hold great promise both for biological diagnostics, where the nanocrystals can provide unique detection signatures, and for nanotechnology, where the information content of the bio-molecule can be harnessed for spatial patterning of nanocrystals. In materials science, assemblies of particles have been constructed by using oligonucleotides as molecular scaffolds for supporting oligonucleotide labeled nanocrystals. In biological research, semiconductor nanocrystals in a range of colors have been used as fluorescent probes for cellular imaging. Due to their reduced photobleaching properties they are especially suitable for dynamic studies in living cells. We show that nanocrystals are actively incorporated by living cells. The uptake is analyzed in dependence of the nanocrystals' size and charge. Dynamic confocal microscopy images suggest, that negatively charged and almost neutral silanized nanocrystals are endo- or phago-cytosed by living cells and arranged in intracellular vesicular compartments.

GRAIN BOUNDARIES IN GALLIUM ARSENIDE NANOCRYSTALS

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We have investigated structural transformation in GaAs nanocrystals using parallel molecular dynamics (MD) simulations. Spherical and faceted nanocrystals of different sizes are studied by suspending them in a liquid and then isothermal-isobaric MD simulations are performed. It is found that the transformation from four-fold (zinc blende) to six-fold (rock salt) coordination is nucleated on the nanocrystal surface and proceeds inwards with increasing pressure. Inequivalent nucleation of the rock salt phase at different sites on the surface leads to non-uniform deformation of the nanocrystals. The transformation is sensitive to initial shape: spherical nanocrystals above a critical diameter ≥ 44 Å always show grain boundaries where as faceted nanocrystals of comparable size do not show grain boundaries in 40% of the cases. The pressure to complete the transformation is found to increase with nanocrystal diameter and approaches the bulk value from below. A thermodynamic explanation for this trend based on nanocrystal-liquid interface enthalpy is attempted. Spatially resolved phonon densities of states correlate with local structure.

This work has been supported by NSF, DOE, AFOSR, DoD-DURINT, NASA and BCVC (Louisiana Board of Regents).

NANOFABRICATION RESEARCH AND CAPABILITIES AT CORNELL NANOFABRICATION FACILITY

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Cornell Nanofabrication Facility (CNF) is a National user facility – a part of the National Nanofabrication User Network (NNUN) funded by a grant from NSF. The goal of CNF and NNUN is to facilitate and support research of others from all around the Nation. With nearly \$30M worth of equipment and 20 members of technical support staff, skillful in any kind of Nanofabrication techniques and processes, CNF services a rapidly growing U.S.-wide research community. This year, nearly 700 users performed Nanofabrication-related projects at CNF. Most of these projects required training, assistance, and, occasionally, design and process development expertise from the CNF technical staff.

This talk will give a brief overview of CNF facilities, modes of interaction with outside users, and give examples of some recent projects performed here. Projects from the fields of chemistry, biology, electronics, mechanics, optoelectronics, and nanostructure physics will be presented with the emphasis on the unique nanofabrication capabilities that are available to outside users at CNF. The unique CNF needs in materials and process simulation at the nanoscale will be addressed, as well.

PROCESS-STRUCTURE-PROPERTY RELATIONSHIPS OF POLYMERIC BIOMATERIALS

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The Process-Structure-Property-Performance paradigm of material science is well known and is routinely used to define and optimize synthetic polymers for specific applications. One of the underlying themes of the Medical Device Concept Laboratories is to apply this paradigm to the emerging field of bioerodable, polymeric biomaterials. Our specific objectives are:

- Understanding the origins of the biological and material properties exhibited by these materials as function of their chemistry, morphology and surface characteristics
- Quantifying the effects of processing on the development of structural features
- Developing characterization techniques relevant to in-vivo use

The combinatorial library of desaminotyrosyl polyarylates developed by Professor Joachim Kohn of Rutgers University, is being investigated as a model system. Selected library polymers are melt formed into uniform fibers and films defining a range of structural and performance characteristics. Existing thermal analysis, microscopic and spectroscopic techniques are utilized as platforms for developing biorelevant data sets, capable of extrapolation to in-vivo performance prediction. The influence of structural features, from the nanoscale through the macroscale, on biological performance is being investigated.

Results to date indicate that the Kohn library is extraordinarily rich in structural features and performance options. It was found that some library polymers form novel, mesogenic nanostructures of interest to the polymer physics community independent of the impact of this structure on biological activity. Cell culture studies are currently underway to quantify the effects of this novel morphology on cellular growth. The impact of controlled mechanical properties and dimensional stability on the efficacy of these materials as ACL repair scaffolds is being investigated in collaboration with Professor M. Dunn of the RWJ Medical School.

SHORT AND INTERMEDIATE RANGE ORDER IN DISORDERED $\text{Ge}_x\text{Se}_{1-x}$ SYSTEMS

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Interest in disordered $\text{Ge}_x\text{Se}_{1-x}$ systems is motivated by the peculiar structural changes exhibited over the whole compositional range, which reflect variations in the nature of bonding. On the Se rich side ($x=0.2$, GeSe_4 and $x=0.33$, GeSe_2), intermediate range order (IRO) which establishes on length scales significantly more extended than nearest neighbor distances gives rise to the presence of a first sharp diffraction peak (FSDP) in the total neutron structure factor. First principle molecular dynamics studies have shown that liquid GeSe_4 is a chemically ordered system [1], i.e. the number of heteropolar bonds is maximized. On the other hand, in liquid GeSe_2 the chemical order is broken due the presence of miscoordinated atoms and homopolar bonds which coexist with GeSe_4 tetrahedra[2]. The existence of homopolar Ge-Ge bonds for this composition has also been recently firmly established for amorphous GeSe_2 .

To highlight the intimate relationship between bonding and intermediate range order in disordered network-forming systems, liquid GeSe_2 has been investigated by adopting two distinct functionals for exchange and correlation within density functional theory. It was found that a generalized gradient approximation (GGA) is required to reproduce a FSDP in the total structure factor, while, when the local density approximation (LDA) is used, the FSDP is absent.

