DYNAMIC FRACTURE TOUGHNESS DETERMINED USING MOLECULAR DYNAMICS

J. G. Swadener, M. I. Baskes and M. Nastasi
Materials Science and Technology Division, Los Alamos National Laboratory, Los Alamos, NM 87545 USA

ABSTRACT

Molecular dynamics (MD) simulations of fracture in crystalline silicon are conducted in order to determine the dynamic fracture toughness. The MD simulations show how the potential energy released during fracture is partitioned into surface energy, energy stored in defects and kinetic energy. First, the MD fracture simulations are shown to produce brittle fracture and be in reasonable agreement with experimental results. Then dynamic fracture toughness is calculated as the sum of the surface energy and the energy stored as defects directly from the MD models. Models oriented to produce fracture on either (111) or (101) planes are used. For the (101) fracture orientation, equilibrium crack speeds of greater than 80% of the Rayleigh wave speed are obtained. Crack speeds initially show a steep increase with increasing energy release rate followed by a much more gradual increase. No plateau in crack speed is observed for static energy release rates up to 20 J/m^2. At the point where the change in crack speed behavior occurs, the dynamic fracture toughness (J_d) is still within 10% of two times the surface energy ($2\gamma_0$) and changing very slowly. From these MD simulations, it appears that the change in crack speed behavior is due to a change in the kinetic energy generation during dynamic fracture. In addition, MD simulations of facture in silicon with defects were conducted. The addition of defects increases the inelastic dissipation and the energy stored in defects.

1 INTRODUCTION

As a crack grows dynamically, potential energy is converted into surface energy, energy stored in defects and kinetic energy. The loss of potential energy can be calculated per unit of crack extension as the strain energy release rate. The kinetic energy is dissipated as heat, and the surface energy can be estimated from the area of the new crack surfaces, although this is complicated if a tortuous crack path results or if crack branching occurs. In previous experimental studies of fracture in silicon [1, 2], it was shown that surface energy alone does not satisfy the energy balance. The kinetic energy and stored defect energy are difficult to measure experimentally, but straight forward to calculate using molecular dynamics. In order to obtain a clearer picture of the relationship between the energy conversion and dynamic fracture toughness, more information is needed on the distribution of the energy converted during dynamic fracture. In this study, we determine the surface energy and defect energy for fracture in a silicon single crystal using molecular dynamics (MD).

We have previously shown [3] that the modified embedded atom method (MEAM) [4] results in brittle fracture in silicon and is in better agreement with experiments than other potentials [1, 5-7]. Here we make one modification to the original MEAM silicon potential to increase the vacancy formation energy. The resulting potential will be shown to produce brittle fracture with crack speeds in agreement with experiments. The surface energy and defect energy are then calculated and compared to the static energy release rate and the kinetic energy.

2 METHODS

The original MEAM potential for silicon gave the vacancy formation energy as 2.8 eV [4]. Changing the MEAM parameters $\beta^{(1)}$ and $t^{(1)}$ to 8.0 and 4.10, respectively increased the vacancy formation energy to 3.90 eV. This new value is in agreement with experimental values and more

recent ab initio values of 3.6 to 4.0 eV [8]. This modification also increased the surface energies on the (111) and (100) surfaces by approximately 15% to 1.43 J/m^2 and 1.66 J/m^2, respectively. The new MEAM surface energies are 10-20% higher than the majority of experimental values, but considering the uncertainty of the experimental surface energy and the better agreement with the vacancy formation energy, this seems like a reasonable compromise.

