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**EMBEDDED MICROCLUSTERS IN ZEOLITES AND
CLUSTER BEAM SPUTTERING -- SIMULATION
ON PARALLEL COMPUTERS**

Final Progress Report

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FINAL PROGRESS REPORT (1992-96)

PROPOSAL TITLE: Embedded Microclusters in Zeolites and Cluster Beam Sputtering – Simulation on Parallel Computers

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EXECUTIVE SUMMARY

This report summarizes the research carried out under DOE supported program (DOE/ER/45477) at the Concurrent Computing Laboratory for Materials Simulations at Louisiana State Universities. Large-scale molecular-dynamics (MD) simulations were performed to investigate: i) sintering process, structural correlations, and mechanical behavior including dynamic fracture in microporous and nanophase Si_3N_4 ; ii) crack-front propagation in amorphous silica; iii) phonons in graphitic tubules; and iv) amorphization and fracture in nanowires. The simulations were carried out with highly efficient multiscale algorithms and dynamic load-balancing schemes for mapping irregular atomistic simulations on distributed-memory parallel architectures. These research activities resulted in fifty-three publications and fifty-five invited presentations. Two graduate students are completing dual-degrees--Ph.D. in physics and a M.S. from the Department of Computer Science--during the course of this project.

This DOE project involved three faculty members, two graduate students, and a postdoc over a three-year period (1992-1996). It also involved interactions/transitions with researchers at governmental laboratories and industry.

TABLE OF CONTENTS

EXECUTIVE SUMMARY	i
TABLE OF CONTENTS	ii
§1 BACKGROUND	1
§2 RESEARCH ACCOMPLISHMENTS	1
§2.1 STRUCTURE AND MECHANICAL PROPERTIES OF NANOPHASE Si_3N_4	1
§2.2 CRACK-FRONT PROPAGATION IN NANOPHASE SILICON NITRIDE	3
§2.3 SINTERING OF SILICON NITRIDE NANOCLUSTERS	5
§2.4 FLOPPY MODES AND THERMAL TRANSPORT IN MICROPOROUS Si_3N_4	5
§2.5 DYNAMIC FRACTURE IN A GRAPHITE SHEET	6
§2.6 AMORPHIZATION AND FRACTURE IN NANOWIRES	7
§2.7 STRUCTURAL CORRELATIONS AND BRITTLE/DUCTILE BEHAVIOR IN AMORPHOUS SILICA	7
§2.8 ATOMISTIC PROCESSES IN SILICON CARBIDE AND ALUMINA	8
§2.9 PARALLEL MULTIREOLUTION MOLECULAR-DYNAMICS SIMULATIONS	10
§2.10 DYNAMIC LOAD-BALANCING SCHEME FOR IRREGULAR APPLICATIONS	10
§3 INTERACTIONS/TRANSITIONS	11
§4 EDUCATIONAL ACCOMPLISHMENTS: TRAINING OF GRADUATE STUDENTS	12
§5 PUBLICATIONS	14
§6 INVITED TALKS	19

§ 1 BACKGROUND

Advanced ceramics are excellent materials for applications requiring extreme operating conditions. The capability to withstand high temperatures, combined with their high strength and low weight, makes them highly desirable for energy technologies such as high thrust-to-weight ratio turbine engines, hypersonic aerospace vehicles, and environmental applications. These materials are also very useful for surface transportation, electronics, and advanced manufacturing industries.

The fundamental issue concerning ceramics is the relationship between the microscopic structure, atomic diffusion, and mechanical and thermal properties. An understanding of this relationship on the atomic scale is critical for the design of novel ceramics with application-specific properties.

This DOE project involved the investigation of properties and processes in nanostructured ceramics. Using large scale molecular-dynamics (MD) simulations, we investigated:

- Structural correlations and mechanical behavior, including crack-front propagation, in crystalline and nanophase silicon nitride;
- Growth of pore interfaces and brittle and ductile behavior in amorphous silica;
- Mechanical properties, thermal transport, and low-frequency floppy modes in microporous silicon nitride;
- Early stages of sintering of ceramic nanoclusters;
- Crack propagation in graphite;
- Strain effects and phonons in graphitic tubules;
- Amorphization and fracture in nanowires.

These MD simulations were executed with highly efficient, portable and scalable, multiresolution algorithms including the fast multipole method for the long-range Coulomb interaction and a dynamic load-balancing scheme for mapping irregular applications on parallel machines. *These research activities have resulted in 53 papers and 55 invited presentations.* The next section provides an overview of our research accomplishments.

§ 2 RESEARCH ACCOMPLISHMENTS

§ 2.1 STRUCTURE AND MECHANICAL PROPERTIES OF NANOPHASE Si_3N_4

Advanced ceramics such as Si_3N_4 , SiC , SiO_2 , and Al_2O_3 are highly desirable materials for applications requiring extreme operating conditions. Light weight, elevated melting temperatures, high strengths, and wear and corrosion resistance make them very attractive for applications in energy technologies and advanced manufacturing industries. 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 nanophase materials are fabricated by in-situ consolidation of nanometer size clusters.) Despite a great deal of research, many perplexing questions concerning nanophase ceramics remain unanswered. Experiments have yet to provide information regarding the morphology of pores or the structure and dynamics of atoms in nanophase ceramics. As far as modeling is concerned, only a few atomistic simulations of nanophase materials have been reported thus far. (This is due to the fact that these simulations are computationally very demanding: A realistic simulation of a nanophase

solid requires 10^5 - 10^6 time steps for processing and $\sim 10^6$ atoms, since each nanocluster itself consists of 10^3 - 10^4 atoms.)