An analysis of the bonding configurations indicates that liquid GeSe_2 is a defective network consisting of predominant Ge-centered tetrahedral units but Ge- and Se-centered triads and homopolar bonds occur in nonnegligible amounts. The number of Ge-Ge homopolar bonds and of ordered fourfold rings compare favorably with experimental estimates. Chemical disorder manifests through an important percentage of Se-rich odd membered rings. We characterized the intermediate range order by studying the relation between real-space distances and the FSDP. We found that this feature appears when correlations beyond 5\AA are accounted for. The evaluation of bond lifetimes reflect the higher stability of Ge-Se bonds with respect to homopolar bonds, consistent with the predominance of tetrahedral units [5].

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NANOSCALE INHOMOGENEITIES IN MULTICOMPONENT OXIDE GLASSES: MOLECULAR DYNAMICS SIMULATION STUDY

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We present results of molecular dynamics simulations on a wide variety of multicomponent network-forming glasses, i.e., oxide glasses with doped alkali oxides such as Na/Si/O, Li/Si/O, and Na/B/O. The simulations are based on the Born-Mayer-Huggins potentials totally characterized by the charges and sizes of ions. Such a simple model is able to account for essential features of the glassy networks modified by alkali ions. It is one of central issues how the network-modifier cations are distributed in the glasses. The same method[1] as used to identify Ag clusters in Ag/Ge/Se glasses is applied to the multicomponent glasses to address that issue. We define clusters of the alkali modifiers and then calculate their size distribution. The clustering tendency in each glass is discussed in reference to the cluster-size distribution in a corresponding system with randomly distributed particles. The Na ions embedded in the glassy SiO₂ matrix show clustering behavior similar to that of Ag in g-GeSe₂, while no clustering of the Na ions in g-B₂O₃ at all. Many glass systems show metastable immiscibility in certain compositional range. The immiscibility behavior of alkali silicate glasses clearly depends on the strength of the Coulomb interaction between oxygen and alkali ions: smaller alkalis show a greater tendency to phase separation than larger alkali ions. Comparison of the clustering behavior between Na/Si/O and Li/Si/O glasses accommodates the phase separation tendency. Alkali silicate glasses are inhomogeneous on nanoscale even outside the compositional range of immiscibility although those have been regarded as homogeneous. Relationship of the clustering nature to the dynamical properties in the glasses is also discussed.

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"NANO" AND "BIO" AT THE DEPARTMENT OF ENERGY

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The two prefixes "nano" and "bio" are generating exciting possibilities within the materials community. I will give a provincial view (from Basic Energy Sciences) of the response within the Department of Energy. Although DOE is a large supporter of very wide-ranging scientific research, it is still a mission-oriented agency. Within this context, one defines the scope and opportunities of these new emphasis. However, I claim absolutely NO clairvoyance!

DIRECTED ASSEMBLY OF FUNCTIONAL NANOSTRUCTURES

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The past decade has seen explosive growth worldwide in the synthesis and study of a wide range of nanostructured materials, the substance of nanotechnology. An overview of nanoscience and nanotechnology and their relationship to novel functional materials assembled from nanoscale building blocks will be presented within the framework of the 2001 United States National Nanotechnology Initiative and our new National Science Foundation Nanoscale Science and Engineering Center for Directed Assembly of Nanostructures at Rensselaer. Several examples from our recent research results will be presented including investigations of functional nanocomposites that could find use in a variety of structural, electrical, and biomedical applications.

NANOMETRIC ASPECTS OF ENERGETIC CRYSTAL PROPERTIES/TESTING

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Energetic crystals exhibit an interesting combination of mechanical properties: being elastically soft (because of their molecular/hydrogen bonding); plastically hard (because of the mutual interference to dislocation movement of adjacent interposed molecules in low symmetry crystal lattices); and brittle (because of relatively low, anisotropic, surface energies)¹. The large displacement vectors of dislocations lead to low dislocation densities in solution-grown crystals that are predicted on a continuum mechanics comparison of volumetric elastic strain energy versus substituted surface free energy to contain “worm holes” running along the cores of the dislocation lines --- at larger hole diameters than apply for the smaller nanometric dimensions at which the surface energy and volume free energies are equivalent. A continuous indentation hardness stress-strain basis has been developed for assessing the combined elastic/plastic/cracking behaviors of energetic crystals in comparison with those behaviors of other crystal structure types² --- and the method necessarily involves nanometric-scale force/displacement measurements for assessing the connected behaviors. In particular, crystal size dependent pile-ups of only a few dislocations are predicted to be involved in the production of “hot spots” associated with cracking and the initiation of chemical decomposition. Smaller crystals are known at micrometer dimensions to be less sensitive to impact initiation, consistent with greater strength levels occurring for finer microstructures. Such model consideration shows that energetic crystals are especially susceptible to hot spot development on the basis of their combined [crack initiation/thermal conductivity] properties --- relating also to the general property of shear banding in structural materials.

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ADAPTIVE ABERRATION CORRECTION IN CONFOCAL MICROSCOPY

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The confocal microscope is becoming an instrument of choice in many laboratories in both the life and physical sciences since its optical sectioning property permits the images of volume structures to be rendered in three-dimensions. In order to achieve this volume rendering a series of through-focus images must be recorded at different focal depths within the specimen. An inevitable consequence of this is that aberrations are unavoidably introduced. Aberrations, due to refractive index mismatch are further introduced by using, for example, an oil immersion objective to image a watery specimen. In order to overcome this fundamental problem we will describe an adaptive optics approach in which a novel wavefront sensor is used both to measure the aberrations introduced and to provide control signals to an adaptive element for correction. The system works in closed loop and permits diffraction limited resolution to be restored at depth. Examples will be shown from both the biological sciences and the physical sciences where the system will be applied to the reading of three dimensional optical memory materials.