Two MD models constructed in a strip geometry were used to simulate fracture on (111) and (101) planes. Knauss [9] showed that the strip geometry produces a constant energy release rate when the crack tip is at least 1.5H from either end. The model oriented for fracture on a (111) plane is shown in Fig. 1 and has dimensions 450 x 15 x 147 Å. The model oriented for fracture on a (101) plane with the crack propagating in the [10$\bar{1}$1] direction is similar with dimensions 492 x 16 x 150 Å. To apply load, uniform tensile strain in the z-direction was applied to the model which increased the separation of the upper and lower surfaces by an amount V. At the same time, compressive strains equal to -25% of the z-direction strain were applied in the x- and y-directions. (These compressive strains were applied to prevent premature failure at the corners of the model and did not affect the fracture results.) The upper and lower surfaces were then held fixed and the crack was allowed to propagate. Initially, the models were relaxed through 2000 minimization steps to allow the formation of the crack tip stress field and the growth of a "starter" crack. Then the atoms were given a kinetic energy distribution equal to a temperature of 300 K, and the model was run dynamically with the temperature of the upper third and lower third of the model maintained at 300 K using a Nosé-Hoover thermostat on only the velocities in the x- and y-directions. After the initial temperature distribution, no temperature control was used in the middle third of the model where the crack propagated.

Elastic strains of up to 14% were imposed on the model in order to obtain relatively high energy release rates. At strains of this magnitude, the material response is no longer linear. Hence linear elastic formulas cannot be used. The energy release rate was calculated from the potential energy in MD models. First, the change in energy (ΔU) from the imposed state of strain to the relaxed state (no stress in the z-direction) was determined from the MD energy calculations. Then the static energy release rate (J_s) was calculated from the formula:

$$J_s = H(\Delta U)/2\Omega, \tag{1}$$

where H is the height of the model, ΔU is the change in energy per atom, and Ω is the atomic volume. In the nonlinear strain region, the elastic constants and the Rayleigh wave speed (c_R) also varies with strain. Since c_R is an important parameter in dynamic fracture, it was calculated from the elastic constants (determined from MD models) for the various strain levels used in the simulations. For example, at a strain of 0.096 in the z-direction (and -0.024 in the x- and y-directions), c_R = 3.86 km/s for the (111) orientation, and c_R = 3.93 km/s for the (101) orientation.

3 RESULTS AND DISCUSSION

For $J_s \leq 4$ J/m^2, cracks would not grow in either of orientations studied, despite the fact that this energy is 20-30% greater than two times the surface energy ($2\gamma_0$). The difficulty with initiation of fracture is similar to previous results [1, 6] and may be due to the time scales used in the MD simulations. For slightly greater values of J_s, cracks propagated dynamically in both model orientations, and accelerated to approximately constant speeds within 2 ps. Average crack speeds were determined for crack growth beginning at 2 ps and continuing for 5-10 ps while the crack was within the region where the static energy release rate is constant. Steady state crack speeds normalized by the Rayleigh wave speed (v/c_R) are plotted versus J_s for the (111) model orientation in Fig. 2. Experimental results from Hauch et al. [1] are also shown in Fig, 2 for comparison. The MD and experimental results agree within experimental uncertainty. For the (110) model

orientation, normalized crack speeds are shown in Fig. 3 and compared to the experimental results of Cramer et al. [2]. While the normalized MD crack speeds are approximately 10% less than the average speeds measured experimentally, the agreement is still within the experimental uncertainty. For both model orientations, the crack speeds initially increase quickly with J_s, then increase at a much slower rate, similar to the experimental results. A possible reason for this behavior will be discussed below.