Using 1.08 million particle MD simulations we have investigated the structure and mechanical behavior of nanophase Si_3N_4 . The MD simulations are performed with effective two- and three-body interatomic potentials: The two-body terms consist of steric repulsion between atoms, screened Coulomb potentials due to charge transfer between Si and N, and a charge-dipole interaction that takes into account the large electronic polarizability of nitrogen; the three-body potential in Si_3N_4 takes into account covalent effects through bond-bending and bond-stretching terms. To establish the validity of this interaction scheme, we compare the MD results with a variety of experimental measurements. We find: i) the bond lengths and bond-angle distributions in crystalline and amorphous Si_3N_4 are in excellent agreement with experiments; ii) the positions and relative heights of the peaks in the static structure factor for amorphous Si_3N_4 are in good agreement with neutron scattering measurements; iii) the phonon density-of-states of crystalline α - Si_3N_4 agrees well with inelastic neutron scattering experiments; iv) the specific heat of crystalline α - Si_3N_4 is in excellent agreement with experiments over a wide range of temperatures; and v) the bulk modulus and Young's moduli along different directions in α - Si_3N_4 deviate less than 10% from the experimental values.

Figure 1: Snapshot of a configuration of nanophase Si_3N_4 before consolidation (left). The other picture shows the system consolidated with an applied pressure of 15 GPa. The density of the consolidated system is 2.94 g/cc which is 92% of the density of the α - Si_3N_4 crystal.

Nanophase Si_3N_4 is generated by consolidating a random cluster configuration (108 clusters with 10,052 atoms each) with the constant-pressure MD approach. Figure 1 shows the nanophase systems before and after consolidation under an applied pressure of 15 GPa. Pair-distribution functions and bond-angle distributions reveal that interfacial regions in the consolidated nanophase Si_3N_4 are amorphous and they contain a large number of undercoordinated Si atoms. Systems sintered at low pressures (~ 1 GPa) have percolating pores whose surface roughness exponents (0.46 and 0.86) are in excellent agreement with experiments. We also find that the dependence of elastic moduli on porosity and grain size in nanophase Si_3N_4 can be understood in terms of a three-phase model for heterogeneous materials (please see Fig. 2).

Figure 2: Porosity dependence of the bulk modulus (K) and shear modulus (G). Open circles denote the MD results for the bulk modulus of nanophase silicon nitride with cluster size $D=60\text{\AA}$; open triangles and squares represent the MD results for bulk and shear moduli, respectively, of the nanophase system with $45\text{\AA}$ clusters. Solid circles and triangles denote bulk moduli and solid squares represent shear moduli calculated from the multicomponent model [Budiansky, J. Mech. Phys. Solids 13, 223 (1965)]. The solid, dashed, and dotted lines are drawn to guide the eye.

§2.2 CRACK-FRONT PROPAGATION IN NANOPHASE SILICON NITRIDE

Understanding the role of microstructures in fracture is one of the most challenging problems in materials science. Nanophase materials are ideal systems to examine this issue at the atomistic level since microstructures in these materials are only a few nanometers in dimension. Using 1.08 million particle MD simulations, we have investigated the morphological and dynamic aspects of fracture in nanophase Si_3N_4 . Figure 3 shows snapshots of the crack front at various values of the external strain. The crack front consists of pores connected to the notch (shown in magenta; the remaining disconnected pores are shown in orange). Figure 3 (a) shows a snapshot taken 10 ps after the notch is inserted. We observe initial development of the crack front and the growth of a few crack branches in the system. These local branches and nanoclusters tend to arrest the motion of the crack front, and further crack propagation is only possible if additional strain is applied. Figure 3(b) shows a snapshot of the crack front in the nanophase system under 11% strain. Comparing with Fig. 3(a), it is evident that the crack front has advanced significantly and coalesced with the pores in the center. We also observe that pores and interfacial regions allow the crack front to meander and form a branched structure. Figure 3(c) shows a crack-front snapshot 10 ps after the system was strained to 14%. At this time a secondary crack (top left hand corner of the figure) with several local branches merges with the primary crack. With further increase in the strain the secondary front advances toward the initial notch while the crack keeps growing laterally. When the strain reaches 30%, the crack finally separates the material into two disconnected parts and the system is now completely fractured. It should be noted that the critical strain (30%) at which the nanophase system fractures is enormous compared to what the crystalline Si_3N_4 system can sustain (at an applied strain of only 3% the crystal undergoes cleavage fracture). This is due to: i) plastic deformation in interfacial regions; ii) deflection and arrest of cracks by nanoclusters; and iii) multiple crack branching. None of these mechanisms are operative in the crystalline system. This demonstrates the dramatic effect of nanostructures on fracture.

To compare the toughness of nanophase and crystalline systems, we have calculated the fracture energy per unit area in both nanophase and crystalline Si_3N_4 systems (with the same geometry). For the $(10\bar{1}0)$ surface of an atomically sharp mode I crack (film surface was (0001)) in an $\alpha\text{-Si}_3\text{N}_4$ crystalline film, the stress distribution was calculated using the MD method. From the prefactor of the $r^{-0.5}$ term of the local stress (r is the distance from the crack tip), we have estimated the critical stress-intensity factor. This analysis gives a value which is close to our MD

estimate of the intrinsic toughness ($1.3 \text{ MPa}\cdot\text{m}^{0.5}$). From the calculations of the fracture energy per unit area, we estimate that the toughness of the nanophase Si_3N_4 is six times larger than that of the crystal.