THE USE OF ‘EXTREMOPHILE’ PROTEINS IN BIO-NANO-TECHNOLOGY

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The kinds of “weird effects” that were once Feynman and are now you and me and the whole biosphere are ultimately dependent on the physics and chemistry going on at the nanometer (molecular) scale. As the nano-scale becomes a focus for engineering, a role for ‘bio-nano-technology’ is emerging to address fundamental engineering problems on that scale. We have been exploring the potential of using a class of proteins known as ‘heat shock proteins’ (specifically HSP60s) for producing nano-structures with industrial applications. This class of proteins self-assemble into double-ring structures with seven, eight, or nine protein subunits per ring. Through the use of HSP60 genes from ‘extremophiles’ (i.e., organisms living in extreme environments—near-boiling temperatures and at pH 2.0), we are developing simple and effective methods for obtaining industrial quantities of these proteins. By using tools of crystallography and molecular biology, we are exploring the range of structures that can be created using the HSP60 double rings as building blocks.

THE CONVERGENCE OF BIOLOGY AND NANOSCIENCE: AN OPPORTUNITY FOR MOLECULAR DEVICES BUILT WITH BIOLOGICAL MOLECULES

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Nanoscience and biology are discrete disciplines that contribute substantially to each other. Their intersection creates an opportunity for hybrid nanodevices, with nanoscience providing a pallet of precise (primarily) structural nanomaterials, and biology providing a vast menu of functional nanostructures. Successful hybrid devices (called nanobiological, nanobiotechnological devices or biologic nanodevices) have common features and their construction can be codified into a set of steps applicable to a broad sweep of devices. Initial applications of the approach have been predominantly biomedical, but nanobiological devices will not be limited to those applications in the long run, and hybrid devices will ultimately be applicable to many tasks of importance. Emerging and established engineering and biological paradigms inform device design, synthesis and use, and engineering of their components, which should allow broad commercialization of nanotechnology. Nanobiotechnology allows construction of commercial quantities of nanodevices without recourse to self-replication, avoiding an oft-sited concern about the safety of nanotechnology. Continued commitment to nanoscience, biology and the technology and areas at their interface is essential to assure the legitimate human aspiration for a better, more sustainable world.

PHAGE AS ENGINEERED SELF-REPLICATING SELF-ASSEMBLING SYSTEM FOR NANOFABRICATION OF BIOSELECTIVE SENSORS

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Filamentous phage, such as M13, f1 and fd, are thread-shaped bacterial viruses. Their outer coat is composed of thousands of 50-residue α -helical subunits of the major coat protein pVIII, which overlap one another to form a tube encasing the viral DNA. We have shown that filamentous phage can serve as a scaffold, able to form on its surface an indefinite number of potential antigen-binding sites by displaying random peptides fused to major coat protein pVIII. We constructed libraries with random peptides fused to pVIII in various formats, and selected phages that act as substitute antibodies specific for a panel of test antigens and model "threat agents" (Petrenko, 1996, 2000; Romanov, 2001). Because the viral carrier is infective, phage borne bio-selective probes can be cloned individually; thus, either whole libraries or individual clones can be propagated indefinitely without needs of their chemical synthesis or reconstructing (Smith & Petrenko, 1997). can bind biological agents and, as a part of an analytical platform, generates a detectable signal. As elements of field-use detectors, they are superior to monoclonal antibodies, since they are inexpensive, highly specific and strong binders, resistant to unfavorable environmental conditions.

This work is a first demonstration of the use of landscape phages as bio-selective ligands in biosensors. As substitute antibodies phages demonstrate many features (high affinity, field stability, low cost etc.), which allow considering them as prospective ligands in a new generation of sensors for food safety control and environmental in-a-real-time monitoring.

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PATTERN FORMATION AND CELL SIGNALING AT AN INTERMEMBRANE SYNAPSE

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Spatial organization of proteins is an emerging theme of broad significance in cell recognition and signal transduction. Cells from the immune system and nervous system, among others, engage target cells through highly organized patterns of proteins that assemble at the intercellular synapse. Recent studies have revealed dynamic patterns within the immunological synapses formed when either T- or NK-cells engage their respective target cells. Though still controversial, there is mounting evidence indicating that specific synaptic patterns correlate with cellular activation. We are exploring the physical mechanisms behind synaptic pattern formation at intermembrane junctions in an effort to elucidate their role in cell recognition and signaling.

The fundamental problem we address is the collective interaction of populations of receptors and ligands in apposing lipid bilayer membranes. The membrane introduces a fluctuating two-dimensional reaction environment in which topographical constraints and restricted component access strongly influence receptor binding and spatial organization. From theoretical studies, we have found that these membrane constraints modulate the collective receptor ligand binding such that patterns on the nanometer and micrometer scale can emerge spontaneously. Our theoretical predictions have proven to correspond with observations of synaptic patterns in living T-cells.

In order to address this problem experimentally, we have initiated development of a totally reconstituted inter-membrane junction between a supported membrane and a second membrane patch, which is deposited from a giant vesicle. Incorporation of different fluorescent probe lipids into each of the two membranes enables a variety of fluorescence imaging capabilities which we employ to obtain both lateral and topographical information about the junction. We have demonstrated that fluorescence resonance energy transfer (FRET) between the two membranes when they are closely apposed (< 5 nm) leaves a footprint, which maps the contact zone. Larger topographical features can be observed when the membrane system is supported on an oxidized silicon wafer. Near-field interference effects set up optical standing waves that provide contour mapping of the membrane topography with resolution in the nanometer range extending over a micron from the surface. Topographical patterns are a critical feature of cell-cell contacts that are not easily measured by current real-time imaging techniques. This new membrane system and combined imaging strategies will form an important component of our experimental platform for further reconstitution and analysis of inter-membrane synapse formation.

PHYSICAL OBSERVATION / COMPUTATIONAL STRUCTURAL INTERFACES OF INFO-BIO-NANO TECHNOLOGY

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In this paper, we will be concerned with interfaces that have high density gradients over large transition distances. First, we will consider real material interfaces, for situations that involve biological systems and for situations that involve functional (engineering) material systems. Second, we will be concerned with virtual interfaces between the bio-, nano-, and information technologies, especially the manner in which real information is used to conceptualize multiphysics phenomena at multi scales of geometry to describe and predict system behavior.

