

# ATOMISTIC MULTISCALE SIMULATIONS OF FRACTURE

Noam Bernstein  
Center for Computational Materials Science,  
Naval Research Laboratory Code 6390,  
Washington, DC 20375, USA.

## ABSTRACT

Computer simulations can give us atomic resolution information about fracture processes that are very hard to study experimentally, because they happen deep inside a material at speeds too high for any atomic-resolution probe. However, the range of length scales involved, from elastic strain fields to interatomic bonds, makes such simulations challenging. I present our coupling of length scales approach that addresses some of these difficulties by combining different simulation methods in different parts of the system. I discuss some general issues of such coupling approaches, and present our results using an implementation that combines two different atomistic simulation methods: a quantum-mechanical model of bonding near the crack tip, and an empirical interatomic potential far from the crack tip. Using this coupled method we have carried out extensive simulations of fracture in single crystal silicon at low temperatures that show brittle fracture in agreement with experiment. The critical loading for fracture is slightly above the Griffith criterion prediction, indicating that lattice trapping is small but significant. I present a model for the lattice trapping energy barrier that explains the low barrier when tight binding is used to describe the bond breaking process. This model also explains the qualitative failure of several popular empirical potentials for silicon in their description of fracture.

## 1 INTRODUCTION

Structural materials need to retain their shape under mechanical loading. If the loading is too large, the material fails. One of the most common modes of failure is fracture, where a crack grows under the applied strain until the material breaks. During fracture the elastic load on a macroscopic system is concentrated at the crack tip, and this provides the driving force that breaks the bonds between atoms ahead of the crack. Since what ultimately controls the strength of the materials is the bonding between the atoms, understanding fracture requires an understanding of the atomic scale processes at the crack tip. Getting such information experimentally is quite difficult: although some very nice work has been done under special conditions (Bouchaud [1]), the fracture process usually happens deep inside the material, and the crack can move quite quickly compared with the speeds of atomic-resolution probes such as HRTEM or AFM. Atomistic simulations can provide exactly this type of information, but there are many challenges. The simulation must describe the interatomic bonding accurately. Since the bonding is mediated by the valence electrons a quantum-mechanical (QM) description would be the most accurate, but the computational cost limits QM methods to a few thousand atoms for dynamic simulations. Such a small number can perhaps describe the crack tip region, but the elastic strain field extends much farther. Empirical potential (EP) simulations that approximate the interatomic interactions without an explicit QM description can simulate millions of atoms, but it is not clear if EPs are accurate enough to describe the bond breaking process. Since even the smallest experimental system comprises many more than  $10^6$  atoms, a full description will require another method, perhaps a continuum elasticity approach that does not explicitly consider the atomistic nature of the material.

Combining different simulation methods can help describe this wide range of length scales. The QM description of bonding can be used near the crack tip. An EP description can be used farther away, where the issue of accuracy in bond breaking is not relevant. The long-range strain fields can then be described by a continuum approach such as the finite element method (FEM). This *coupling of length scales* approach was developed by a number of groups, although in most cases only EP and FEM descriptions were used (Hoover [2], Rafii-Tabar [3], Mullins [4], Abraham [5], Ogata [6]). Here I present a method that uses an accurate QM description of bonding near the crack tip, coupled to an EP description of bonding far from the crack. The two methods are used in a molecular dynamics (MD) simulation to simulate the time evolution of the atomic positions.