A detail of a typical MD fracture simulation is shown in Fig. 4. Numerous defects are seen on and near the fracture surfaces. Dislocations were sometimes generated at the crack tip, or slightly ahead of or behind the crack tip. For the larger values of J_s studied, crack branching occurred, occasionally leaving microcracks on the fracture surfaces. The energy consumed by the formation of these defects and rough fracture surfaces represents the dynamic fracture toughness, J_d – the energy consumed by the crack itself. This energy was calculated from the MD models after the crack has passed. After the crack had traveled through the model, the atoms were relaxed to their minimum energy configuration. The energy of all the atoms in a volume measuring 100 Å along the crack line by 140 Å high by the width of the model. The difference between the energy of these atoms and an equal number in a perfect crystal was determined. Dividing the difference by the product of 100 Å and the model width gives the dynamic fracture toughness. J_d is plotted as a function of J_s in Fig. 5 for both model orientations. For the lowest energy release rate, the dynamic fracture toughness is only 2% greater than $2\gamma_0$. Initially, J_d increases slowly with J_s. Then, for higher energy release rates, J_d increases more rapidly in a nonlinear manner. Using the original MEAM silicon potential, J_d initially showed an approximately linear increase with J_s, but changed to a similar nonlinear increase at higher energy release rates [3]. The values shown in Fig. 5 for the greatest energy release rates may be affected by the large applied strains. These values will be checked by running a larger model at lower strains to produce the same J_s. Looking at the first three points for each model in Fig. 5, we note that J_d increases by less than 10%. However, this was the region where the crack speed behavior changed (see Fig. 2 and 3). Since the dynamic fracture toughness only shows a small gradual change in this region, the change in the crack speed behavior should be due to a change in the kinetic energy. Such a change would not occur with a continuum model, but occurs with the atomistic model due to the discrete nature of atomic debonding as the crack grows. When the crack speed is greater than $\sim 0.5c_R$, atomic debonding occurs at such a rate that more of the released strain energy is transformed into kinetic energy, which manifests itself in the observed change in crack growth behavior.

In addition to simulation of fracture in perfect crystalline silicon, we have also run MD simulations of fracture in silicon with defects. When defects are present, the strain field in the vicinity of the crack tip interacts with the defect causing additional energy dissipation through inelastic deformation and enlarging of the defects. However, no clear trend in the energy dissipation has yet emerged.

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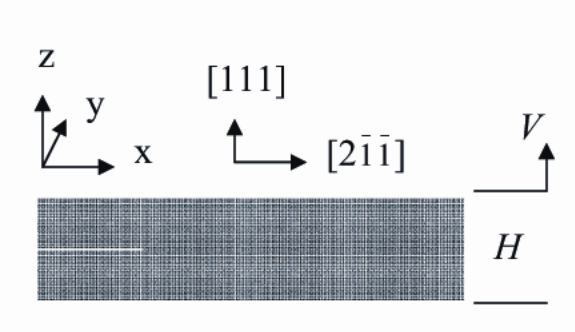

Figure 1: 60 000 atom molecular dynamics model oriented with crystallographic axis as shown. Crack lies in the (111) plane and propagates in the positive x-direction.