We will begin with physical interfaces in the field of biotechnology. Two examples will be considered. The first is the composite interfaces formed in the complex systems used for tissue scaffolding, and the relationship of the constituents to the global function of the tissue. The second is the interface between prosthetic implants and human bone, with specific reference to hip implants. Specific attention will be paid to the situation wherein the bone is induced to “grow into” the surface of the prosthetic. An attempt will be made to define the interface details at the nano-scale which influence / control global behavior, and to define the multi-physics phenomena associated with those details.

We will then extend the multi-physics concept to composite interfaces in fuel cells, in which the system function is defined by the nano-details of the local geometry, the local physics of the electro-chemistry, the local mechanics of heat and energy management, and the chemistry of the fuels and oxidants. We will show similarities with the bio-system that result from consideration of nano-details, and illustrate the analogy with a set of multi-scale (in time and geometry) solutions to the equation set that controls the performance of the fuel cells.

Finally, we will address the question of information in these problems, especially the question of how to identify physical measureables (observables) at the nano-level that can be used as inputs to the equation sets that describe nano-phenomena and behavior. A discrete element simulation approach is used to investigate the deformation characteristics of an interface between two porous materials. A boundary value problem is formulated on a finite size element across the interface and the effective interface properties are calculated through a novel averaging process. A particular aspect of special interest will be the discussion of micro- or nano-analysis simulation methods that can be used for porous nano-structures that do not have repeating geometric units, and therefore cannot be correctly approached with the usual homogenization methods. Examples of this approach will be illustrated for a distributed, random porous material nano-structure and compared to available estimates from the literature.

HIGH RESOLUTION 3D VISUALIZATION OF ATHEROSCLEROSIS

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Atherosclerosis is the leading cause of morbidity and mortality in the United States and other industrialized countries. Several methods are currently used to detect and quantitate atherosclerosis, such as angiography, ultrasonography, computed tomography and magnetic resonance imaging. The resolutions of these clinical imaging methods are in the orders of millimeters or sub-millimeters. High resolution imaging of atherosclerosis is necessary for studying the morphological changes of diseased artery, especially for small sized plaques, which may be formed in the early stage of atherosclerosis. In this paper, we present morphologies of atherosclerosis by using synchrotron radiation computed microtomography with a spatial resolution of several microns. We studied 6 atherosclerosis samples from three patients aged from 51 to 70 in their native forms, and their corresponding bypass arteries. Atherosclerotic lesions such as the plaques were identified in both native and bypass samples. Cross section and 3D visualization of the atherosclerosis in the x-, y- and z- direction will be displayed. 3D volumetric images of deposited plaques will be rendered. The morphological differences among the samples with one another were recognized and the extent of the atherosclerotic plaque will be defined.

DYNAMICAL PROCESSES IN GREEN FLUORESCENT PROTEIN

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Green fluorescent protein (GFP) extracted from the bioluminescent jellyfish *Aequorea Victoria*[1] and its mutants form a nanoscale cylindrical (3 x 5 nm) structure in which the chromophore is embedded in the center of the cylinder. These proteins have been shown to exhibit desirable linear and nonlinear optical properties[2]. In this paper we use time resolved linear and nonlinear spectroscopies to investigate dynamical processes in fluorescent proteins in both aqueous solution and an organic polymer matrix. Experimental results were analyzed in terms of a Brownian oscillator model[3] and by comparison to computer simulations.

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FRictional PROPERTIES OF SELF-ASSEMBLED MONOLAYERS

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Results from molecular dynamics simulations of alkylsilane monolayers on silica and alkylthiol monolayers on gold will be presented. The dependence of the normal forces between surfaces containing self-assembled monolayers will be studied for various chain lengths ranging from 6 to 18 hydrocarbons and for different end-groups. The results will be compared to experiments from atomic and interfacial force microscopy. The frictional forces between the surfaces are studied at normal loads of 0.2 and 2 GPa for velocities ranging from 0.02 to 20.0 m/s. We find that for well-ordered monolayers there is stick/slip motion at all loads and velocities, and that the dependence on velocity and chain length is weak. As all experimental systems contain defects, we have also performed shear simulations in which defects have been added to the monolayers. The defects include the removal of randomly selected chains from the crystalline surface, as well as the inherent disorder in chains bonded to an amorphous silica surface. We find that in all cases the introduction of defects destroys the stick/slip motion. We have also investigated possible finite size effects in our simulations by varying the surface area by a factor of sixteen and find that larger system sizes result only in decreased noise.

CRACKS AND CRAZES: FROM MOLECULAR SIMULATIONS TO THE MACROSCOPIC TOUGHNESS OF POLYMERS

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Understanding the molecular origins of macroscopic mechanical properties such as the fracture toughness G_c is a fundamental scientific challenge. In tough materials, the work G_c required to propagate a crack through a unit area is 3 to 4 orders of magnitude higher than the equilibrium interfacial free energy G_{eq} of the crack surfaces. Efforts to calculate this large toughness enhancement have been frustrated, because phenomena on many length scales must be treated simultaneously. In the case of glassy polymers considered here, the toughness is mainly due [1] to the formation of an intriguing craze structure around the crack tip. Polymer chains (nm in diameter) are bundled into a dense network of fine fibrils (5-30 nm in diameter) that are separated by voids. Crazes can grow up to 50 μ m in width before they break.

In this paper, we bridge length scales by combining an MD calculation of model polymers [2] with a continuum fracture model [3] for the onset of crack propagation to predict the macroscopic toughness of glassy polymers. Key input parameters for the fracture mechanics model are obtained from simulations of the mechanical properties of the polymer in the different regions illustrated in Fig. 1. Craze widening proceeds by drawing fibrils separated by a characteristic spacing D_0 out of the dense polymer glass. (Drawing occurs within a narrow “active zone” at constant drawing stress S . The volume of the material is increased by a constant extension ratio λ , which is determined by the entanglement length [1]. The toughness can be obtained from the work performed on the polymer during crazing, which is S times the increase in width of the crazed region from an initial value of d/λ to a final width d .

