Multimillion Atom Simulations of Dynamics of Wing Cracks and Nanoscale Damage in Glass, and Hypervelocity Impact Damage in Ceramics

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Abstract

We have developed scalable parallel algorithms for first-principles based predictive atomistic simulations of materials. We have achieved parallel efficiency 0.998 for 134 billion-atom molecular dynamics (MD), 1.06 billion-atom reactive force-field MD, and 11.8 million-atom (1.04 trillion electronic degrees-of-freedom) quantum-mechanical MD in the framework of the density functional theory on 131,072 BlueGene/L processors. We have performed up to 540 million-atom MD simulations to study: 1) initiation, growth and healing of wing cracks in confined silica glass; and 2) damage initiation during hypervelocity impact on advanced ceramics.

Key words: molecular dynamics; quantum mechanics; density functional theory; parallel computing; wing cracks; hypervelocity impact

1. Introduction

There is growing interest in large-scale molecular dynamics (MD) simulations involving million-to-billion atoms, in which interatomic forces are computed quantum mechanically to accurately describe chemical reactions. Emerging petaflops computers, combined with scalable parallel computing technology, could potentially extend the realm of quantum mechanical (QM) simulation to the macroscopic scales to understand microscopic mechanisms that govern macroscopic materials behavior. This paper summarizes our research efforts to develop scalable parallel MD and QM simulation technologies as well as their application to the study of atomistic damage mechanisms in glasses and advanced ceramic materials.

2. Scalable parallel simulation algorithms

In the past several years, we have developed a unified embedded divide-and-conquer (EDC) algorithmic framework to design a suite of linear-scaling MD algorithms, in which interatomic forces are computed with varying accuracy and complexity [1]: 1) classical MD involving the formally $O(N^2)$ N-body problem [2]; 2) reactive force-field (ReaxFF) MD involving the $O(N^3)$ variable N-charge problem; 3) quantum mechanical (QM) calculation based on the density functional theory (DFT) to provide approximate solutions to the exponentially complex quantum N-body problem [3]; and 4) adaptive hierarchical QM/MD simulations that embed highly accurate QM simulations in MD simulation only when

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and where high fidelity is required [4,5]. These algorithms include:

– Algorithm MRMD: space-time multiresolution molecular dynamics [2].
– Algorithm F-ReaxFF: fast reactive force-filed molecular dynamics [6].
– Algorithm EDC-DFT: embedded divide-and-conquer density functional theory on multigrids for quantum-mechanical molecular dynamics [7].

We have also developed a tunable hierarchical cellular decomposition (HCD) framework for mapping the $O(N)$ EDC algorithms onto massively parallel computers with deep memory hierarchies. The HCD maximally exposes data locality and exploits parallelism at multiple decomposition levels, while providing performance tunability through a hierarchy of parameterized cell data/computation structures.

The EDC algorithms are portable and have been run on various high-end parallel supercomputers such as IBM BlueGene/L and SGI Altix 3000. The EDC algorithms expose maximal data locality and thus achieved high parallel efficiency on all tested architectures. The largest benchmark tests of the EDC algorithms on 131,072 BlueGene/L processors include 133,982,846,976-atom MRMD, 1,056,964,608-atom F-ReaxFF, and 11,796,480-atom (1,035,825,315,840 electronic degrees-of-freedom) EDC-DFT calculations with parallel efficiency as high as 0.998 (Fig. 1) [8].

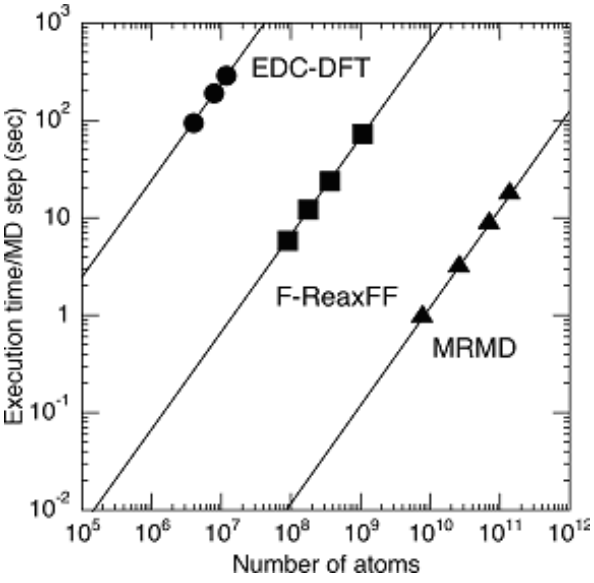

Fig. 1. Benchmark tests of reactive and nonreactive MD simulations on 131,072 BlueGene/L processors. The execution time per MD step is shown as a function of the number of atoms for: quantum-mechanical MD based on the embedded divide-and-conquer density functional theory (EDC-DFT, circles); fast reactive force-field MD (F-ReaxFF, squares); and nonreactive space-time multiresolution MD (MRMD, triangles). Lines show $O(N)$ scaling

