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This project deals with properties and processes in high-temperature materials (HTMs) that are vital to the DoD technology base. In this project, molecular-dynamics (MD) simulations have been performed to investigate: i) sintering of nanostructured SiC and high-pressure structural transformation in SiC; ii) dynamic fracture in nanostructured systems; iii) structure of amorphous Al2O3; and iv) reactive wetting of Al2O3 surface by Al. Our joint MD/neutron-scattering study of nanostructured SiC exhibits the onset of sintering at temperature 1,500 K, which is much lower than the bulk sintering temperature. We have proposed a new transition path for the zinc-blende-to-rocksalt transformation of SiC at high pressures. This new mechanism involves no bond breakage and is characterized by a much lower activation barrier compared with previously proposed mechanisms. MD simulations of nanostructured amorphous silica (n-SiO2) reveal that the crack propagates through interfacial regions between silican nanoparticles. A reliable interatomic potential model has been developed for MD simulations of Al2O3. Simulation results for amorphous Al2O3 show predominantly tetrahedral coordination of Al atoms, which agrees with recent experimental results. Our MD simulations on reactive wetting reveal that oxygen atoms from the substrate difuse into the droplet to form a continuous layer of reaction product at the interface.

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HIGH TEMPERATURE MATERIALS SIMULATIONS ON PARALLEL COMPUTERS

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TABLE OF CONTENTS

COVER PAGE		i
TABLE OF CONTENTS		ii
§1	ABSTRACT	1
§2	RESEARCH ACCOMPLISHMENTS	1
§2.1	SINTERING AND HIGH-PRESSURE STRUCTURAL TRANSFORMATION IN SiC	1
§2.2	DYNAMIC FRACTURE IN NANOSTRUCTURED SYSTEMS	3
§2.3	STRUCTURE AND DYNAMICS IN Al_2O_3	4
§2.4	REACTIVE WETTING OF Al_2O_3 BY Al	6
§3	TRAINING OF GRADUATE STUDENTS: DUAL-DEGREE PROGRAM	7
§4	COMPUTATIONAL FACILITIES	7
§5	PERSONAL SUPPORTED	8
§6	PUBLICATIONS	8
§7	INTERACTIONS/TRANSITIONS	10
A.	PARTICIPATION/PRESENTATIONS AT MEETINGS, CONFERENCES, SEMINARS	10
B.	CONSULTATIVE AND ADVISORY FUNCTIONS TO GOVERNMENT LABORATORIES AND AGENCIES	13
C.	TRANSITIONS	13
§8	NEW DISCOVERIES, INVENTIONS OR PATENT DISCLOSURES	14
§9	HONORS AND AWARDS	14

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HIGH TEMPERATURE MATERIALS SIMULATIONS ON PARALLEL COMPUTERS

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§1 ABSTRACT

This project deals with properties and processes in high-temperature materials (HTMs) that are vital to the DoD technology base. In this project, molecular-dynamics (MD) simulations have been performed to investigate: i) sintering of nanostructured SiC and high-pressure structural transformation in SiC; ii) dynamic fracture in nanostructured systems; iii) structure of amorphous Al_2O_3; and iv) reactive wetting of Al_2O_3 surface by Al. Our joint MD/neutron-scattering study of nanostructured SiC exhibits the onset of sintering at temperature 1,500 K, which is much lower than the bulk sintering temperature. We have proposed a new transition path for the zinc-blende-to-rocksalt transformation of SiC at high pressures. This new mechanism involves no bond breakage and is characterized by a much lower activation barrier compared with previously proposed mechanisms. MD simulations of nanostructured amorphous silica (n-SiO_2) reveal that the crack propagates through interfacial regions between silica nanoparticles. A reliable interatomic potential model has been developed for MD simulations of Al_2O_3. Simulation results for amorphous Al_2O_3 show predominantly tetrahedral coordination of Al atoms, which agrees with recent experimental results. Our MD simulations on reactive wetting reveal that oxygen atoms from the substrate diffuse into the droplet to form a continuous layer of reaction product at the interface.

§2 RESEARH ACCOMPLISHMENTS

§2.1 Sintering and High-Pressure Structural Transformation in SiC

Advanced structural ceramics are highly desirable materials for applications in extreme operating conditions. Light weight, elevated melting temperatures, high strengths, and wear and corrosion resistance make them very attractive for high-temperature and high-stress applications. The only serious drawback of ceramics is that they are brittle at low to moderately high temperatures.

In recent years, a great deal of progress has been made in the synthesis of ceramics that are much more ductile than conventional coarse-grained materials. These so called

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nanostructured materials are fabricated by *in-situ* consolidation of nanometer size clusters. Despite a great deal of research, many perplexing questions concerning nanostructured ceramics remain unanswered. Experiments have yet to provide information regarding the morphology of pores or the structure and dynamics of atoms in nanostructured ceramics. As far as modeling is concerned, only a few atomistic simulations of nanostructured materials have been reported thus far.[3-7] This is due to the fact that these simulations are highly compute-intensive: A realistic MD simulation of a nanostructured solid requires 10^5-10^6 time steps and ~ 10^6 atoms (each nanocluster itself consists of 10^3-10^4 atoms).

