Journal of the Mechanics and Physics of Solids 57 (2009) 840–850

Contents lists available at ScienceDirect

Journal of the Mechanics and Physics of Solids

journal homepage: www.elsevier.com/locate/jmps

Mechanics of nanocrack: Fracture, dislocation emission, and amorphization

Shan Huang [a], Sulin Zhang [b], Ted Belytschko [c], Sachin S. Terdalkar [d], Ting Zhu [a,*]

[a] *Woodruff School of Mechanical Engineering, Georgia Institute and Technology, Atlanta, GA 30332, USA*
[b] *Department of Engineering Science and Mechanics, The Pennsylvania State University, University Park, PA 16802, USA*
[c] *Department of Mechanical Engineering, Northwestern University, Evanston, IL 60201, USA*
[d] *Department of Mechanical Engineering, University of Arkansas, Fayetteville, AR 72701, USA*

ARTICLE INFO

Article history:
Received 23 September 2008
Received in revised form
15 December 2008
Accepted 16 January 2009

Keywords:
Nanocrack
Fracture
Lattice trapping
Brittle-to-ductile transition

ABSTRACT

Understanding the nanoscale fracture mechanisms is critical for tailoring the mechanical properties of materials at small length scales. We perform an atomistic study to characterize the formation and extension of nano-sized cracks. By using atomistic reaction pathway calculations, we determine the energetics governing the brittle and ductile responses of an atomically sharp crack in silicon, involving the competing processes of cleavage bond breaking, dislocation emission, and amorphization by the formation of five- and seven-membered rings. We show that the nanoscale fracture process depends sensitively on the system size and loading method. Our results offer new perspectives on the brittle-to-ductile transition of fracture at the nanoscale.

1. Introduction

Nanoscale fracture experiments and simulations demonstrate the potential to probe and exploit the ultimate strength of materials (Belytschko et al., 2002; Han et al., 2007; Khare et al., 2007; Lee et al., 2008; Peng et al., 2008; Pugno and Ruoff, 2004; Yu et al., 2000; Zhang et al., 2005). These studies also point to the need for an understanding of the mechanisms governing the formation and extension of nanometer-sized cracks in a broad range of fields and applications (Celarie et al., 2003; Gao et al., 2003; Guin and Wiederhorn, 2004; Mielke et al., 2007; Ritchie et al., 2004). Here we present an atomistic study of nanoscale fracture mechanisms under ultra-high stresses, being close to but below the ideal tensile strength, i.e., the athermal limit of instantaneous fracture. Such high stresses can easily arise in materials with nanometer-sized cracks. While the nanocrack response in this sub-critical load range controls the fracture behavior of small-volume materials, only few theoretical studies have emerged in recent years (e.g., Bernstein and Hess, 2003; Perez and Gumbsch, 2000a, b; Zhang et al., 2007). This is largely because from an atomistic-modeling standpoint, the fracture under a sub-critical load is hardly accessible by direct molecular dynamics (MD) simulations due to the time-scale constraint (Voter et al., 2002). To overcome the time-scale limitation of MD, we adopt the nudged elastic band (NEB) method (Jonsson et al., 1998) to model the sub-critical fracture in terms of the energetics of nanocrack formation and extension.

The quantification of atomic-level energetics clearly reveals an essential feature of fracture in crystals: the lattice discreteness causes the atomic-scale corrugation of the energy landscape, giving rise to the lattice-trapping effect (Thomson et al., 1971). Specifically, under an applied load, a crack can be locally “trapped” in a series of metastable states with different crack lengths and crack-tip atomic structures. The time-dependent kinetic crack extension then corresponds

---

* Corresponding author.
E-mail address: ting.zhu@me.gatech.edu (T. Zhu).

0022-5096/$ - see front matter © 2009 Elsevier Ltd. All rights reserved.
doi:10.1016/j.jmps.2009.01.006

to the transition of the system from one state to the other via thermal activation (Rice, 1978). This lattice-trapping effect is expected to play an increasingly important role in fracture with reduced system size, though its significance varies for different crystals, depending on the bonding characteristics such as the interaction range and shape of the interatomic force law (Curtin, 1990; Sinclair, 1975; Zhang et al., 2007). From the atomistic-modeling perspective, the existence of lattice-trapped states enables us to capture and examine in detail various brittle and ductile responses, including the competing processes of cleavage fracture, dislocation emission, and amorphization (Bernstein and Hess, 2003; Warner et al., 2007; Zhu et al., 2004, 2006).

In this paper, we examine the thermodynamic driving forces and activation barriers associated with growth of a crack, dislocation emission, and amorphization at a crack tip subjected to either stress or strain loading. We show that for a Stillinger–Weber (SW) potential of silicon (Stillinger and Weber, 1985), amorphization is most favored both thermodynamically and kinetically. Based on this result, amorphization is expected to be the dominant crack-tip response. This prediction is consistent with direct MD simulations (Bernstein and Hess, 2003; Buehler et al., 2007), but is valid for a much wider range of stresses, temperatures, and loading rates. We further investigate the energy landscape beyond the initial formation of dislocations and five/seven-membered rings. Our results exhibit energy barriers that govern the subsequent defect migration and nucleation. The competition of these defect processes dictates stress relaxation at a crack tip, and controls fundamentally the brittle-to-ductile transition of fracture.