The final width d of the craze is limited by the stress concentration near the crack tip. This diverges as $d^{1/2}$ [3] and when the stress reaches a maximum value S_{max} the fibrils fail and the crack tip propagates through the craze. The magnitude of the stress concentration was determined from the elastic properties of the craze (Fig. 1B), and S_{max} was obtained from the stress where fibrils fail through pullout or chain scission. Our results for the final craze width and the toughness enhancement are in good agreement with experimental values. A key parameter is the ratio of the length of the chains to the entanglement length. When this ratio is less than about 2, crazes do not form and the toughness is small. As the ratio rises above 2, G_c/G_{eq} rises rapidly. G_c/G_{eq} saturates at 2000 to 5000 for long chains because they break rather than pulling out when the craze fails.

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UNITED-ATOM MODELS OF POLYMERIC MATERIALS: A UNITED ATOM MODEL OF POLYETHYLENE WITH THE MODIFIED EMBEDDED ATOM METHOD

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Nanotechnology developments are driving a need for a greatly improved understanding of polymeric material behavior. The behavioral range of interest encompasses polymer-inorganic interfaces, as well as bulk material behavior. Among the major issues in bulk materials is the influence of environmental factors such as solvent quality, pH and dielectric properties. Such influence virtually electron density of the polymer and any solvent be part of a model of these materials. Current polymer model typically neglect any explicit modeling of the valence electron density. The modified embedded atom method (MEAM) does explicitly model valence electron density. This presents the possibility of a unique modeling approach to polymer-polymer and polymer-solvent interactions. We present a united-atom model of polyethylene as a simple illustration of this modeling approach. Two valence-electron density parameters naturally lend themselves to regulating the interaction of a polymer chain with other chains and solvent molecules. Through these parameters, the polymer tack and folding behavior as a function of environmental variables. The regulation of polymer tack and folding without solvents will be illustrated here.

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YIELDING PMMA - A SIMULATION STUDY

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Thermotropic materials have important applications in industry and are both used pure or in a composite. Mechanical response to deformation of those materials is of great interest, e.g. to be able to make predictions about fatigue due to constant deformation. Previous computer simulations by J. Rottler et al. have shown that model systems composed of beads connected by springs exhibit similar behavior to that observed in experiments.

PMMA is a real world material with a simple chemical structure which is well suited to be investigated in respect to its response to deformation, the more so as it has been well studied in experiments. Two different force fields have been applied in this study, the Polymer Consistent Force Field by MSI treats all atoms, while Okada's et al. forcefield neglects hydrogens and uses united atoms instead. First the glass transition of temperatures of PMMA of both force fields have been compared to each other in order to validate their use. Later the viscoelastic behavior, yield points and stresses produced in simulation have been put into relation with experimental data.

AN OVERVIEW OF MAGNETIC NANO-PINNING AT TEXAS A&M UNIVERSITY

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We are exploring the use of high temperature superconductors as nano-pinning devices for magnetic flux. This talk presents an overview of the various materials science/magnetic flux/positioning/simulation research being performed at Texas A&M University to explore and characterize various magnetic flux arrangements. Since pinning in HTSC's takes place on the nanoscale, pinned vortices offer a variety of opportunities for electronic nanoscale technologies such as information storage. A review will also be given of progress and the challenges that lay ahead.

MONTE CARLO SIMULATION ON THE RKKY INTERACTIONS OF Co-DOPED ZnO FILM

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Monte Carlo simulations using a three-dimensional lattice model studied the RKKY indirect exchange interaction of doped magnetic Co ions in ZnO films. The results of the calculations show that the RKKY interaction in Co-Doped ZnO is long-ranged and its magnitude is proportional to R^{-1} . The sign oscillates with a frequency that depends on the carrier's concentration. The long-distance sum of the RKKY indirect exchange energies is positive indicating that these materials are ferromagnetic, in direct correlation with previously reported results.

QUANTUM ENERGY TRANSPORT IN NANOSCALE SYSTEMS

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We give an overview of our recent theoretical investigations of thermal transport in mesoscopic and nanoscale systems. Recently, a quantization of the thermal conductance in freely suspended one-dimensional dielectric wires was observed [1], analogous to the well-known electrical conductance quantization in one-dimensional mesoscopic conductors. In the present work we consider mesoscopic thermal transport through a wire or weak link in the limit where the phonon transmission probability through the wire is small and the thermal conductance is much less than the quantized value [2]. We find that the thermal current is determined by a product of the local vibrational spectral densities of the two bodies, and derive a general expression for the energy flux that is a thermal analog of the well-known formula for the electrical current through a tunneling barrier.

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PHONONS IN A NANOPARTICLE MECHANICALLY COUPLED TO THE ENVIRONMENT

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The discrete nature of the vibrational modes of an isolated nanometer-scale solid dramatically modifies its low-energy electron and phonon dynamics from that of a bulk crystal. However, nanocrystals are usually coupled, even if only weakly so, to an environment consisting of other nanocrystals, a support matrix, or a solid substrate, and this environmental interaction can dominate the vibrational properties at low frequencies. We will discuss our recent investigation the modification of the vibrational modes of an isolated spherical nanoparticle caused by a weak mechanical coupling to a semi-infinite solid substrate. As a probe of the modified nanoparticle phonon spectrum, we consider an electron in a localized impurity state in the nanoparticle, and calculate the rate of low-energy nonradiative energy relaxation provided by the substrate interaction.

CARBON NANOTUBES IN NANOELECTRONICS AND SENSOR DEVELOPMENT

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Carbon nanotubes (CNT) exhibit extraordinary mechanical properties and unique electronic properties and thus are being investigated widely for applications in nanoelectronics, sensors, composites, nanoelectromechanical systems to name a few. We have focused on controlled growth of CNTs using CVD for applications in device and sensor fabrication. Both p- and n- type CMOS transistors using CNTs have been fabricated and used to develop an inverter -a building block towards future nanotube based logic circuits. We have also been developing a biosensor based on CNTs for cancer diagnostics. The tasks on this development call for growth of vertically aligned nanotube arrays, functionalization of this array with DNA or PNA probe molecules, and electrochemical signal generation due to hybridization events. All these have been successfully accomplished and this talk will provide an overview of the research above. In addition, computational nanotechnology issues at every stage would be identified which can complement the experimental work by providing insight into mechanisms.

Contributions from Alan Cassell, Bin Chen, Lance Delzeit, Jie Han, Jun Li, Cattien Nguyen, Deepak Srivastava, and Ramsey Stevens are acknowledged.