We have performed large-scale MD simulations to investigate sintering, structure, and mechanical behavior of nanostructured SiC. Figure 1 shows the results of the first joint experimental and MD study of sintering of nanostructured SiC (n-SiC). In both experiment (solid diamonds) and simulation (open circles), the onset of sintering is around 1,500K. The MD simulations provide a microscopic picture of how the morphology of micropores in n-SiC changes with densification. The fractal dimension and the surface roughness exponent of micropores are found to be 2.4 and 0.45, respectively, over the entire pressure range between 0 and 15GPa. Small-angle neutron scattering at low wavevectors yields a fractal dimension of 2 for pores in n-SiC. MD calculations of pair-distribution functions and bond-angle distributions reveal that interfacial regions between nanoparticles are highly disordered with nearly the same number of 3-fold and 4-fold coordinated Si atoms. The effect of consolidation on mechanical properties is also investigated with the MD approach. The results show a power-law dependence of elastic moduli on the density with an exponent of 3.4 ± 0.1.

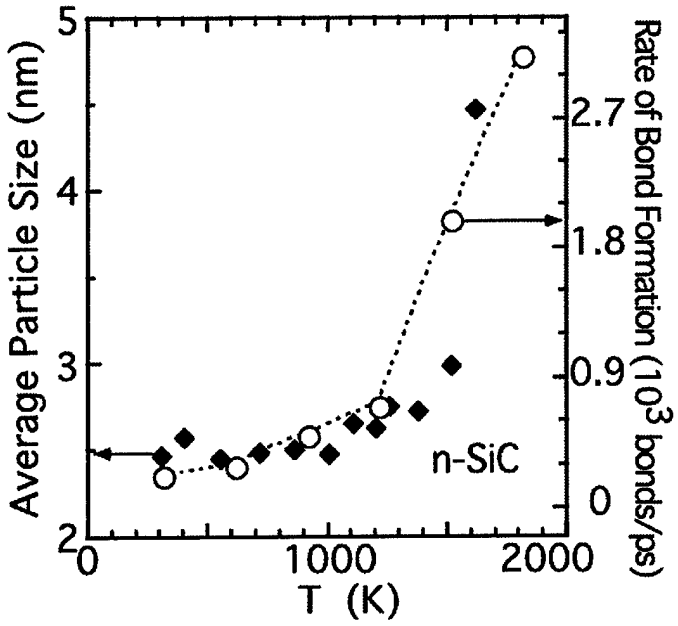

Fig. 1: The onset of sintering is indicated by an increase in the average particle size in the neutron data (◆) and an increase in the rate of bond formation between nanoparticles in the MD results (o). The dotted line is a guide to the eye for the MD results.

Despite numerous experimental and theoretical studies, structural transformations in SiC at high pressures are not well understood at the atomistic level. We have investigated the

mechanisms of these transformations using an isothermal-isobaric MD approach and the interatomic potential schemes mentioned above. In SiC, a reversible transformation between the four-fold coordinated zinc-blende structure and the six-fold coordinated rocksalt structure is found at a pressure of 100 GPa. The calculated volume change at the transition and the hysteresis are in good agreement with experimental data. The atomistic mechanism for the structural transformation is a cubic-to-monoclinic unit-cell transformation and a relative shift of Si and C sublattices in the [100] direction. The new transition path does not involve any bond breaking and it has a significantly lower activation energy compared with a previously proposed transformation mechanism (see Fig. 2).

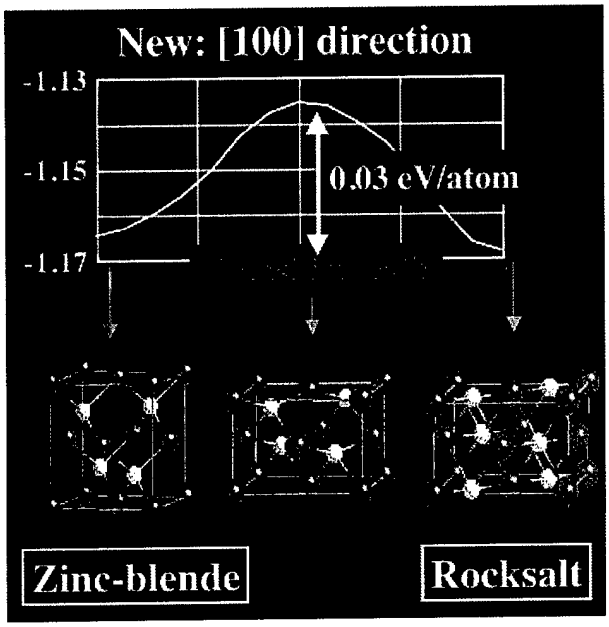

Fig. 2: The newly proposed transition path for the pressure-induced zinc-blende-to-rocksalt transformation in SiC (right) involves a relative shift of Si and C sublattices in the [100] direction. It has a small activation enthalpy (0.03 eV/atom).

§2.2 Dynamic Fracture in Nanostructured Systems

We have investigated crack propagation and fracture in bulk amorphous silica (a-SiO_2) and nanostructured amorphous silica (n-SiO_2) and silicon nitride (n-Si_3N_4) with MD simulations ranging between 1 million and 113 million atoms (see Fig. 3). These large-scale simulations have played a vital role in our understanding of mechanical failure. The simulations have provided valuable information at the crack tip and the surrounding region up to submicron length scales.