The coupling allows for dynamics simulations of the propagation of a crack through the material. The FEM is not used because it adds complications to the coupled method and it is unnecessary for this work. The difficulty in coupling FEM and atomistic simulations is primarily in the description of the material: the FEM uses a continuous field of strains or displacements, while the atomistic method treats the atoms as point masses. Most of the gain in efficiency in the FEM comes from the ability to coarsen the mesh of elements used to solve the continuum equation. However, a mesh with different resolution at different regions can introduce artifacts into the dynamics. Finally, a constitutive law must be provided for the continuum equation, and for dynamic simulation including the nonlinear and temperature dependent material properties is quite difficult. In addition to these technical difficulties, the FEM region is simply not needed. The typical time for a QM calculation of a MD step is of order 10 s. A run time of 1 day translates to about  $10^4$  time steps, or about 10 ps. Since the rate at which information travels in the material is the speed of sound, this time scale implies a length scale of 40 nm (assuming a sound speed in silicon of about 4 km/s). A 40 nm system can be simulated using EPs, without the complexity entailed in coupling an atomistic description to a continuum field description.

## 2 METHOD

The dynamically coupled EP and TB (DCET) method (Bernstein [7]) uses a minimal-basis tight-binding total energy method to simulate interatomic bonding in a small region. Our simulations use the TB model for Si of Bernstein and Kaxiras (Bernstein [8]). To enable the calculation of forces using TB in a finite part of a large system we use a linear scaling Green's function based computation of the electronic density matrix (Bernstein [9]). The environment dependent interatomic potential (EDIP) is used in the rest of the simulated system (Justo [10]). The system is partitioned into a TB region and an EP region, with a boundary region between the two. The TB problem is solved in the TB and boundary regions, subject to the constraint that Green's function matrix elements involving atoms in the boundary region are fixed to their bulk Si values (Bernstein [9]). The EP forces are calculated on all atoms. The time evolution of the system is computed using the molecular dynamics method with the velocity-Verlet time-integration algorithm (Allen [11]), which requires the force on each atom. Atoms in the TB region are propagated using TB-calculated forces, while atoms in the boundary and EP regions are propagated using EP forces (Bernstein [7]). While this approach does not have a well-defined total energy, the TB forces are in practice more accurate than previous implementations (Abraham [5]) that used severe approximations to compute the TB forces in a formulation that did have a well-defined total energy. We find that this trade off of increased accuracy of forces in exchange for uncertainty in energy conservation results in more accurate simulations.

Initializing the simulation requires the position and velocity of every atom in the system. We use a single-crystal Si structure of a crack under mode-I (tensile) loading in plane-strain. The crack is initialized as a thin slit parallel to the (1 1  $\bar{2}$ ) direction, exposing (1 1 1) faces, with a (1  $\bar{1}$  0) crack front. The whole sample of 54000 atoms is about 40 nm by 23 nm by 1.1 nm, and

the crack is initially 20 nm long. A TB region of about 5.5 nm by 1.7 nm surrounds one of the crack tips, surrounded by a 0.65 nm thick boundary region. Free boundary conditions are used in the two large dimensions, while periodic boundary conditions are used along  $(1 -1 0)$  to obtain plane-strain conditions. The initial atomic positions are computed by applying the displacement field of an infinitely thin crack in an infinite plate loaded in tension (pulled along the  $(1 1 1)$  direction) (Broberg [12]) to the initial positions. Velocities are chosen randomly with a mean corresponding to a temperature of 200 K. Atoms along the edges parallel to the crack face are held fixed to apply the tensile load.