BUILDING ORGANIZED ARCHITECTURES WITH CARBON NANOTUBES

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This talk will focus on the directed assembly of multiwalled carbon nanotubes on planar substrates into highly organized structures that include vertically and horizontally oriented arrays, ordered fibers and porous membranes. The concept of growing such architectures is based on growth selectivity on certain surfaces compared to others. Selective placement of ordered nanotube arrays is achieved on patterned templates prepared by lithography or oxide templates with well-defined pores. Growth of nanotubes is achieved by chemical vapor deposition (CVD) using hydrocarbon precursors and vapor phase catalyst delivery. The new technique developed in our laboratory allows enormous flexibility in building a large number of complex structures based on nanotube building units. The understanding of the early stages of nanotube film growth during this CVD process will be discussed. It is observed that there are select pathways during the growth process of nanotube films on substrates, influencing the final morphology of the films developed, and these pathways can be tailored by tuning the catalyst concentration in the vapor phase. We will also discuss some of our recent efforts in creating nanotube junctions selectively and controllably.

EFFECTS OF STRUCTURAL DEFORMATION AND CHIRALITY ON ELECTRON TRANSPORT IN CARBON NANOTUBES

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Recent experiments (Ref. 1) showed that the conductance of a nanotube suspended between two leads decreased by two orders of magnitude upon deformation with an AFM tip. In this work we provide a theoretical explanation for the conductance drop observed. Atomistic simulations using a combination of classical forcefield and Density-Functional-Theory (DFT) show that carbon atoms remain essentially sp² coordinated in either bent tubes or tubes pushed by an atomically sharp AFM tip. Subsequent non-orthogonal tight-binding Green's function calculations reveal that for arm- chair tubes there is no significant drop in conductance, while for zigzag tubes the conductance can drop by several orders of magnitude in AFM-pushed tubes. We conclude that the effect can be attributed to simple stretching of the tube concurrent with the tip deformation, which opens up an energy gap at the Fermi surface throughout the tube.

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**AB-INITIO MOLECULAR DYNAMICS STUDIES OF
NANOSTRUCTURES AND BIOMOLECULES**

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InAs/GaAs SQUARE NANOMESAS: MULTIMILLION-ATOM MOLECULAR DYNAMICS SIMULATIONS ON PARALLEL COMPUTERS

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Surface energies of GaAs and InAs for the (100), (110), and (111) orientations have been calculated. Both molecular dynamics (MD) method and conjugate gradient method are used and the results are in excellent agreement. Surface reconstructions on GaAs(100) and InAs(100) are studied via the conjugate gradient method. We have developed a new model for GaAs(100) and InAs(100) surface atoms. Not only does this model reproduce well surface energies for the (100) orientation, it also yields (12) dimer lengths in accordance with ab initio calculations. We have performed large-scale molecular dynamics simulations to investigate the mechanical stresses in InAs/GaAs nanomesas with {101}-type sidewalls. The in-plane lattice constant of InAs layers parallel to the InAs/GaAs(001) interface are found to exceed the InAs bulk value at the 12th monolayer (ML) and the hydrostatic stresses in InAs layers become tensile above ~ 12 ML. Hence, it is not energetically favorable to have InAs overlayers thicker than 12 ML. This may explain the experimental findings of the growth of flat InAs overlayers with self-limiting thickness of ~ 11 ML on GaAs nanomesas. We have also investigated the lateral size effects on the stress distribution and morphology of InAs/GaAs square nanomesas using MD simulations. Two nanomesas with the same vertical size but different lateral sizes are simulated. For the smaller mesa, a single stress domain is observed in the InAs overlayer, whereas two stress domains are found in the larger mesa. This indicates the existence of a critical lateral size for stress domain formation in accordance with recent experimental findings. It is found that the InAs overlayer in the larger mesa is laterally constrained to the GaAs bulk lattice constant but vertically relaxed to the InAs bulk lattice constant.

EXPLOITING NANOFILM COATINGS IN MICROFLUIDIC DEVICES FOR BIOSENSING

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This talk will explore new combinatorial methods inside microfluidic devices for biosensor applications. Fluid heterogeneous coatings on the nanometer scale provide the key to multivalent ligand receptor attachment a cell surface mimics. Several innovative new architectures will be described.

TECHNIQUES FOR GUIDING THE ASSEMBLY OF FCC, BCC, HCP, TETRAGONAL AND TRICLINIC PHOTONIC CRYSTALS

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This paper describes a technique to guide the assembly of colloidal spheres into crystalline structures. We have several geometric molds to guide colloidal spheres into face centered cubic (FCC), tetragonal, body centered cubic (BCC), hexagonal close packed, and triclinic crystalline structures. Our work has focused on FCC, triclinic and tetragonal crystals. Here we lay down the basic geometry to yield all of the above structures and show how FCC, tetragonal and triclinic originate from a similar template. We also introduce an inexpensive method that we have been developing over the last year and a half for creating these crystalline structures up to 1 cm long with colloidal spheres 5 μ m or larger. It has recently been demonstrated possible to form the FCC structure with colloidal spheres smaller than 5 μ m, however, our focus and the thrust of our research is to develop an inexpensive technique to create these structures with 200nm or larger spheres.

A MECHANISTIC EVALUATION OF MECHANISMS OF “NEAR-NANOSCALE” HIGH-CYCLE FATIGUE FAILURES IN POLYSILICON THIN FILMS FOR MEMS

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The fracture and fatigue resistance of micron-scale silicon-based, structural films are important mechanical properties for the design, reliability and long-term durability of micromechanical devices, especially MEMS. Contrary to conventional wisdom on the mechanisms of fatigue, recent work has established that such brittle thin films of single- and poly-crystalline silicon are susceptible to premature failure under cyclic loading conditions, with failure occurring at long lives ($>10^9$ cycles) at approximately one half of the single-cycle fracture strength. However, the mechanism(s) of such failures have remained a mystery. In this presentation, a mechanism is presented for the fatigue of thin-film LPCVD polysilicon based on extensive stress-life fatigue testing and high-voltage transmission electron microscopy. It is proposed that the fatigue process is "surface dominated" and involves the mechanically-induced thickening of the native oxide film, followed by environmentally-assisted subcritical cracking of the thickened film. It is further shown that this mechanism is only specific to thin films and can not cause failure in bulk silicon.