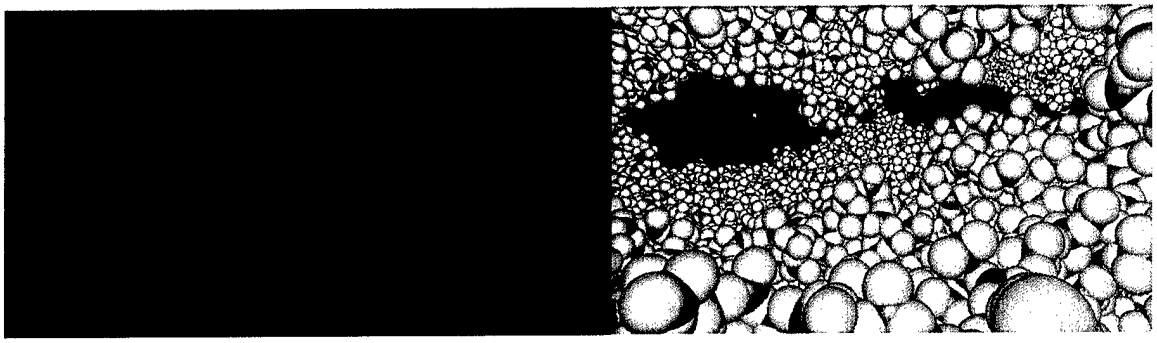

Fig. 3: A snapshot of 113 million-atom MD simulation of fracture in amorphous SiO_2 (left) and a close-up of the crack front showing cavity opening, where red and green spheres are silicon and oxygen atoms, respectively (right).

The interatomic interaction potentials for ionic-covalent materials such as silica and silicon nitride comprise two-body and three-body terms. The two-body terms include steric repulsion, Coulomb interaction due to charge transfer, and charge-dipole interaction due to electronic polarizabilties of atoms. The three-body terms take into account bond-bending and bond-stretching interactions. Comparing MD simulation results for structural and mechanical properties and vibrational spectra with experimental measurements and DFT calculations validates these potentials.

Figure 4 (top) shows the MD results for crack propagation in a-SiO_2. We find nucleation and growth of nanometer scale cavities approximately 5 nm ahead of the crack tip and the cavities coalesce and merge with the advancing crack to cause failure. These MD results are in agreement with recent AFM studies, which also reveal nanocavitation and coalescence of cavities with the crack to be the mechanism of fracture in glasses; see Fig. 4 (bottom). Our estimate of the critical stress intensity factor, K_{1C}, in a-SiO_2 is 1 MPa.$m^{1/2}$ and the experimental values range between 0.8 MPa.$m^{1/2}$ and 1.2 MPa.$m^{1/2}$.

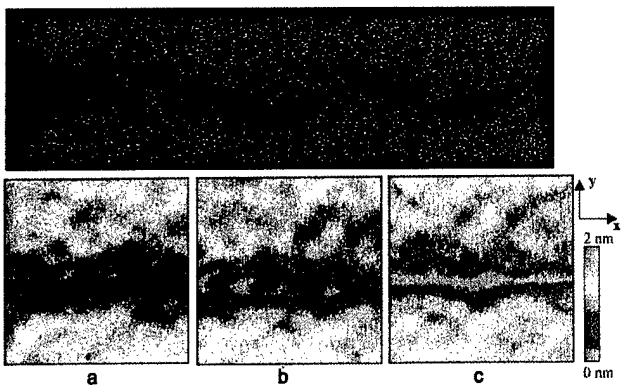

Fig. 4: (Top) MD configuration of fractured amorphous SiO_2. (Bottom) AFM images of fracture in a glass by E. Bouchaud's and collaborators.

MD simulations of nanostructured amorphous silica (n-SiO_2) reveal that the crack propagates through interfacial regions between silica nanoparticles. At small values of the applied strain, these regions have a few isolated nanocavities. As the applied strain is increased, we observe nanocavities grow and coalesce and new nanocavities form ahead of the crack in interfacial regions. The crack meanders through interfacial regions and coalesces with cavities in its path. This is the primary mechanism of fracture in n-SiO_2. MD simulations of dynamic fracture in nanostructured Si_3N_4 (n-Si_3N_4) also reveal nanoscale cavitation, crack meandering, and crack branching.

We have examined the morphology of fracture surfaces and have found scaling behavior akin to that observed experimentally. Fracture surfaces are self-affine objects with the height-height correlation function varying as:

$$\Delta h(r) = < (x(z+r) - x(z))^2 >_z^{1/2} \propto r^{\zeta},$$

where x is the height of the fracture profile normal to the plane of crack propagation and $<...>_z$ implies an average over z. The MD calculation in n-Si_3N_4 reveals two distinct power-law regimes, with exponents $\zeta = 0.58$ and 0.84 below and above a cross-over length, ξ_c, respectively. The smaller exponent (0.58) is due to intra-pore correlations while the larger one (0.84) results from inter-pore correlations and pore-crack coalescence. The cross-over length, ξ_c, is close to the size of the nanoparticle.

Fracture experiments on various metals, alloys, ceramics, and glasses reveal similar scaling behavior. The experimental value of the lower exponent is around 0.5 while the larger exponent is always close to 0.8, independent of the material or its microstructure. The cross-over length ξ_c is, however, a material characteristic which decreases with an increase in the crack velocity.