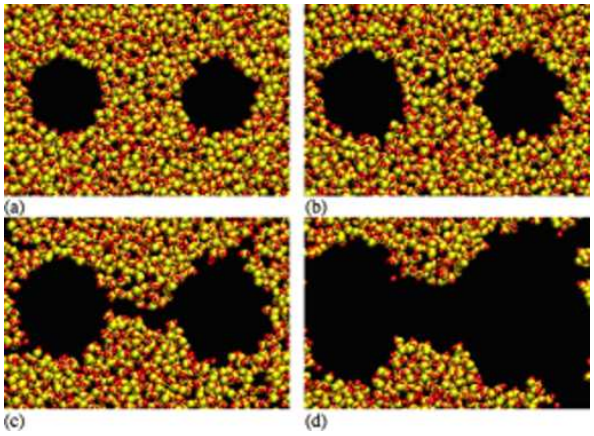

Fig. 2. Snapshots of void coalescence causing fracture in silica glass: (a) Initial MD configuration with two voids of diameter 3 nm each, separated by 3 nm; (b) formation of nanovoids in the inter-void region; (c) a ligament connecting the two voids and nanoscale cracks on the void surfaces at an applied strain of 7 %; and (d) failure caused by void coalescence and damage spreading through the glass at a strain of 11.2 %.

3. Wing cracks in silica glass

We have used the scalable parallel MD simulation technology described in the previous section to perform multimillion-atom simulations of various materials properties and processes. An example is the study of damage initiation and fracture of glasses.

Atomic force microscopy experiments on stress corrosion cracking of silica and silicate glasses in the presence of water reveal that damage in these glasses is predominantly in the form of nanocavities [9,10]. It is observed that damage nanocavities nucleate and grow in front of the crack tip and that they coalesce not only with one another but also with the advancing crack front to cause failure. Our MD simulations on silica glass under applied tensile loads also reveal the formation, growth and coalescence of damage nanocavities and failure due to crack-cavity coalescence [10]. Cavitation and crack-cavity coalescence are known to be the mechanisms for ductile fracture in metallic systems. So the key issue in damage and fracture of glasses is how cavities coalesce and whether the coalescence is similar to that in metals.

We have performed MD simulations to investigate this issue in silica glass. Each system contains two nanovoids of the same size—diameters between 2 nm

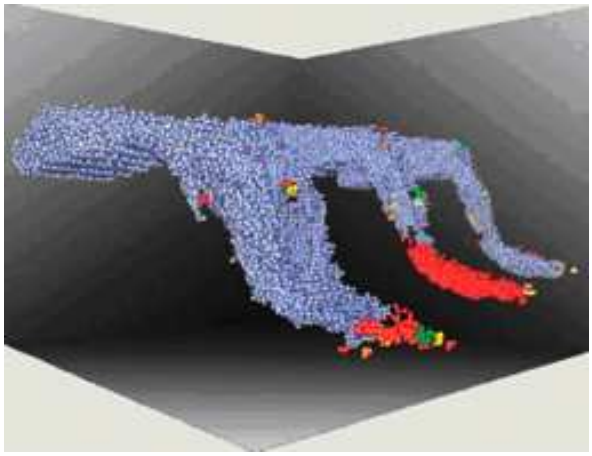

Fig. 3. Snapshots of the wing crack and nanocavities. (Right) wing crack turned in the direction of the applied load. (Middle) a large cavity (red) splits off the wing crack. (Left) after 4 ps the wing crack and the cavity rejoin and the crack recedes by 6 nm.

and 5 nm and the intervoid distances between 2/3 and 3 times the void diameter. We apply dilatational strain with strain rates of 10^8 and 10^9 s^{-1}. Fig. 2 shows the initial configuration of two voids of diameter 3 nm each separated by 3 nm. With increasing strain, we observe: 1) the nucleation of nanovoids between the two voids (Fig. 2b); 2) a ligament joining the two voids (Fig. 2c); 3) the nucleation of cracks on the void surfaces; and 4) failure by coalescence of voids and cracks. We have observed these features in other simulations as well. Our results suggest that damage and fracture in glasses are similar to those in metals, albeit at the nanometer scale.