We have also investigated the morphology of crack fronts in the fractured nanophase Si_3N_4 . In recent years this issue has drawn a great of experimental attention. Measurements on a variety of brittle and ductile solids have revealed that the widths of fracture profiles scale with the lengths as $w \sim L^\zeta$. For out-of-plane fracture profiles, the roughness exponent, $\zeta_\perp$, above a certain length scale, has a value of 0.8 in three and 0.7 in two spatial dimensions. Many experiments indicate that these values of $\zeta_\perp$ may be independent of the material or the mode of fracture. At small length scales or when the crack front propagates quasi statically, the roughness exponent crosses over to a smaller value ~ 0.5 . Recently it has also been pointed out that there is another distinct roughness exponent, $\zeta \approx 0.6$, associated with in-plane fracture profiles.

To investigate the nature of self-affine fracture surfaces in nanophase Si_3N_4 , we calculate the height-height correlation functions both in and out of the fracture plane y - z . Figure 4a shows that the best fit to the out-of-plane height-height correlation function $g_{xx}(z)$ ($= \langle [x(z+z_0) - x(z_0)]^2 \rangle^{1/2}$) for the fracture profile $x(z)$ requires two roughness exponents: $\zeta_\perp = 0.84 \pm 0.12$ above a certain

length scale ($64\text{\AA}$) and $\zeta_{\perp} = 0.58 \pm 0.14$ otherwise. For the other out-of-plane height-height correlation function $g_{xz}(y)$, the roughness exponent $\zeta_{\parallel} = 0.75 \pm 0.08$. The MD results for $\zeta_{\perp}$ and $\zeta_{\parallel}$ are very close to experimental values. We have also determined the roughness exponent, ζ , for the in-plane fracture profile $y(z)$: Figure 4b shows that the best fit to the corresponding height-height correlation function gives $\zeta = 0.57 \pm 0.08$. Measurements of ζ in Al-Li and Super α_2 Ti₃Al-based alloys yield 0.60 ± 0.04 and 0.54 ± 0.03 , respectively [E. Bouchaud, J. Phys. Cond. Matter].

§2.3 SINTERING OF SILICON NITRIDE NANOCLOUDS

Figure 5: Snapshots showing sintering of Si₃N₄ nanoclusters at 2,000K: (a) nanocrystals at time $t = 0$; (b) sintered nanocrystals at $t = 200$ ps; and (c) sintered amorphous nanoclusters at $t = 400$ ps.

The study of structural and mechanical properties of nanophase Si₃N₄ was preceded by MD simulations of sintering of silicon nitride nanoclusters (each cluster consisting of 20,335 atoms). Our MD calculations provide a microscopic view of neck formation during early stages of sintering (Fig. 5). In the case of Si₃N₄ nanocrystals at 2000K, we initially observe considerable relative motion of clusters. Subsequently a few Si and N atoms join the two nanocrystals and, thus bound, they continue to rotate relative to each

other for 100 ps. In the next 100 ps, the relative motion subsides and we observe a steady growth of an asymmetric neck between the two nanocrystals. In the neck region, there are more four-fold than three-fold coordinated Si atoms. We have also investigated the sintering of amorphous silicon nitride nanoclusters at 2,000K. The neck between amorphous nanoclusters is much more symmetric than the neck between thermally rough nanocrystals. The neck region between amorphous nanoclusters has nearly the same number of three- and four-fold coordinated Si atoms. For both nanocrystals and amorphous nanoclusters, sintering is driven by diffusion of surface atoms. The diffusion in the neck region of amorphous clusters is four times faster than in the neck between nanocrystals.

§2.4 FLOPPY MODES AND THERMAL TRANSPORT IN MICROPOROUS Si₃N₄

Physical properties of Si₃N₄ are greatly influenced by voids. (They are usually present in the system as a result of synthesis by chemical vapor deposition or other processes.) Using MD simulations we have investigated the effect of porosity on mechanical properties and thermal conductivity of amorphous Si₃N₄. Under uniform dilation, pores begin to form at a mass density of $\rho = 2.6$ g/cc. With further decrease in the density, the number of pores and their sizes increase dramatically and around 2.0 g/cc the largest pore percolates through the system. Near percolation the average pore volume diverges as $(\rho - \rho_c)^{-\gamma}$ with $\gamma = 1.95 \pm 0.17$. This is consistent with the percolation theory.

The thermal conductivity of microporous Si₃N₄ is calculated from the heat current-current correlation function and a non-equilibrium MD approach. Between 300 and 1500K, the thermal

conductivity scales as ρ^t where $t \approx 1.5$. Experimental data on carbon and silica aerogels are in agreement with this result. The MD results for Young's modulus E vary as ρ^τ with $\tau \approx 3.6$. This is also close to the experimental value of τ for silica aerogels.

The nature of low-energy floppy modes in microporous Si_3N_4 has also been investigated with the MD approach. Floppy modes appear continuously in amorphous Si_3N_4 as the network connectivity is reduced; in the crystal they appear suddenly at 20% volume expansion. We find that their contribution to density-of-states varies linearly with energy and they significantly enhance the specific heat of microporous Si_3N_4 .

§2.5 DYNAMIC FRACTURE IN A GRAPHITE SHEET

Recently we have also investigated crack propagation in a graphite sheet using million-atom MD simulations on parallel machines. (These simulations are also based on the reactive bond order potential of Brenner.) Fracture dynamics is investigated under a constant applied strain after inserting a notch of length $20\text{\AA}$. We consider two different orientations of the graphite sheet, which exhibit completely different behavior during crack-front propagation:

- Under an applied uniaxial strain of 12% the system G(1,1), in which a fraction of covalent bonds are parallel to the strain (Fig. 6b), undergoes cleavage-like fracture;
- For the G(1,0) orientation, the crack front develops multiple secondary branches and overhangs (Fig. 6a) when its speed reaches approximately half the Rayleigh wave speed. Within the same secondary branch the crack-front profile has a roughness exponent $\zeta = 0.5$, whereas for interbranch fracture surface profiles $\zeta = 0.7$. The scenario of multiple local branches and the values of the roughness exponents are in agreement with recent experimental investigations of fracture.