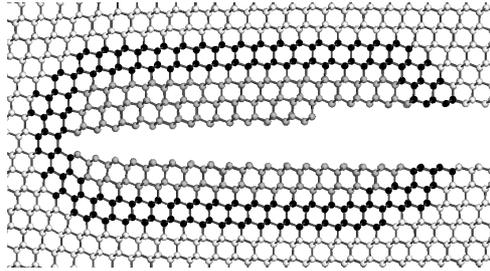


Figure 1: Visualization of cracked system

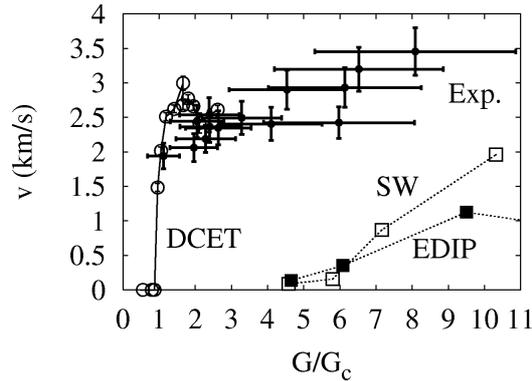


Figure 2: Crack speed as a function of applied load

### 3 RESULTS

When the system is allowed to evolve in time the crack propagates by cleaving bonds between two  $(1 1 1)$  planes. The crack remains atomically sharp, and the exposed surfaces remain on the same pair of crystallographic planes. A visualization of the system is shown in Fig. 1. This behavior is clearly consistent with brittle fracture, which is experimentally observed for Si at low temperatures. In addition to these qualitative observations, it is possible to quantitatively study the crack propagation process as a function of applied loading. A plot of the crack propagation speed as a function of loading, measured in terms of the energy release rate  $G$ , is shown in Fig. 2. The  $x$ -axis is normalized by the Griffith criterion critical energy release rate  $G_c$ , which is the minimal load for fracture that satisfies energy conservation (Griffith [13]). The experimental results (From Hauch [14]) are normalized by the best-known value for  $G_c$  using a first-principles calculation of the surface energy of Si. It is clear from the graph that both experiment and our DCET simulations show fracture very near the Griffith critical load, while the two EPs we tested, EDIP and the Stillingier-Weber (SW) potential (Stillingier [15]) only fracture at much higher loads. In fact, these

two EPs do not show brittle fracture at all: the crack only propagates when dislocations are emitted and the material near the crack tip becomes amorphous.

#### 4 DISCUSSION

To understand the reason for the differences between the DCET and EP results we begin with an important observation: for the EPs there is a wide range of loadings that are above the Griffith criterion critical load, but below the load needed to create any bond breaking events at the crack tip. When this event occurs, it is a dislocation nucleation. For the DCET simulation, in contrast, this range of strains is small, and the bond-breaking event is the propagation of the crack by one lattice spacing. The resistance of the EP simulation to crack propagation even above  $G_c$  is called lattice trapping (Thomson [16]). It is a manifestation of the discrete nature of the atomic structure of the material.

To analyze the source of the lattice trapping we develop a model for the bond breaking process that separates the energy into two parts: bond breaking, and elastic relaxation. This model is similar to the work of Curtin (Curtin [17]), although different assumptions (discussed below) lead us to different conclusions. To quantify these two contributions we perform a series of constrained EP simulations that force the bond ahead of the crack tip to break. By tracking the energy of the system as the bond breaks, we measure the energy barrier to crack propagation. The bond-breaking contribution to this energy barrier can be extracted from a simulation that separates a bulk solid into two semi-infinite slabs. Once this contribution is subtracted from the energy barrier, the remainder is the elastic energy relaxation. By repeating this process for different EPs, we find that the elastic energy contribution is universal up to two normalization factors: the magnitude of the energy (i.e. the energy release rate  $G$ ), and the opening of the crack one lattice spacing behind the crack tip. This model reproduces the energy barrier for the empirical potential simulations. To apply the model to the DCET simulation, we calculate the bond breaking energy using a conventional periodic-boundary condition TB simulation. Combining this energy with the scaled universal elastic energy contribution gives a small but finite lattice trapping energy barrier for TB. The energy scaling factor is computed from the EP (EDIP) elastic constants, while the crack-opening distance is extracted from a sub-critical crack simulation.