§2.3 Structure and Dynamics in Amorphous Al_2O_3

Alumina (Al_2O_3), the principle oxide of aluminum, is well established as a technologically useful material. Due to its important properties, such as, hardness (~25 GPa microindentation hardness), high electrical resistivity (>10^4 Ωm at 1,000 °C), and high melting point (2,054 °C), alumina is used as a basis for a wide variety of wear-resistant and electrically insulating components, furnace insulation and metal reinforcement, and even biomedical applications. The α-phase, the best defined crystalline form of aluminum oxide, is a corundum structure that consists of hexagonal close-packed layers of oxygen atoms with aluminum atoms occupying two-thirds of the octahedrally coordinated sites surrounded by six oxygens in a rhombohedral cell. The metastable γ-Al_2O_3 phase is described by a defect spinel structure in which Al coordination varies from three to five, with tetrahedral Al predominating. Due to such diverse bonding structures in crystals, understanding the structure of amorphous and liquid alumina is highly nontrivial. Consequently, extensive experimental works have been performed recently to investigate structures of amorphous and liquid alumina.

We performed MD simulations of liquid and amorphous alumina using a new interatomic potential. The potential consists of two-body and three-body terms, and it is validated by comparing the MD simulation results for crystalline α-Al_2O_3 with various experiments including the lattice constant, cohesive energy, elastic constants, and melting temperature. Figure 5 compares calculated and neutron-scattering experiment results for the phonon density of states of α-Al_2O_3. (The experiment was performed by Dr. C. Loong at Argonne National laboratory.) The spectra extend up to 110 meV, and the high-energy modes above 60 meV are mostly due to the vibration of oxygen atoms. The low-energy excitations below 60 meV in the MD result agree well with the experiment.

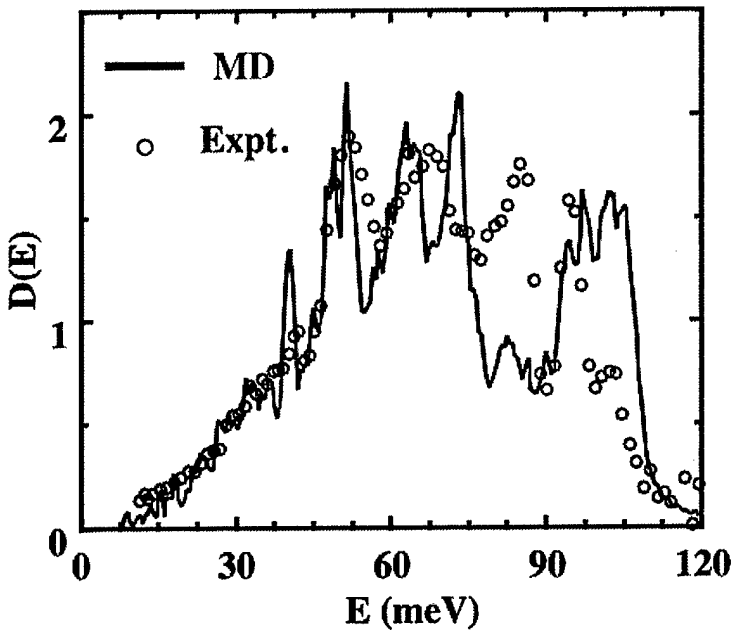

Fig. 5: Phonon density of states in α-Al_2O_3. The solid curve is the MD result, and the circles represent the result of the neutron-scattering experiment.

We have studied the structure of liquid Al_2O_3 at density 3.175 g/cm^3 and temperature 2,500 K. The calculated Al-O distance, 1.79 Å, is in reasonable agreement with an experimental value, 1.76 Å.[‡]

We have obtained an amorphous system by gradually lowering temperature of the liquid through successive cooling and thermalization. Figure 6 shows partial pair distribution functions of amorphous Al_2O_3 of the same density at temperature 300 K. The calculated average Al-O distance, 1.85 Å, agrees well with experimental values, 1.8-1.9 Å. The calculated coordination number of Al is 4.67, which is in good agreement with experimental values, 4.1-4.8. This suggests the predominance of tetrahedrally-coordinated Al atoms in amorphous alumina. The calculated coordination number of O is 3.12.

[‡]S. Krishnan and D. L. Price, "X-ray diffraction from levitated liquids," *J. Phys.: Condens. Matter* **12**, R145 (2000).

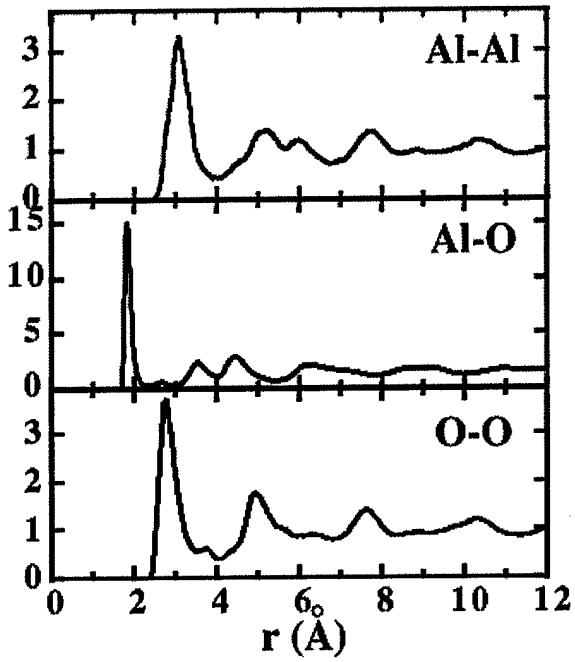

Fig. 6: Partial pair distribution function of amorphous Al_2O_3 of density 3.175 g/cm^3 at temperatures 300 K.