Figure 6: Multiple branches in a fractured graphite sheet with 1.1 million atoms. Applied strain is 16%, and the orientation is G(1,0).

We have also determined the fracture toughness of the graphite sheet in the G(1,1) orientation using the MD approach. The system with a notch of $50\text{\AA}$ was subjected to different strains. Applying the Griffith criterion, with the surface energy determined from the final fracture surface, the critical stress is estimated to be 71 GPa. The crack starts propagating at a stress of 66 GPa, which corresponds to a critical strain of 10%. From these results, the value of the fracture toughness (defined as $\sigma_F \sqrt{c}$, where σ_F is the

critical stress at which the crack starts propagating and c is the length of the notch) is found to be $4.7\text{ MPa}\cdot\text{m}^{1/2}$. We have also calculated the local-stress distribution around the notch just before

the onset of crack propagation. The data are well-described by $1/\sqrt{r}$ dependence with a stress-intensity factor of $6 \text{ MPa}\cdot\text{m}^{1/2}$. The angular dependence of the local stresses is also in good agreement with the elasticity theory.

§2.6 AMORPHIZATION AND FRACTURE IN NANOWIRES

Silicon diselenide is an important chalcogenide material. It is one of the basic solid electrolytes for advanced high-energy electrochemical cells. Recently we investigated the dynamics of amorphization and fracture in SiSe_2 nanowires using large-scale MD simulations. The calculations are based on interatomic potentials which combine charge-transfer, electronic polarizabilities, steric effects, and three-body covalent interactions. The validity of the interaction scheme is established by comparing the MD results with various available measurements. We find: structural correlations in both crystalline and amorphous systems are in excellent agreement with experiments; the calculated melting temperature ($1250\pm 20\text{K}$) is very close to the experimental value ($1233\pm 5\text{K}$); and the vibrational spectra of crystalline and amorphous SiSe_2 are also in good agreement with neutron scattering measurements.

Figure 7: Snapshots showing fracture in an $800\text{\AA}$ long segment of a 64-chain silicon diselenide nanowire. The total length of the wire is $\sim 4,000\text{\AA}$.

The MD simulations for SiSe_2 nanowires reveal that the critical strain ($\sim 15\%$) of fracture is independent of the number of chains in the nanowire. Also fracture is preceded by amorphization in nanowires. At first, bonds between edge-sharing tetrahedra break in the chains at the outermost layer. These broken chains form corner-sharing tetrahedra by cross-linking with neighboring chains. Local amorphization propagates across the nanowire to form a sandwich-like structure with an amorphous region in the middle. Cracks then nucleate at the boundaries and propagate inward from the nanowire surface until the nanowire fractures (Fig. 7).

§2.7 STRUCTURAL CORRELATIONS AND BRITTLE/DUCTILE BEHAVIOR IN AMORPHOUS SILICA

Silica has numerous technological applications in microelectronic devices and micro-electro-mechanical systems (MEMS). Atomistic simulations have been used to study the behavior of silica. We have investigated the fracture process in vitreous SiO_2 by applying the parallel multiresolution MD approach to a system of 1.18 million atoms. The calculations are based on an interatomic potential which includes the effects of charge transfer, electronic polarizabilities, and steric repulsion through two-body terms; covalent effects are included via three-body bond-bending and bond-stretching terms. Figure 8 shows a comparison between the MD and neutron-scattering results for the static structure factor, $S(q)$, of amorphous silica. Clearly the simulation

results for $S(q)$ are in very good agreement with experiments. The calculations for elastic moduli and the phonon density-of-states of amorphous SiO_2 are also in good agreement with experimental measurements.

Figure 9 shows the MD results for fracture (snapshots of crack fronts) in amorphous silica at 300K and 900K. It is evident that the system undergoes cleavage fracture at 300K. At the critical strain for fracture (8%), the crack tip reaches a terminal speed of 1.40 km/s which is nearly half the Rayleigh wave speed. (At 600K, the fracture is again cleavage-like with the terminal crack-tip speed reaching a value of 0.85 km/s.) In contrast, at 900K the amorphous silica system shows plastic behavior up to a strain of 17%. Currently we are investigating sintering, structural correlations, and mechanical properties of nanophase amorphous silica system.

§2.8 ATOMISTIC PROCESSES IN SILICON CARBIDE AND ALUMINA

Silicon carbide and alumina are excellent structural ceramics for applications requiring extreme operating conditions. We are investigating properties and processes in these materials using large-scale MD simulations. The SiC simulations are based on an empirical bond-order potential

proposed by Tersoff [Phys. Rev. B **39**, 5566 (1989)]. The MD results for structural properties (bond lengths, bond angles, etc.), elastic moduli, and the cohesive energy of crystalline SiC are in excellent agreement with experiments. The melting temperature obtained from MD simulations using Tersoff's potential agrees well with the result of the electronic-structure calculations. Currently we are performing MD simulations to understand the crack-front morphology and the effect of strain rate on dynamic fracture in crystalline and amorphous SiC systems. Preliminary results of these fracture simulations are shown in Fig. 10.

The MD simulations for aluminum oxide are based on an interaction scheme proposed by Streitz and Mintmire [Phys. Rev. B **50**, 11996 (1994)]. This potential allows the local atomic charges to vary with the environment. The dynamic charge transfer and the resulting electrostatic interaction is merged with an embedded-atom potential yielding a scheme which can simultaneously treat FCC aluminum and α -alumina systems. This potential has been optimized to reproduce the bulk structural and mechanical properties of FCC aluminum and α -alumina. Additionally, the potential yields reasonable values for surface energies and surface relaxations.