2. Nanocrack formation and size effect

Consider a central crack in an otherwise perfect crystal of silicon under a uniform far-field load. We use the standard supercell setup with periodic boundary conditions (Parrinello and Rahman, 1981). The silicon atoms form a diamond-cubic crystalline network, characterized by localized and directional covalent bonds that generally enhance the lattice-trapping effect (Sinclair, 1975). Consider the silicon under a high stress of 10 GPa, about 1/4 of the ideal tensile strength in the $\langle 111 \rangle$ direction, 38 GPa, as predicted by the SW potential (Zhu et al., 2006). We determine the atomic geometry and energetics of formation and extension of a nano-sized crack. Here we focus on quasi-2D fracture and ignore the 3D mechanism of crack advancement by double-kink formation and migration along the crack front (Marder, 1998; Sinclair, 1975; Zhu et al., 2004).

Fig. 1(a) shows the system energy per unit cell along the crack front as a function of crack length under both the stress-controlled (red) and strain-controlled (blue) loading conditions. In this calculation, the supercell is 18.3 nm wide, 20.1 nm high, and 3.8 nm thick, with a total of 1680 atoms. In Fig. 1(a), circles represent the local energy minima at different crack lengths, i.e., different numbers of broken bonds. These metastable states arise because of the lattice-trapping effect. They are numerically obtained by using the constrained energy minimization method, as detailed in Appendix A2. The attainment of these states enables us to quantitatively evaluate the applicability of the Griffith theory to nanoscale fracture. According to this theory (Lawn, 1993), fracture occurs at a critical crack length when the system energy maximizes. From the envelop curve connecting circles (dashed line), we determine the Griffith crack lengths for stress-controlled and strain-controlled fractures; both are close to $2a_c \approx 2.8\,\text{nm}$. On the other hand, the critical crack length can be predicted based on the Griffith formula. Namely, the critical energy release rate G_c and the stress intensity factor K_c satisfy the condition of $G_c = K_c^2/E' = (\sigma\sqrt{\pi a_c})^2/E' = 2\gamma_s$; using the surface energy ($\gamma_s = 1.45\,\text{J/m}^2$) and effective Young's modulus in the $\langle 111 \rangle$ direction ($E' = 148.6\,\text{GPa}$) given by the SW potential (Zhu et al., 2006), one predicts $2a_c = 2.74\,\text{nm}$, as indicated by the vertical line in Fig. 1(a). The agreement between the two methods of predicting the critical crack length, with a difference less than one atomic spacing of 0.33 nm, suggests that the Griffith formula is applicable to nanoscale fracture. Note that the above estimate of the stress intensity factor, $K = \sigma\sqrt{\pi a}$, ignores the finite-size effect of the system. We have validated this approximation, as shown later in the study of the image-crack effect.

In Fig. 1 (a), each curve connecting two adjacent circles measures the energy variation along the minimum energy path (MEP) (Jonsson et al., 1998) for breaking or healing one crack-tip bond, i.e., crack extension or receding by one bond distance. These MEP curves are calculated from the nudged elastic band method, as detailed in Appendix A. Each MEP involves a forward and a backward transition. We extract the energy barriers along the thermodynamically favorable directions of transition. So the activation energies shown in Fig. 1(b) are the barriers of crack extension when $a > a_c$, and the barriers of crack healing when $a < a_c$.

Fig. 1 also reveals the size effect on nanoscale fracture. In Fig. 1(c), we compare the energies governing the stress-controlled fracture in two supercells, 18.3 nm × 20.1 nm (red curve) and 9.1 nm × 10 nm (brown curve). Fig. 1(d) shows the energetics of strain-controlled fracture in two supercells, 18.3 nm × 20.1 nm (blue curve) versus 9.1 nm × 10 nm (green curve). Comparing Figs. 1(c) and (d), one sees a significant size effect on strain-controlled fracture, whereas stress-controlled fracture is not sensitive to the system size.

To further reveal the effects of loading method and system size, we regroup the curves in Figs. 1(c) and (d), and show in Fig. 1(e) the energies of stress-controlled (brown) and strain-controlled (green) fracture in the size-reduced system (9.1 nm × 10 nm). In contrast to Fig. 1(a), the two loading methods lead to considerably different energy curves. This difference arises because the strain-controlled fracture is more sensitive to the system size. Fig. 1(f) shows the energy barriers of crack extension, extracted from Fig. 1(e). Particularly, when $a > a_c$, the energy barrier for strain-controlled fracture (green circles) first decreases and then increases as the crack further extends. This trend differs qualitatively from