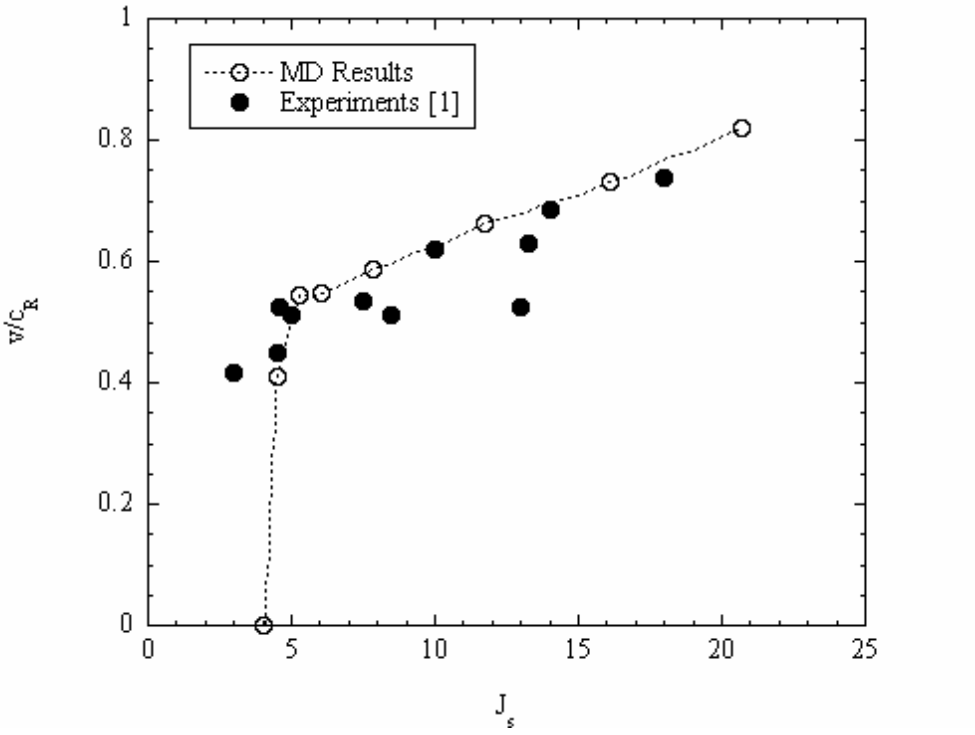

Figure 2: Comparison of normalized crack speeds from MD simulations (open symbols) with experimental results (full symbols) [1] for (111) fracture orientation.

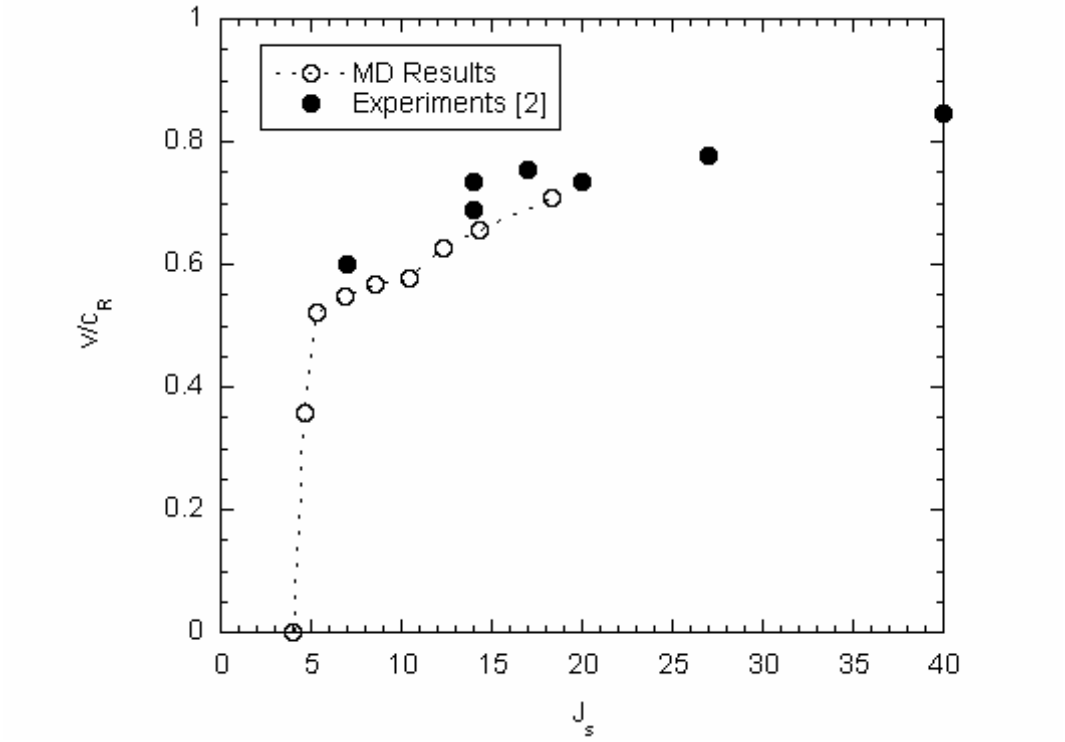

Figure 3: Comparison of normalized crack speeds from MD simulations (open symbols) with experimental results (full symbols) [2] for (101) fracture orientation.