We have implemented the MD simulations for Al_2O_3 using an extended Lagrangian scheme in which the charges are treated as dynamical variables. The long-range Coulomb interaction is implemented with an $O(N)$ fast multipole method (FMM). We have already determined the phonon density-of-states (DOS), infrared spectrum, and Raman spectrum of α - Al_2O_3 crystal. The MD results compare well with experimental measurements. Currently, we are investigating the behavior of $\text{Al}/\text{Al}_2\text{O}_3$ interface. The preliminary results are shown in Fig. 10.

Figure 10. The figure on the left shows the onset of fracture in a million atom MD simulation of crystalline SiC under 7% strain at 300K. The other figure shows dynamic charge transfer at $\text{Al}/\text{Al}_2\text{O}_3$ interface. The interface involves (111) Al and (0001) Al_2O_3 surfaces. The white circles show the atomic positions (the small circle is aluminum and the large circle is oxygen). The color bar shows the valence of aluminum atoms.

§2.9 PARALLEL MULTIREOLUTION MOLECULAR-DYNAMICS SIMULATIONS

Atomistic simulations discussed in §2.1 - §2.9 require considerable computational resources because of long processing times, large systems, and compute-intensive interatomic interactions (e.g. long-range Coulomb and three-body covalent forces). These simulations are not feasible without efficient algorithms or massively parallel machines.

We have designed a highly efficient, multiresolution molecular-dynamics (MRMD) approach to carry out large-scale materials simulations on parallel machines. This approach includes the fast multipole method (FMM)--a divide-and-conquer scheme which reduces the computational cost for the Coulomb interaction from $O(N^2)$ to $O(N)$. The FMM is based on a hierarchical subdivision of space (Fig. 11), where at each spatial scale the influence of a large collection of charges is approximated to any desired precision by a multipole expansion. The method is well-suited to parallel architectures: Unlike the direct method which must communicate the locations and strengths of a large number of charges between distant processors, the FMM transmits a compressed representation of this information, namely the coefficients of the multipole expansion. In addition to FMM, the MRMD approach includes a multiple time-scale algorithm for short-ranged, two-body interactions and a separable scheme for three-body covalent interactions.

Figure 11: Multilevels in the FMM for a 2D system (left); execution (solid curves) and communication times (dashed curves) per MD time step for the MRMD approach (right). p is the number of processors.

Figure 11 shows the performance of the MRMD approach on the 512-node Touchstone Delta machine at Caltech and the 128-processor IBM SP system at Argonne National Laboratory. The execution time scales linearly with the system size and the computation time dominates the communication time. Using MPI (Message Passing Interface), the MRMD has been ported to other parallel platforms as well.

§2.10 DYNAMIC LOAD-BALANCING SCHEME FOR IRREGULAR APPLICATIONS

In many atomistic simulations (e.g. porous materials or fracture) one encounters a non-uniform spatial distribution of atoms. Regular partitioning of such a system into subsystems of equal volume and then one-to-one mapping of subsystems on processors of a parallel machine leads to an imbalance of the computational workload among the processors. A load-balancing scheme has been designed by one of our students, Tim Campbell, in collaboration with Dr. Aichihiro Nakano in the Department of Computer Science. In this scheme, the computational workload is distributed

equally among the processors and the interprocessor communication is minimal. In this scheme, the atomic coordinates are transformed into curvilinear coordinates:

$$\xi = x + \sum_Q a_Q \exp(i Q \cdot x), \quad (1)$$

and in the curvilinear space the system is partitioned uniformly into subsystems which are mapped onto the processors of a parallel machine. Using the simulated annealing approach, the parameters $\{a_Q\}$ are varied so that processors have equal workloads and also the interprocessor communication is minimal. (When structural rearrangement occurs during a simulation, the variational parameters are updated dynamically to adjust the boundaries of subsystems.) Figure 12 shows the performance of this dynamic load-balancing algorithm on 36 nodes of the in-house Digital Alpha system on two GIGA SWITCHES. Evidently the algorithm performs very well even when the size of the system increases from 25 to 125 million atoms. Recently this load balancer has been further improved by replacing the plane-wave basis by orthonormal wavelets.

§ 3 INTERACTIONS/TRANSITIONS

Government Laboratories

We have a number of collaborations with scientists at government laboratories: i) We are working with Drs. Joseph Lichtenhan and Stephen Rodgers at the Phillips Laboratory; and ii) with Dr. Jeremy Broughton and his research group at the Naval Research Laboratory. We are also collaborating with a number of scientists at Argonne National Laboratory: Dr. C. Loong at the Intense Pulsed Neutron Source Division and Drs. T. Disz, W. Gropp, and R. Stevens in the Mathematics and Computer Science Division.

Industries

In collaboration with Drs. James Patterson, Joseph Manke, Daniel Curtis, Benjamin Dembart, and Thomas Wicks at Boeing Corporation, one of our students, Timothy Campbell, developed a parallel implementation of electromagnetic scattering calculations using the Fast Multipole Method (FMM).

Universities

Recently we put together an outstanding, multidisciplinary team consisting of: i) D. Brenner (North Carolina State); ii) E. Kaxiras (Harvard Univ.); iii) J. Broughton (NRL); iv) A. Madhukar (Univ. of Southern California); v) L. Greengard (Courant); and vi) T. Disz, W. Gropp, and R. Stevens (Argonne). One of our goals is to develop a materials simulation software repository

which will include: i) Multiresolution schemes to carry out large-scale MD simulations based on interatomic potentials derived from electronic-structure calculations; ii) new integration algorithms that will allow MD simulations to reach microsecond time scales; iii) extensions in the areas of dynamic process support, remote memory operations, and various latency-hiding operations that will allow substantial progress in computations on heterogeneous parallel platforms; and iv) interactive and immersive visualization tools for materials simulations.