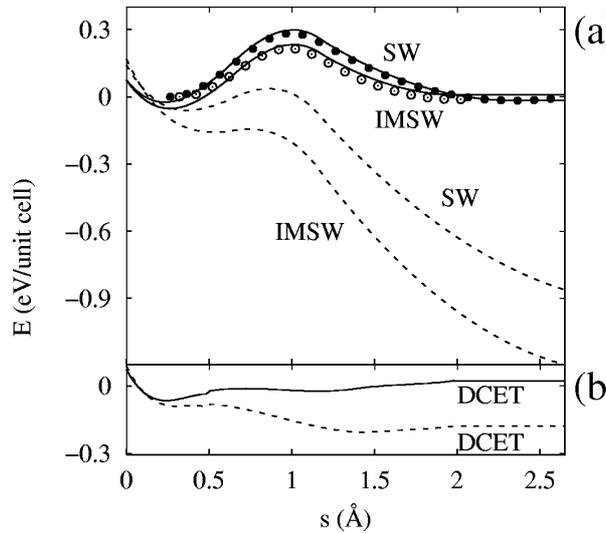


Figure 3: lattice trapping energy barrier as a function of crack opening  $s$

The results of the direct calculations of the barrier and the model are shown in Fig. 3. The two upper lines show the direct calculation (circles) and model prediction (solid lines) for the SW potential, and for a modified form of SW (IMSW) (Holland [18]), at the Griffith critical load. The two dashed lines in the upper panel show the energy barrier at the actual critical load, which corresponds to dislocation nucleation for SW and brittle fracture for IMSW. The lower panel shows the energy barrier for the DCET simulation at  $G_c$  (solid line) and at the observed critical load for brittle fracture (dashed line). From this plot it is clear that the reason the SW simulations do not show brittle fracture is that they have excessive lattice trapping. Even at high loadings (indicated in the graph as a low energy at large crack opening), high enough to nucleate a dislocation, SW still shows a significant energy barrier to crack propagation. The modified form of SW also shows a large barrier at  $G_c$ , but the modification suppresses dislocation nucleation and allows brittle fracture to occur, albeit at much too high a load. The DCET simulation, on the other hand, shows only a small barrier that disappears at the observed critical load.

The energy barrier occurs because of the interplay between bond breaking and elastic relaxation. These two processes each have a length scale, and it is variations in both length scales that explain the differences between the different simulations. The bond breaking distance varies because of the different physical descriptions of bonding. In particular, the EPs are relatively short ranged, because it has proven challenging to find a functional form that captures the physics of covalent bonds in the bulk, which occur only between nearest neighbors, without ignoring the long range interactions that occur as the crack-tip bond is breaking. The crack-tip opening distance also varies significantly among the models. This indicates that there is some deviation from linear elasticity (which predicts a particular opening) and/or that the precise location of the hypothetical continuum crack tip relative to the lattice is different in the different models. The DCET simulation, because of the use of TB at the crack tip, has a longer distance for bond breaking, and a smaller crack opening. Both of these factors combine to reduce the lattice-trapping barrier as compared with the EP simulations. Curtin (Curtin [17]) also noted these two length scales, but perhaps because of his choice of materials he assumed that the bond breaking length is always much larger than the crack opening distance.

## 5 CONCLUSION

Atomistic simulations of fracture can reveal microscopic detail of crack-tip processes, but only if the wide range of length scales involved can be adequately addressed. Coupling different methods in different parts of the system has proven to be an effective approach for doing this in dynamical simulations. While three different methods have obvious applicability to different parts of a fracturing system, scaling arguments show that often only two need to be used in a single simulation. Using an atomistic simulation method that couples an accurate TB description of bonding near the crack tip to an EP description of bonding far from the crack tip, we have simulated brittle fracture in silicon at low temperatures. Our simulations show brittle fracture, in agreement with experiment, at a load very near the Griffith criterion critical load. These results are a qualitative improvement over several popular empirical potentials that show dislocation nucleation and plasticity at the crack tip. Since this work was originally published there has been one EP simulation using the modified embedded atom method that shows brittle fracture with moderate amount of lattice trapping (Swadener [19]). Unfortunately, direct comparison to experiment is nearly impossible: estimates of error in the experimentally measured energy release rates are too large, and there is no technique for measuring the surface energy. A final resolution of the true magnitude of lattice trapping in Si will await more precise experiments and better first principles calculations of the surface energy for input into the Griffith criterion prediction.

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