§2.4 Reactive Wetting of Al_2O_3 by Al

Recently, we have studied reactive wetting of Al_2O_3 (0001) surface by an Al nano-droplet using the variable-charge MD approach (see Fig. 7).

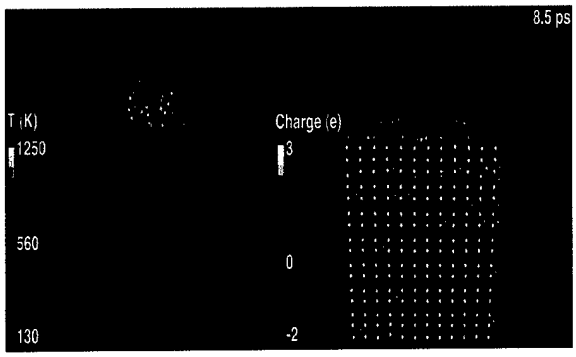

Fig. 7: Snapshots of temperature distribution (left) and atomic charges (right) taken after 8.5 ps in a simulation of reactive wetting of α-Al_2O_3 (0001) surface by an Al droplet. The larger and smaller spheres are oxygen and aluminum atoms, respectively.

Wetting of ceramic substrates by liquid metals is important for various applications such as coating, joining, and composite processing. In metal-ceramic systems, the wetting process is governed by interfacial energies, which depend strongly on chemical reactions at the metal/ceramic interfaces. During the wetting of an alumina (α-Al_2O_3) substrate by a liquid aluminum (Al) droplet, for example, the interfacial energy acts as a driving force for the diffusion of oxygen atoms from the α-Al_2O_3 substrate into the liquid Al, through which the interfacial energy is lowered. In fact, large amounts of oxygen atoms have been observed experimentally within Al droplets, where the droplets join α-Al_2O_3 substrates. This dissolution of oxygen atoms may be a major source of the adhesion between Al and α-Al_2O_3.

In our variable-charge MD simulations, we have found that oxygen atoms from the substrate diffuse into the droplet to form a continuous layer of reaction product at the interface. The number density of oxygen atoms at the 5 top layers of the substrate decreases substantially. As a result, the structural correlations near the reactive region differ considerably from those in

the bulk substrate. The diffusion length of oxygen atoms into the spherical Al droplet of radius 2.3 nm is ~ 0.73 nm. Heat generated in the reactive region is found to be sensitive to the droplet shape.

§3 TRAINING OF GRADUATE STUDENTS: DUAL-DEGREE PROGRAM

Our graduate students have pursued the dual-degree program, *i.e.*, Ph.D. in physics and an MS in computer science. This program provides students with broad-based training in high performance computing and communications (HPCC) and the physical sciences. In connection with this program, we have introduced two graduate courses in computational physics, which are cross-listed with computer-science courses and three HPCC courses in Computer Science. We are planning to introduce a course on data mining and a course on interactive and immersive visualization. Students have access to a number of in-house parallel machines to gain hands-on experience and they use massively parallel architectures at DoD's Major Shared Resource Centers to perform research on large-scale computational projects. Recently, the computational physics course was simultaneously taught at LSU and the Delft University of Technology in the Netherlands. LSU students were paired up with Delft students to jointly work on computational projects using various parallel computers and immersive and interactive 3D-visualization platforms. Similar global courses will be developed with Niigata University in Japan and the Federal University of São Carlos in Brazil. These courses will help us develop modules that will be disseminated through the Web.

Our students also have excellent opportunities to broaden their research experience beyond the traditional university based environment. They are involved in our collaborative efforts with computational and experimental scientists at government laboratories, industries, and other universities. These interactions have significantly enhanced the research capabilities of students.

§4 COMPUTATIONAL FACILITIES

Our group has access to excellent in-house computational facilities in the Concurrent Computing Laboratory for Materials Simulations (CCLMS). The CCLMS consists of two parallel computing laboratories, one in the Department of Physics and Astronomy and the other in the Department of Computer Science. With $2.5 million in infrastructure enhancement grants from the State of Louisiana, these labs have been equipped with the following parallel machines (see Fig. 8):

- **PC cluster**—166 PCs (550-800 MHz Pentium III) linked by a network fabric with gigabit and fast ethernet switches;
- **Digital Alpha cluster**—64 Alpha processors on two Gigaswitches and a Fast Ethernet switch;
- **Intel iWarp**—a 64-cell systolic architecture.

For the CCLMS the University provided 5000 sq. ft. of space, $200K for space renovation, and a systems manager.