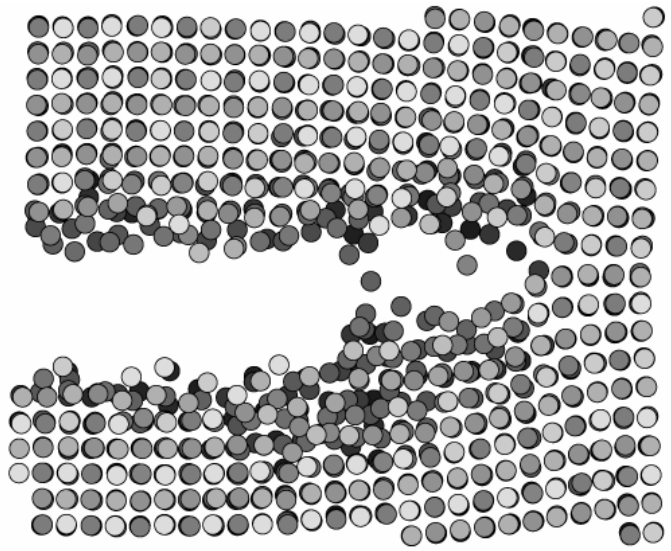

Figure 4: Detail of an MD fracture simulation in the (101) fracture orientation for J_s = 10.4 J/m^2. Shading indicates atoms at the same depth.

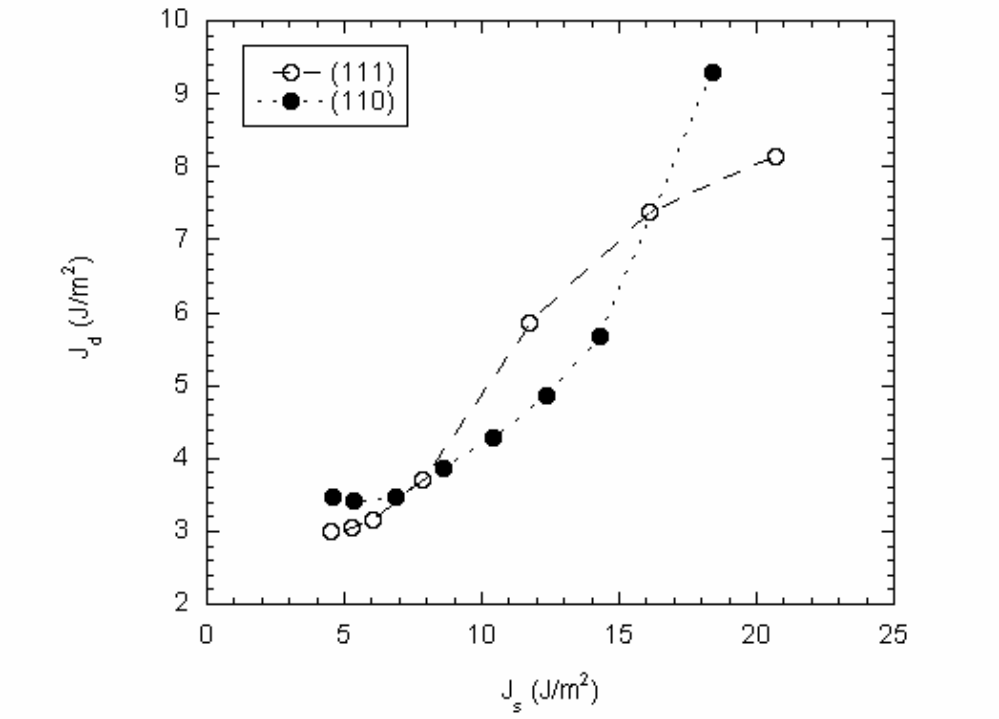

Figure 5: Dynamic fracture toughness (J_d) from MD calculations as a function of static energy release rate (J_s) for (111) and (101) fracture orientations.