AN ATOMIC STUDY OF DYNAMIC BRITTLE FRACTURE IN SILICON

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Abstract

Dynamic fracture has been modeled using a modified embedded atom method (MEAM) potential for silicon. For Mode I dynamic fracture along (111) crystallographic planes, the molecular dynamics model predicts crack speeds and fracture energies in agreement with previous experimental results [1]. In this orientation, fracture occurs almost exclusively along (111) planes for energy release rates up to 30 J/m². For Mode I fracture oriented initially on (110) planes, fracture occurs by cleavage on (110) planes for a static energy release rate (Jₛ) less than 8 J/m². For greater values of Jₛ, the fracture surfaces switch to alternating (111) planes, which is in agreement with previous experimental results [2]. Crack speed predictions for the (110) orientation are somewhat less than the high speeds observed experimentally.

In the atomistic simulations, the dynamically propagating cracks generate dislocations, which are primarily produced on the (111) and (110) planes. Differences in the type and quantity of dislocations produced have been observed for different orientations. Molecular dynamics has the ability to calculate the energy consumed by dislocations and other lattice defects produced during fracture and the total surface energy of the main crack, side branches and secondary cracks. The sum of the surface energy and the energy consumed by lattice defects determines the dynamic fracture toughness, J(v). The dynamic fracture toughness has been found to vary linearly with Jₛ. For the (111) orientation with cracks propagating in the [211] direction, J(v) asymptotically approached a value of 1/3 of Jₛ. The remainder of the strain energy that is released during fracture is converted into kinetic energy at the crack tip during the fracture process, which occurs atom by atom.

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Outline

• MD Models and Methods
• Fracture Simulations
  – Crack speeds compared with experiments
  – Cleaved and faceted fracture surfaces
  – Dynamic fracture toughness
• Conclusions
Models and Orientations

- [111] (H = 15 nm, H = 24 nm)
- [211] (H = 15 nm, H = 24 nm)
- [101] (H = 15 nm, H = 24 nm)
- [101] (H = 15 nm, H = 30 nm)
- [011] (H = 15 nm)

Dimensions:
- 2.5H - 3H
- H
Molecular Dynamics Model

Cracks propagated at constant energy release rate

MEAM potential used to describe directional bonding in silicon

Temperature: 300 K
Calculations

Static Energy Release Rate

\[ J_S = \frac{1}{2} \varepsilon_{zz}^2 HE^* \]

\[ \frac{1}{2} \varepsilon_{zz}^2 E^* = \frac{\Delta U}{\Omega} \]

\[ J_S = H \frac{\Delta U}{\Omega} \]
Variation of Moduli and Rayleigh Wave Speed

\( C_{33} \) and \( C'_{33} \) (GPa)

\( \varepsilon_{zz} \)

\( c_R \) (km/s)

(111) \( H = 15 \) nm
MD Crack Speeds for (111) Fracture

![Graph showing crack speed vs. J_s (J/m^2)]
Dynamic Fracture Results Match Experiments

![Graph showing dynamic fracture results matching experiments. The graph plots v/c_R against J_s (J/m^2). The data includes points for MD, H = 24 nm, MD, H = 15 nm, and Hauch et al., 1999.]
MD Crack Speeds for (110) Fracture

Crack Speed (km/s) vs. $J_s$ (J/m$^2$)

- <101> $H = 15$ nm
- <101> $H = 24$ nm
- <100> $H = 15$ nm
- <100> $H = 30$ nm
MD Results Close to Experiments

![Graph showing the relationship between $v/c_R$ and $J_s$ (J/m²). The graph includes data points for different values of $H$ and a reference to Cramer et al., 2000.]
Fracture Surfaces for (101)[101] Fracture

\[ J_s = 6.3 \text{ J/m}^2 \]
Facets on (111) Surfaces

\[ J_s = 9.7 \text{ J/m}^2 \]
Fracture Surfaces for (011)[100] Fracture

\[ J_s = 6.3 \text{ J/m}^2 \]

\[ J_s = 9.7 \text{ J/m}^2 \]
Larger (111) Facets at Greater $J_s$

$J_s = 18.4 \text{ J/m}^2$
Dynamic Fracture Toughness (111)

\[ J(y) = 0.97569 + 0.32622x \quad R = 0.99059 \]
Dynamic Fracture Toughness (110)

\[ J(v)/J_f \]

\[
\begin{align*}
\text{\( <101> \) } H = 15 \text{ nm} \\
\text{\( <100> \) } H = 15 \text{ nm}
\end{align*}
\]

\[
y = 0.79009 + 0.53761x \quad R = 0.99106
\]

\[
2\gamma_0
\]
Kinetic Energy Increase (111)<211>

\[ J_s = 19 \, \text{J/m}^2 \]
Conclusions

- MEAM Potential Produces Brittle Fracture
- Crack Speeds Within 20% of Experiments
- Faceted Fracture Surfaces Observed
- Calculated Dynamic Fracture Toughness