Virtual Environment Laboratory

We have received $180K from the AFOSR via a DURIP grant and $90K + $218K in matching funds from the University to establish a virtual environment (VE) laboratory. The VE lab features an interactive and immersive visualization platform called *ImmersaDesk*, which is driven by a multiprocessor SGI Onyx2/InfiniteReality2 and an Octane/MXE graphics servers. Via high-speed networks, it is fully integrated with the existing parallel machines at the CCLMS and with massively parallel computers at national computer centers. In 2001, we received $3.9 million from the State of Louisiana to start a Biological Computation and Visualization Center that has made it possible to establish an immersive Virtual Environment (VE) and Access Grid (AG) Environment.

DoD Challenge Application Award

We have been allocated 2 million processor-hours of computing per year under a DoD Challenge Application Award entitled "Computational Assisted Development of High Temperature Structural Materials". We are performing large-scale materials simulations on IBM SP4 and Compaq AlphaServer computers at DoD's NAVO (Naval Oceanographic Office) and ERDCS (Engineer Research and Development Center) MSRCs (Major Shared Resource Centers).

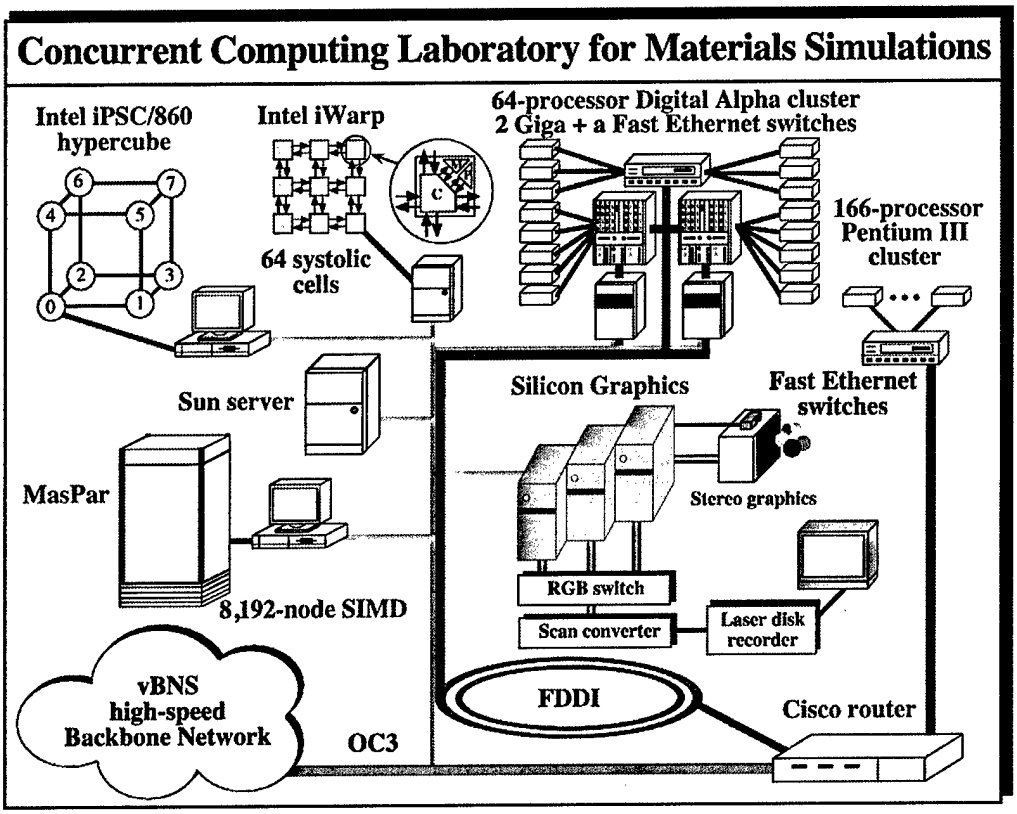

Fig. 8: Computational infrastructure at the CCLMS.

§5 PERSONNEL SUPPORTED

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§6 PUBLICATIONS

Journals and Proceedings

1. "Nanoindentation of silicon nitride: a multimillion-atom molecular dynamics study," P. Walsh, A. Omeltchenko, R. K. Kalia, A. Nakano, and P. Vashishta, Applied Physics Letters 82, 118-120 (2003).

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10. "Million-atom molecular dynamics simulation of flat InAs overlayers with self-limiting thickness on GaAs nanomesas," X. Su, R. K. Kalia, A. Madhukar, A. Nakano, and P. Vashishta, Applied Physics Letters 78, 3717-3719 (2001).

11. "Critical lateral size for domain formation in InAs/GaAs square nanomesas: a multi-million-atom molecular dynamics study," X. Su, R. K. Kalia, A. Madhukar, A. Nakano, and P. Vashishta, Applied Physics Letters 79, 4577-4579 (2001).

12. "Multimillion atom simulation of materials on parallel computers—nanopixel, interfacial fracture, nanoindentation, and oxidation," P. Vashishta, M. E. Bachlechner, A. Nakano, T. J. Campbell, R. K. Kalia, S. Kodiyalam, S. Ogata, F. Shimojo, and P. Walsh, Applied Surface Science 182, 258-264 (2001).

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15. "Linear-scaling density-functional-theory calculations of electronic structure based on real-space grids: design, analysis, and scalability test of parallel algorithms," F. Shimojo, R. K. Kalia, A. Nakano, and P. Vashishta, Computer Physics Communications 140, 303-314 (2001).