We have also investigated initiation, growth and healing of wing cracks in confined silica glass by MD simulations [11]. Under dynamic compression, frictional sliding of pre-crack surfaces nucleates nanovoids, which evolve into nanocrack columns at the pre-crack tip. Nanocrack columns merge to form a wing crack, which grows via coalescence with nanovoids in the direction of maximum compression. Lateral confinement arrests the growth and partially heals the wing crack. Growth and arrest of the wing crack occur repeatedly, as observed in dynamic compression experiments on brittle solids under lateral confinement (Fig. 3). We find the temperature elevation in front of the wing crack decays as $1/r$, where r is the distance from the wing crack tip. This is in accordance with the Rice-Levy model.

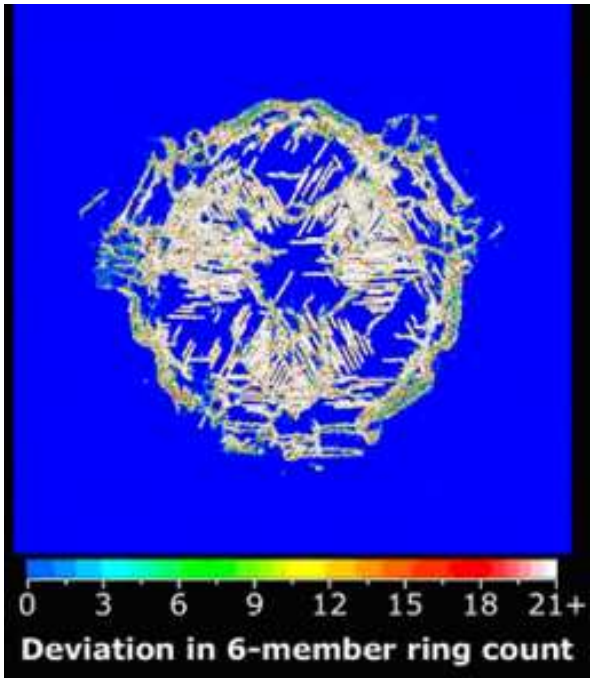

Fig. 4. A thin slice of a 540 million-atom alumina target 40nm in front of the projectile during hypervelocity impact simulation. Deviation in the number of 6-member rings from perfect crystalline atoms (blue) is color-coded using the gradient bar above.

4. Hypervelocity impact damage in ceramics

We have also performed 200-540 million-atom MD simulations to study hypervelocity impact damage of advanced ceramics (AlN, SiC, and Al_2O_3). Our MD simulation on AlN reveals atomistic mechanisms of fracture accompanying structural phase transformation (SPT) in AlN under hypervelocity impact [12]. We found that a shock wave generated by impact splits into an elastic wave and a slower SPT wave that transforms the wurtzite structure into the rocksalt phase. Interaction between the elastic wave reflected from the specimen boundaries and the SPT wave front generates nanovoids and dislocations into the wurtzite phase. Nanovoids coalesce into mode I cracks while dislocations give rise to kink bands and mode II cracking. Such simulations help design thermal and radiation protection systems of aerospace vehicles, which are tolerant to micrometeorite impacts (where impact speeds are as high as 40 km/s).

Recently, we have studied hypervelocity impact on α-alumina (0001) surface using 540 million-atom MD simulation (Fig. 4). The weak planes in α-alumina cause 6-fold intrusion pattern of the

projectile, which in turn initiates a mixture of 3-fold deformation modes in the substrate. These deformation modes include basal slip, basal twin, pyramidal slip, rhombohedral twin and slip-twin-slip composite. We have also investigated cracking mechanisms under the impact loading. As compressive loading introduces defects through deformation mechanisms such as slips and twins, tensile stresses during unloading initiate pores from the defects, which coalescence into cracks. The cracking process is accelerated during the spallation phase and chunks of material are ejected from the substrate as the cracks connect into an hourglass-shaped surface.

In a snapshot of a thin slice of material 40nm in front of the projectile in Fig. 4, our shortest-path ring analysis reveals rhombohedral twinnings (colored as white) forming in three possible orientations within a circle of pyramidal slips (colored as red or green), as both types of deformation give different ring numbers from normal crystalline atoms (colored as blue) [13]. While pyramidal slips cause deviation in coordination number as well, rhombohedral twinning can effectively be identified only by ring analysis. We are currently extending these simulations to ultrahard and tough nanophase ceramic materials [14].

5. Conclusion

In the past several years, significant progresses have been made in simulation methods, linear-scaling algorithms, and scalable parallel computing technologies. Petaflops computers are expected to push the spatiotemporal scale of high-end atomistic simulations, thereby bringing in further new scientific knowledge for the rational design of advanced materials.

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