§4 EDUCATIONAL ACCOMPLISHMENTS: TRAINING OF GRADUATE STUDENTS

Recently we introduced an interdisciplinary program which allows graduate students to obtain a Ph.D. in physics and a M.S. from the Department of Computer Science.

Figure 13: Computational infrastructure at our *Concurrent Computing Laboratory for Materials Simulations* (CCLMS). The CCLMS consists of two parallel computing laboratories, one in Physics and Astronomy and the other in 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: **Digital Alpha cluster** - 40 Alpha nodes (46 processors consisting of eight 275-MHz and thirty-eight 165-MHz processors) connected via two Giga switches; **Intel iWarp** - a 64-cell systolic architecture; **MasPar** - an 8192-node SIMD (Single Instruction Multiple Data) machine; **Intel iPSC/860** - a distributed-memory MIMD (Multiple Instructions Multiple Data) machine. The CCLMS also has visualization facilities which include a Silicon Graphics workstation, an 8-processor Silicon Graphics Power Center, and stereo-graphic equipment. Efforts are underway to establish a virtual environment (VE) laboratory which will feature an interactive and immersive *ImmersaDesk* for visualization.

The aim of this program is to provide students with broad-based training in high performance computing and communications (HPCC) and the physical sciences. In connection with this program, we have introduced a number of high performance computing courses in the Physics and Computer Science Departments. The Department of Physics has two graduate courses in

computational physics which are cross-listed with computer-science courses. The first course deals with classical and quantum simulations on parallel architectures. The second course, designed for advanced graduate students, covers special topics such as multiscale phenomena, multigrid methods, wavelets, etc. In the Department of Computer Science we have introduced three new HPCC courses. Two more courses will soon be added to the computer-science curriculum: a) Heterogeneous Computing; and b) Scientific Visualization. The courses we have introduced emphasize parallel computing and algorithm design for large-scale scientific applications. Students have access to a number of parallel machines to gain hands-on experience and to perform research on large-scale computational projects.

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. Through these contacts, students also have access to excellent parallel computing and visualization facilities at other institutions.

DOE SUPPORTED PUBLICATIONS

1. Structure of Rings in Vitreous SiO₂
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2. Structural Correlations in Porous Silica: Molecular Dynamics Simulation on a Parallel Computer
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3. Computer Simulation of Network Glasses and Molecular Dynamics Algorithm on SIMD and MIMD Machines
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8. Classical and Quantum Simulations for Large Systems on Parallel Computers
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9. Structure, Fragmentation, and Phonons in Silicon Microclusters
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19. Dynamic Correlations in Nanoscale Devices: Quantum Dynamics Simulations on Parallel
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21. Molecular Dynamics and Quantum Molecular Dynamics Simulations on Parallel Architectures
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23. Computational Approach to Nanotechnology on Parallel Architectures
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24. Structural Transformation in Densified Silica Glass: A Molecular-Dynamics Study
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25. Massively Parallel Algorithms for Computational Nanoelectronics Based on Quantum Molecular Dynamics
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26. Molecular Dynamics and Quantum Molecular Dynamics Simulations on Parallel Architectures
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27. Structural and Dynamical Correlations in Stishovite and High Density Silica Glass
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36. Low-Energy Floppy Modes in High-Temperature Ceramics
P. Vashishta, R. K. Kalia, and I. Ebbsjö
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37. Dynamics and Morphology of Brittle Cracks: A Molecular-Dynamics Study of Silicon Nitride
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38. Crystal Structure and Phonon Density of States of High Temperature Ceramic Silicon Nitride
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39. Molecular-Dynamics Simulations of Covalent Amorphous Insulators on Parallel Computers
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41. Phonons in Graphitic Tubules--A Tight-Binding Molecular Dynamics Study
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42. Simulations of Crack Propagation and Fracture in Silica and Silicon Nitride Films on Parallel Computers
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43. Tight-Binding Molecular Dynamics Study of Graphitic Tubules on Parallel Computers
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"High Performance Computing 1995 Grand Challenges in Computer Simulations", ed. A. Tentner (SCS, Phoenix, 1995), p. 116.
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46. Molecular Dynamics Simulations of Ceramic Films on Parallel Computers
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47. Million-Particle Simulations of Fracture: Multiresolution Molecular Dynamics Approach on Parallel Architectures
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48. Phonons in Solid C₆₀ and Graphitic Tubes
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Proc. of the Teraflop Computing and New Grand Challenge Applications Conference, eds. R. K. Kalia and P. Vashishta (Nova, 1995), p. 139.
49. Million Atom Simulations of Materials on Parallel Computers--Silica, Silicon Nitride, and Ceramic Films
A. Nakano, R. K. Kalia, and P. Vashishta
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50. Computer Simulation of Materials on Parallel Architectures: Glasses, Solid C₆₀, and Graphitic Tubules
P. Vashishta, R. K. Kalia, W. Jin, J. Yu, and A. Nakano
"Elementary Processes in Dense Plasmas", edited by S. Ichimaru and S. Ogata (Addison-Wesley, Reading, 1995), p. 359.
51. Structure, Mechanical Properties, and Thermal Transport in Microporous Silicon Nitride -- Molecular Dynamics Simulations on a Parallel Machine
Andrey Omeltchenko, Aiichiro Nakano, Rajiv K. Kalia, and Priya Vashishta
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52. Early Stages of Sintering of Silicon Nitride Nanoclusters: A Molecular Dynamics Study on Parallel Machines
Kenji Tsuruta, Andrey Omeltchenko, Rajiv K. Kalia, and Priya Vashishta
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53. Crack Propagation and Fracture in Ceramic Films -- Million Atom Molecular Dynamics Simulations on Parallel Computers
Priya Vashishta, Aiichiro Nakano, Rajiv K. Kalia, and Ingvar Ebbsjo
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Invited Talks on DOE Research