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§7 INTERACTIONS/TRANSITIONS

A. PARTICIPATION/PRESENTATIONS AT MEETINGS, CONFERENCES, SEMINARS

- "Multimillion Atom Simulations of Nanostructured Materials on ParallelComputers - Sintering and Consolidation, Fracture, and Oxidation," International Conference on Computational Physics, Kanazawa, Japan, October 11-13, 1999.
- "Massively Parallel Materials Simulations," Colloquium in the Department of Chemical Engineering, Univ. of Cincinnati, October 21, 1999.
- "Atomistic Simulations of Nanostructures: Multimillion Atom Molecular Dynamics Simulations on ParallelComputers," Foresight Conference on Molecular Nanotechnology, San Jose, CA, October 15-17, 1999.
- "Parallel Multiscale Simulations of Nanostructred Materials," CERCA, Montreal, Canada, December 8, 1999.
- "Multiscale Simulations of Nanostructred Materials on Massively Parallel Compters, Steacie Institure for Molecular Sciences," National Research Council of Canada, Ottawa, Canada, December 10, 1999.
- "Computational Assisted Development of High-Temperature Structural Materials," Defense Science Board Presentation, Washington, DC, February 4, 2000.
- "Multi-Million Atom Molecular Dynamics Simulations of Metal/Ceramic and Semiconductor/Ceramic Interfaces on Parallel Computers," Workshop on Process Modeling of Laminated Multilayer Ceramic Systems, Motorola University,Tempe, Arizona, March 1, 2000.
- "Mulltimillion Atom Simulation of Nanostructured Materials on Parallel Computers – Sintering and Consolidation and Fracture and Oxidation," The Materials Society (TMS),

Nashville, TN, March 12-16, 2000.

- "Parallel Multiscale Simulations of Nanostructured Materials," CSW 2000, EPOCHAL TSUKUBA International Congress Center, March 13-15, 2000.
- "Molecular Simulations of Solids: Metals, Semiconductors, Ceramics, and Glasses," International Comparative Study of Applications of Molecular and Materials Modeling, Washington, DC, March 14, 2000.
- "Information Technology and the Dual-Degree Program," Amercian Physical Society, Minneapolis, Minnesota, March 20, 2000.
- "Large-Scale Atomistic Simulations of Solid State Materials Modeling Many Millions of Atoms on Parallel Computers," American Physical Society , Minneapolis, March 22-24, 2000.
- "Parallel Multiscale Simulations of Nanostructured Materials," Iowa State University and Ames Research Laboratory, Ames, Iowa, April 3, 2000.
- "Multimillion Atom Simulations of Materials on Parallel Computers - Past, Present and Future," Celebrating the Success of LSU Computer Science, Baton Rouge, LA, April 14, 2000.
- "Multiscale Simulations of Oxidation and Fracture in Nanostructured Solids," HPaC Seminar, TU Delft, The Netherlands, April 14, 2000.
- "Parallel Multiscale Simulations of Nanostructured Materials," MD Meeting, University of Illinois at Urbana, April 16-17, 2000.
- "Multimillion Atom Simulations of Nanophase Materials on Parallel Computers," Seminars on Humanity 3000- Nanotechnology In the Future, Foundation for the Future, Bellevue, WA, April 21, 2000.
- "Massively Parallel Multiscale Simulations Nanostructured Materials," Intel Corporation, May 1, 2000.
- "Massively Parallel Multiscale Simulations of Nanostructured Ceramics," American Ceramic Society Symposium on Advances in Theory, Modeling, and Simulations of Materials, St. Louis, Missouri, May 3, 2000.
- "Computer Simulations of Ceramic Interfaces," AFOSR Meeting on Ceramic Materials and Composites, Saint Louis, MO, May 4-5, 2000.
- "Multimillion Atom Simulations of Materials on Parallel Computers - Past, Present and Future," XXIII Encontro Nacional de Física da Matéria Condensada, São Lourenço, Minas Gerais, Brasil, May 11-13, 2000.
- "Multi-Million Atom Simulation of Sintering and Consolidation on Parallel Computers," SIAM Conference on Mathematical Aspects of Materials Science, Philadelphia, PA, May 23, 2000.
- "Recent Research Activities in Material Sciences at LSU: Introduction to Concurrent Computing Laboratory for Materials Simulations (CCLMS)," Niigata University-LSU

Symposium, Niigata University, Niigata, Japan, May 30, 2000.