CACHE-CONSCIOUS ALGORITHM DESIGN

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The topic of cache performance has been well studied in recent years. It has been clearly shown that the amount of processor-memory traffic is the bottleneck for achieving high performance in many applications. While the topic of cache performance has been well studied, much of the focus has been on dense linear algebra problems. These problems possess very regular access patterns that are known at compile time. In this paper, we take a unique approach to this topic by focusing on other fundamental problems, which have poor cache utilization.

Optimizing cache performance to achieve better overall performance is a difficult problem. Modern microprocessors are including deeper and deeper memory hierarchies to hide the cost of cache misses. The performance of these deep memory hierarchies has been shown to differ significantly from predictions based on a single level of cache. Different miss penalties for each level of the memory hierarchy as well as the TLB also play an important role in the effectiveness of cache-friendly optimizations. These miss penalties vary from processor to processor and can cause large variations in experimental results. In this work, we identify the key issues and demonstrate algorithmic techniques by considering two key problem areas:

- Effective utilization of cache memories is a key factor in achieving high performance in computing signal transforms). Most optimization techniques for computing the Discrete Fourier Transform (DFT) rely on either modifying the computation and data access order or exploiting low level platform specific details, while keeping the data layout in memory static. We propose a high level optimization technique, dynamic data layout (DDL). In DDL, data reorganization is performed between computations to effectively utilize the cache. This cache-conscious factorization of the DFT including the data reorganization steps is automatically computed by using efficient techniques in our approach. An analytical model of the cache miss pattern is utilized to predict the performance and explore the search space of factorizations. Our technique results in up to a factor of 4 improvement over standard FFT implementations and up to 33% improvement over other optimization techniques such as copying on SUN UltraSPARC-II, DEC Alpha and Intel Pentium III. Compared with the best known FFT library (FFTW, MIT) our implementations run up to 2x faster on DEC Alpha and up to 3x faster on UltraSPARC. For the Walsh Hadamard

Transform, compared with the state-of-the-art, our implementations achieve up to 4x performance improvement on DEC Alpha and UltraSPARC.

- Graph problems are fundamental in a wide variety of fields, most notably network routing, distributed computing, and computer aided circuit design. Graph problems, as irregular problems, pose unique challenges to improving cache performance, challenges that often cannot be handled using standard cache-friendly optimizations. We develop the *Unidirectional Space Time Representation (USTR)* and show that using this representation we can develop cache-friendly implementations for a large class of algorithms. This representation is very similar to the space-time representation used in systolic array design, which also deals with partitioning the space as we do. However, such systolic array designs do not have the added challenge of dealing with cache conflicts and multiple levels of memory hierarchy. We also show how this representation can be used to uniquely face the challenges posed by the transitive closure problem. Using this representation we show up to a factor of 2 improvement over a state-of-the-art cache-friendly optimization, including those available in a research compiler. We use the SimpleScalar simulator to demonstrate improved cache performance. We also present a number of optimizations to the Floyd-Warshall algorithm, Dijkstra's algorithm, and Prim's algorithm. For the Floyd-Warshall algorithm we present a recursive implementation that achieves a 6x improvement over the baseline implementation. We also show that by tuning the base case for the recursion, we can further improve performance by approximately 20%. We also show a novel approach to tiling for the Floyd-Warshall algorithm that achieves performance very close to that of the recursive implementation. State-of-the-art research compilers cannot generate these implementations.

The work reported here summarizes ongoing efforts at USC. These efforts are developing algorithmic techniques to improve the performance of signal processing algorithms (Signal Processing algorithms Implementation Research for Adaptable Libraries (SPIRAL) project, www.ece.cmu.edu/~spiral) and algorithmic techniques to improve the performance of data intensive applications on advanced architectures (Algorithms for Data Intensive Applications on Intelligent and Smart Memories, <http://advisor.usc.edu>).

SELF-CONSISTENT MODELING OF WEAKLY IONIZED PLASMAS - CHALLENGES IN QUANTUM AND CLASSICAL MECHANICS

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Weakly ionized plasmas are used in several critical steps in IC processing. They fall into the regime of glow discharges (both normal and abnormal), which are characterized by relatively lower pressures (< 1 Torr), large spatial gradients in electromagnetic fields, and chemically active electronegative gases. These plasmas themselves are sustained by electron induced ionization and chemistry at non-equilibrium conditions. For self-consistent modeling of these plasmas in realistic processes, three components need to be addressed - (1) Quantum mechanics-based calculations of electron impact probabilities, (2) Self-consistent building of reaction data in gas phase and on surfaces, and (3) coupled transport, reactions, and electromagnetics. There has been substantial progress in all the three areas in the last two decades. The paper will examine the status and challenges in each of the areas:- multi-length and time scales in weakly collisional plasmas, difficulties in building a self-consistent chemical dataset for processing gases, the need for efficient algorithms to exploit the recent availability of multi-processor systems, and some application of these techniques to real systems. The intention is to show the numerical and scientific challenges in combining the different techniques and data for using plasma modeling as a predictive tool. The paper will span continuum mechanics, kinetic theory, and quantum techniques and the numerical techniques used in each of the areas.