1. *Structural and Dynamical Correlations in Glasses*
"International Conference on Physics of Strongly Coupled Plasmas",
Rochester, New York, August 17-21, 1992.
2. *Molecular Dynamics Simulation of Strongly Covalent Systems with Coulomb Interactions*
"International Conference on Computational Physics for Condensed Matter
Phenomena", Tokyo, Japan, September 19-21, 1992.
3. *Molecular Dynamics Simulation of Network Glasses & MD Algorithm on Parallel
Computers*
"Second International Conference on Computer Applications to Materials and
Molecular Science and Engineering", Yokohama, Japan, September 22-25, 1992.
4. *Covalent Glasses at Large Positive and Negative Pressures - A Molecular Dynamics
Study*
"New Developments of Computer Based Design of Functional materials",
Osaka, Japan, September 29-30, 1992.
5. *Molecular Dynamics Simulation of Covalent Glasses*
"Southeastern Section American Physical Society Meeting",
Oak Ridge, Tennessee, November 12-14, 1992.
6. *Classical and Quantum Simulations for Large Systems on Parallel Computers*
"Theory and Modeling" Symposium at the Annual Materials Research Society
Meeting, Boston, November 29-December 4, 1992.
7. *Structure and Dynamics of Network Glasses at Very large Positive and Negative
Pressures - A Molecular Dynamics Study*
"Solid State Ionics" Symposium at the Annual Materials Research Society
Meeting, Boston, November 29-December 4, 1992.
8. *Computational approach to nanotechnology on parallel architectures*
"Mardi Gras '93, Concurrent Computing Conference in the Physical Sciences",
Baton Rouge, Louisiana, February 18-20, 1993.
9. *Covalent Glasses at Very Large Positive and Negative Pressures - A Molecular
Dynamics Study*
"The Metallurgical Society of America", Denver, Colorado, February 21-25, 1993.
10. *Structure and Dynamics of SiO₂ at Very Large Positive and Negative Pressures*
"American Chemical Society Meeting", Denver, Colorado, March 28-April 2, 1993.
11. *Molecular Dynamics of Silica Under Very Large Positive and Negative Pressures on
Parallel Computers*
"High Performance Computing - 1993 Simulation MultiConference",
Washington DC, March 29-April 1, 1993.
12. *Molecular dynamics simulations of classical and quantum systems on parallel
architectures*
"Gordon Godfrey Workshop on Computational Approaches for Novel Condensed
Matter Systems", Sydney, Australia, July 12-17, 1993

13. *Molecular dynamics simulations of silica under very large positive and negative pressures*
Institute for Advanced Studies, University of Canberra, Canberra ACT, Australia,
July 22, 1993
14. *Quantum molecular dynamics simulations of solid C₆₀ - the effects of orientational disorder and pressure*
"Symposium in Honor of John Quinn's 60th Birthday", Brown University, Rhode Island, September 3, 1993
15. *Molecular dynamics and quantum molecular dynamics simulations parallel computers*
"Second IMACS Conference on Computational Physics", St. Louis, Missouri,
October 6-9, 1993
16. *Molecular dynamics simulations of structure and dynamics of silica at very large positive and negative pressures*
"The Minerals Metals & Materials Society (TMS) Meeting", Pittsburgh, Pennsylvania,
October 18-21, 1993
17. *Large-scale materials simulations on parallel architectures*
"Symposium at Brown University", Providence, Rhode Island, September 1993
18. *Probing amorphous materials with computer experiments on parallel architectures*
Battelle Pacific Northwest Laboratory, Richland, Washington, November 1993
19. *Materials simulations on parallel architectures*
"Future Directions of Quantum Many Body Theory", Texas A&M University,
College Station, Texas, January 14-16, 1994
20. *Multimillion particle MD simulations of fracture in silica glass*
"Mardi Gras '94 Conference on Toward Teraflop Computing and New Grand
Challenge Applications", Baton Rouge, Louisiana, February 10-12, 1994.
21. *Effect of orientational disorder and pressure on phonons in solid C₆₀ - A tight binding molecular dynamics study*
"High Performance Computing Symposium" at the Society of Computer Simulation
Conference, San Diego, California, April 11-15, 1994
22. *Dynamic correlations in nanoscale devices: Quantum dynamics simulations on parallel architectures*
"SCS Simulation Multiconference", San Diego, California, April 11-15, 1994.
23. *Computer simulation of porous glasses on parallel architectures*
"SCS Simulation Multiconference", San Diego, California, April 11-15, 1994.
24. *Vibrational spectra of solid C₆₀ and graphitic tubules - A tight binding molecular dynamics study on parallel computers*
"Electrochemical Society Meeting", San Francisco, California, May 23-27, 1994
25. *Multimillion particle molecular dynamics simulation of SiO₂ and Si₃N₄ on parallel computers*
"CECAM Workshop on Computer Simulation of the Growth of Semiconducting
Materials", Lyon, France, May 30-June 2, 1994