- "Computational Assisted Development of High-Temperature Structural Materials," DoD High Performance Computing Modernization Program Conference, Albuquerque, NM, June 5-8, 2000.
- "Computational Assisted Development of High Temperature Structural Materials," DoD Challenge User's Group Meeting, Albuquerque, New Mexico, June 8, 2000.
- "Multimillion Atom Simulations of Mechanical Behavior of Nanostructured Materials, Interfaces, and Dynamics of Oxidation," The Society of Materials Science, Japan (JSMS), Osaka, Japan, May 21-26, 2001.
- "Multimillion Atom Simulations of Materials at the Forefront of Information Technology and Nanosciences," National Research Council, National Materials Advisory Board Meeting on "Materials Research for Defense-After-Next", Woods Hole Center of the National Academy of Sciences, MA, June 27-28, 2001.
- "High Performance Computing and Visualization: Opportunities and Challenges at the Information-Bio-Nano Interface," Frontiers in Information Technology, Rensselaer Polytechnic Institute, Troy, NY, November 8, 2001.
- "Scalable multiscale continuum/atomistic/quantum-mechanical simulations of nanosystems," Institut National de Recherche en Informatique et en Automatique (INRIA) School on "Numerical Methods for Atomistic Simulation: from Micro to Meso Scale", November 26-30, 2001, Paris, France.
- "Large-scale atomistic simulations of nanostructured materials and interfaces," 13th Symposium of Materials Research Society of Japan on "Advanced and Interdisciplinary Materials Research for the 21st Century", December 20, 2001, Kawasaki, Japan.
- "Scalable parallel-computing framework beyond Teraflop for high-end computational materials research," Joint Research Center for Atom Technology (JRCAT), Computational Science Workshop 2002, January 9, 2002, Hayama, Japan.
- "Computational materials science on Teraflop-to-Petaflop computers," DOD, DOE, NASA Joint Conference on Mission Critical Computing,Washington DC, February 4-6, 2002.
- "Multimillion atom simulations of nanosystems on parallel computers," International Symposium on Computational Science & Engineering, Tokyo, Japan, March 5-6, 2002.
- "Multiscale simulations of nanosystems," IPNS Nanocomposite Workshop, March 28, 2002, Argonne National Lab, Chicago, IL.
- "Multiscale FE/MD/QMD method and multimillion atom simulations of nanosystems and interfaces on parallel computers," Symposium on Modeling and Numerical Simulation of Materials Behavior and Evolution, MRS Spring Meeting, CA, 2002.
- "Mulstiscale simulations of nanosystems," April 18, 2002, Oak Ridge National Lab, TN.
- "Large-scale molecular dynamics simulations of the oxidation of metallic nanoparticles," Gordon Conference on Energetic Materials, Tilton, NH, June 19, 2002.

- "Multimillion atom simulations of nanosystems on parallel computers - nanopixel, nanoindentation and oxidation," APS Conference on Computational Physics 2002, San Diego, August 25-28, 2002.
- "Multimillion atom simulations of nanosystems on parallel computers - nanopixel, nanoindentation and oxidation of aluminum nanoparticles," CNER-MSI Nanosimulation Workshop, Center for NanoEnergetics Research, Minnesota Supercomputing Institute, Minneapolis, MN, August 26-27, 2002.
- "Large scale atomistic simulations of reactivity of nanosystems - nanostructured materials and oxidation of aluminum nanoparticles, Expanding the Envelope: Nano Materials for Aerospace Symposium, Corpus Christi, Texas, January 27-30, 2003.

B. CONSULTATIVE AND ADVISORY FUNCTIONS TO GOVERNMENT LABORATORIES AND AGENCIES

- Served on the advisory committee of a DOE supported workshop on "Probing Advanced Materials for Extreme Environment: New Experimental Opportunities in Neutron Scattering." The workshop was held in connection with the DOE initiative on Spallation Neutron Source to be built at Oak Ridge.
- Served on NSF Phase I SBIR (Small Business Innovation Research) and STTR (Small Business Technology Transfer) Program Peer Review Panel.
- Editorial board, Journal of Physics: Condensed Matter.
- Associate Editor-in-Chief, Computing in Science and Engineering.
- Served on World Technology Evaluation Center (WTEC) Panel on Applications of Molecular Modeling.

C. TRANSITIONS

Government Laboratories

- Collaborated with Drs. Ronald Kerans and James Larsen at the AFRL (Wright Patterson Research Site).
- Collaborating with Dr. Michael A. Stroscio at Army Research Office on stress-driven phenomena in electronic devices.
- Collaborating with Dr. S. Saini at NASA Ames on algorithm design and implementation of large-scale materials simulations on NASA's Information Power Grid.
- Collaborating with Dr. A. Sayir at NASA Lewis on experimental and simulation studies of hgih-temperature ceramic eutectics.
- Collaborating with Dr. C. Loong at Argonne National Laboratory on a joint neutron scattering and molecular-dynamics study of nanostructured ceramics.

Industry

- Collaborating with Dr. S. Shankar's simulation and modeling group at Intel Corporation on atomistic simulation of electronic devices.

- Collaborating with Dr. David Wilcox's experimental group on multilayer ceramic integrated circuits at the Ceramic Technology Center at Motorola Laboratories

Collaborative Team for Ceramic Research

We continue to interact with Drs. E. Dickey (Univ. of Kentucky), A. S. Argon (MIT), A. Sayir (NASA-Lewis) on eutectic ceramic composites. We continue to develop interaction potentials for more complex ceramic materials to make direct contact with experimental synthesis and property measurements. Dr. C. Loong, Intense Pulsed Neutron Source, Argonne National Laboratory continues to make neutron measurements on amorphous and nanophase alumina. A program on levitated amorphous and liquid alumina is also carried out at Advanced Photon Source at Argonne. We have close contacts with all these experimental efforts. The barriers between synthesis, property measurements, and large-scale simulations are being reduced for productive and fruitful scientific effort leading toward technological applications of advanced ceramic materials.

§8 NEW DISCOVERIES, INVENTIONS OR PATENT DISCLOSURES

None

§9 HONORS AND AWARDS

- The Best Technical Paper Award, IEEE/ACM Supercomputing 2001 Conference (2001).
- Best Papers, IEEE Virtual Reality 2002 Conference (2002).