COUPLED GROOVING AND MIGRATION OF INCLINED GRAIN BOUNDARIES

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Grain-boundary migration controls the growth and shrinkage of crystalline grains and is important in materials synthesis and processing. A grain boundary ending at a free surface forms a groove at the tip, which affects its migration. This coupled grooving and migration is studied for a straight, inclined grain boundary intercepting a horizontal free surface. Surface diffusion is taken to be the mass transport mechanism for grooving. Previous work on a groove migrating at constant speed suggests that the grain boundary is pinned if the inclination angle is small. We find that the grain boundary is never pinned. The coupled motion can be separated into two time regimes. In Regime I, both the grain-boundary and groove profiles grow with time following similarity laws. The groove profile is symmetric about the groove root. The symmetry forces the grain boundary to turn vertically at the tip, and this bending drives the migration. The self-similar profiles are shown to be linearly stable, and they grow continuously into Regime II. In Regime II, the turning relaxes following two different paths depending on s/b , where b is the initial inclination angle of the grain boundary and s is the supplementary dihedral angle ($p - s$ is the dihedral angle). For $b > s/6$, the groove root coordinates $(x_0, y_0) \sim (t^{1/2}, t^{1/6})$ as time $t \rightarrow \infty$, whereas for $b < s/6$, $(x_0, y_0) \sim (t^{1/4}, t^{1/4})$ as $t \rightarrow \infty$. These results come from asymptotic expansions and agree with a finite-difference solution of the coupled equations. They show that the grain boundary is never pinned. The asymptotic solutions also apply to the Sun-Bauer method of measuring grain-boundary mobility, and predict grain-boundary profiles that agree better with experiments.

NUMERICAL TECHNIQUES FOR TIME-DEPENDENT DENSITY FUNCTIONAL THEORY

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Recently developed linear response methods based on time-dependent density functional theory formalisms provide a new tool for calculating excited states properties. These methods examine the response of a system when it undergoes a certain initial periodic perturbation. Two distinct and broad methods are in use in this context. In standard Time-Dependent LDA (TDLDA) (see, e.g., [1]) the Ordinary Differential Equation (ODE) obtained from the time-dependent Kohn-Sham equation is integrated over time. The major part of the cost associated with this technique comes from the need to integrate over (relatively) large time intervals and the requirement to integrate one ODE for each occupied state. A second approach developed in [1] works in Fourier space. It builds a large coupling matrix K and computes its eigenvalues from which transition energies can be obtained. The coupling matrix K is typically dense and can be quite large. The biggest cost associated with this approach lies in the computation of the matrix K which requires solving a Poisson equation for each matrix entry.

FIRST PRINCIPLES STUDY OF ORGANOSULFUR MONOLAYERS ON GOLD

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Self-assembled monolayers (SAMs) of organosulfur molecules on gold and other metal surfaces are intensely studied because of their many potential applications in various areas of nanotechnology, including nanofabrication, chemical sensing, and molecular electronics. In spite of their wide interest, the adsorption structure of most SAMs is not well understood yet. Here I will discuss this issue on the basis of Density Functional slab calculations for a few different organosulfur molecules on the Au(111) and Cu(111) surfaces at various coverages. Results for methanethiol and dimethyl disulfide, trifluoromethanethiol, benzenethiol, and L-cysteine will be presented. The question whether these molecules adsorb as monomers (thiolates) or dimers (disulfides) will be addressed.

PARALLELIZATION AND VISUALIZATION OF COMPUTATIONAL NANOTECHNOLOGY LCAO METHOD

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Accurate atomic-scale quantum theory of nanostructures and nanosystems fabricated from nanostructures enables precision metrology of these nanosystems and provides the predictive, precision modeling tools needed for engineering these systems for applications including advanced semiconductor lasers and detectors, single photon sources and detectors, biosensors, and nanoarchitectures for quantum coherent technologies such as quantum computing. The tight-binding model based upon the Linear Combination of Atomic Orbitals (LCAO) method provides an atomistic theory for nanostructures which is accurate and easy to implement(1). The tight-binding method is ideal for modeling small nanostructures. However, the method becomes impractical to use on sequential computers, due to long run times, for modeling nanostructures with more than 25,000 atoms. Dramatic improvements in run time can be achieved through parallelization. We parallelize this method by dividing the structure into layers. Communication is across layers. First we create the structure. Then we solve the Hamiltonian equation for each atom considering only nearest neighbors using PARPACK(2). This parallel implementation is nearly linear in time. The output of the code is transferred to the NIST immersive environment where we study the structure interactively. This provides us with a detailed inspection and visualization of the structures and the atomic scale variation of calculated nanostructure properties that is not possible with any static graphical representation. We save the interaction with the structure in the immersive environment as a quicktime movie. The parallel implementation can handle arbitrary nanostructure shapes through an input file specification procedure. Structures of up to one million atoms are currently being studied.

[1] G. W. Bryant and W. Jaskolski, *Physica E* 11, 72 (2001).

[2] K. Maschhoff, D. Sorensen, "A portable implementation of ARPACK for distributed memory parallel architectures", Preliminary proceedings, Copper Mountain Conference on Iterative Methods, 1996.

NANOLOGIC: A LOGICAL BRIDGE TO NANOCOMPUTING

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Almost all attempts to introduce nanoscale devices into electronic computers have focused on making the devices operate as logical switches. As the fabrication dimensions drop below 100 nm this is an increasingly difficult and ultimately impossible challenge. We have taken a different approach. Instead of forcing the processor to conform to defined data structures, we propose forcing the data to conform the defined processor structures. The appropriate data structures are neither pure digital nor pure analog, but intrinsically hybrid. By defining the data properly, we can exploit the extraordinarily rich (and growing) inventory of nanoscale devices that have nonlinear, intrinsically hybrid, transfer characteristics. Arrays of such hybrid devices, in which the output from one device is used as the input to the next, will constitute a hybrid computer. Such computers can be built in any applications- specific architecture to further exploit the hybridicity of the data. Computers operating on this nanologic principle will have far greater density, and therefore greater logic throughput than any pure analog or pure digital computer. They will find best applications as simulators of physical systems. They could use direct analog and digital I/O making the choice for sensor arrays. Conservative estimates indicate a nanologic computer would have 2-4 orders of magnitude higher logic throughput than the conventional computers. Applications include military (smart weapons, nuclear design, burst decision-making, etc), industrial (weather prediction, structural and fluid engineering, drug design, etc), commercial (implantable personal IT aids, sensors for the disabled, smart robots, entertainment, artistic creation tools, etc.), and scientific (molecular dynamics, social behavior, morphogenesis, chaotic systems, etc.). We believe that hybrid logic computers, of the nature described here, are inevitable, and that they will be widespread within ten years.

In this presentation, we will describe the technical basis of nanologic computing, current technology for implementing it, the design process for nanologic circuits, and potential applications of the technology.