26. *Morphology of pores and fractured surfaces in porous silica - multimillion particle molecular dynamics simulations*
"XVIII International Workshop on Condensed Matter Theories",
Valencia, Spain, June 6-11, 1994
27. *Effect of Orientational disorder and pressure on phonons in solid C₆₀ and graphitic tubules - A tight binding molecular dynamics study*
"XVIII International Workshop on Condensed Matter Theories",
Valencia, Spain, June 6-11, 1994
28. *Silica under very large positive and negative pressures - Molecular dynamics simulation on parallel computers*
"Twelfth Symposium on Thermophysical Properties",
Boulder, Colorado, June 19-24, 1994
29. *Computer simulation of materials on parallel architectures - Glasses, solid C₆₀, and graphitic tubules*
"Oji International Seminar on Elementary Processes in Dense Plasmas",
Tomakomai, Japan, June 27-July 1, 1994.
30. *Simulation of materials using parallel computers*
Energy Research Laboratory, Hitachi City, Japan, July 4, 1994
31. *Molecular dynamics simulations of covalent amorphous insulators on parallel computers*
"Symposium on Amorphous Insulators", Winter Park, Colorado, August 7-11, 1994
32. *Million particle molecular-dynamics simulations of disordered materials*
"Workshop on Large Scale Simulations in Chemistry and Materials Science",
Dayton, Ohio, September 12-13, 1994
33. *Molecular dynamics simulation of high temperature ceramics*
"Workshop on Large Scale Simulations in Chemistry and Materials Science",
Dayton, Ohio, September 12-13, 1994
34. *Large Scale Simulation of Silica on Parallel Computers*
Quartz Workshop, Naval Research Laboratory,
Washington, DC, September 19-20, 1994
35. *Multi-Million Particle Molecular Dynamics Simulations on Parallel Architectures*
NIST High Performance Computing Series, Gaithersburg, MD, October 17, 1994
36. *Multi-Million Particle Materials Simulations on Parallel Computers*
Materials Research Laboratory, Michigan State Univ., East Lansing, MI,
November 3, 1994
37. *Large Scale Simulations of Disordered Materials on Parallel Computers*
Institute for Theoretical Physics, University of California,
Santa Barbara, Nov. 10, 1994
38. *Multi-Million Particle Simulations of Porous Glasses and Ceramics on Parallel Computers*
Joint Seminar Sponsored by Materials Science, Chemical Technology, and Intense
Pulse Neutron Source Divisions, Argonne National Laboratory, Argonne,
December 7, 1994

39. *Multimillion Particle Molecular-Dynamics Simulations for Amorphous Materials on Parallel Architectures*
Los Alamos National Laboratory, Los Alamos, NM, January 20, 1995
40. *Parallel Molecular-Dynamics Simulation of Amorphous Materials*
8th Annual Workshop on Recent Developments in Computer Simulation Studies in Condensed Matter Physics, University of Georgia, Athens, GA,
February 20-24, 1995
41. *Parallel Molecular Dynamics Simulations of Ceramic Films*
High Performance Technologies and Scientific Applications, LSU, Baton Rouge, LA,
February 23-25, 1995
42. *Multimillion Atom Molecular Dynamics Experiments on Parallel Architectures*
1995 Simulation Multiconference, The Society of Computer Simulation,
Phoenix, AZ, April 9-13, 1995
43. *Molecular Dynamics Simulations of Glasses on Parallel Computers*
1995 Simulation Multiconference, The Society of Computer Simulation,
Phoenix, AZ, April 9-13, 1995
44. *Million Atom Simulations of Materials on Parallel Computers - Silica, Silicon Nitride, and Ceramic Thin Films*
Annual Meeting of the American Ceramic Society, Cincinnati, Ohio, May 1-3, 1995
45. *Studies of Nanoclusters and Amorphous Materials by Parallel Molecular Dynamics Simulations*
Annual Meeting of the American Ceramic Society, Cincinnati, Ohio, May 1-3, 1995
46. *Massively Parallel Computing for Materials Modeling*
Fifth Conference on Computational Research on Materials,
University of West Virginia, WV, May 3-5, 1995
47. *Crack Propagation and Fracture in Ceramic Films -- Million Atom Molecular Dynamics Simulations on Parallel Computers*
European-Materials Research Society, Strasbourg, France, May 22-26, 1995
48. *Large Scale Simulation of Amorphous Materials*
XIX International Workshop on Condensed Matter Theories, Caracas, Venezuela,
June 12-17, 1995
49. *Large Scale Molecular Dynamics Simulation of High Temperature Ceramics*
XIX International Workshop on Condensed Matter Theories, Caracas, Venezuela,
June 12-17, 1995
50. *Fracture and Sintering of Ceramic Materials by Parallel Molecular Dynamics*
High Performance Computational Chemistry Workshop, Pleaston, CA,
Aug. 13-16, 1995
51. *Multiresolution Molecular Dynamics Simulations of Real Materials Using Parallel Architectures*
Livermore National Laboratory, August 15, 1995

52. *Simulation of Crack Propagation and Fracture in Silica and Silicon Nitride Films on Parallel Computers*
Amorphous and Crystalline Insulating Thin Films III Symposium
at the Annual Meeting of Solid State Devices and Materials,
Osaka, Japan, August 21-24, 1995.
53. *Parallel Algorithms for Large Scale Simulations of Real Materials*
Electrical and Electronic Engineering, Faculty of Engineering,
Okayama University, Okayama, Japan, August 25, 1995
54. *Crack Propagation and Fracture Glasses and Ceramics - Million Atom Molecular Dynamics Simulations on Parallel Computers*
Recent Progress in Computational Materials Science Symposium at the IVth
International Conference on Advanced Materials, Cancun, Mexico,
September 4-8, 1995
55. *Massively Parallel Simulations of Nanostructured Materials*
Texas A&M University, College Station, TX, September 21, 1995