Computational Materials Science 136 (2017) 216–222

Contents lists available at ScienceDirect

Computational Materials Science

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

Mixed-mode fracture toughness evaluation of a copper single crystal using atomistic simulations

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ARTICLE INFO

Article history:
Received 4 January 2017
Received in revised form 6 May 2017
Accepted 6 May 2017

Keywords:
Copper single crystal
Atomistic simulation
Mixed mode
Fracture toughness
Crack kinking

ABSTRACT

The fracture toughness and kinking of a cracked Cu single crystal under mixed-mode loads are investigated via atomistic simulations. The embedded-atom-method potential is adopted for modeling the Cu single crystal. The displacement conditions imposed on the simulation cells are the near-tip *K*-field displacements of a crack in a cubic symmetry material obtained from linear elastic fracture mechanics (LEFM). For comparison, an asymptotic problem of a kinked crack in a Cu single crystal is solved by finite element analysis under the LEFM framework. The mixed-mode fracture toughness and preferred orientation of the crack extension for the LEFM approach are evaluated on the basis of a proposed mixed-mode fracture criterion. The crack extension is determined by maximizing the crack extension force, which defined as the ratio of the normalized energy release rate to the normalized surface energy. The discrepancies between the results obtained from the atomistic simulations and the LEFM approach are discussed. The transition of fracture patterns from brittle fracture to fracture after dislocation emission with an increase in mode mixity is the primary reason for such discrepancies.

1. Introduction

When a crack grows under mixed-mode loads, the direction of crack propagation is often kinked relative to the original crack line. Conventionally, linear elastic fracture mechanics (LEFM) is used to solve this kind of problem. Based on LEFM, mode I and mode II stress intensity factors uniquely characterize the crack tip conditions and control the onset of crack growth with kinking. A kinked crack in a linear elastic material has thus received considerable attention from the viewpoint of evaluating the stress intensity factor and energy release rate at the onset of crack kinking. Significant progress has been made in the analysis of kinked cracks in isotropic elastic materials [1] and anisotropic solids [2–4]. However, when crack growth occurs in a plastic zone near the main crack tip, an analysis of crack kinking based on linear elasticity or continuum mechanics is no longer valid. Furthermore, the fracture of a material is intrinsically a multi-scale phenomenon, which originates on the atomic scale through bond breaking between atoms and is affected by the atomistic structures. Therefore, studies based on atomic-level physics are required for investigating the fracture phenomena more precisely.

Atomistic simulations that essentially discern the discrete nature of matter have been successfully applied to the analysis of various crack propagation problems. For example, atomistic simulations of crack propagation in a single crystal under mode I loading were performed for observing a brittle-ductile transition based on the nucleation of dislocations [5–8]. Xu et al. [9] investigated the fracture toughness of a nanoscale crack in a Ni crystal. Xu and Deng [10] examined void nucleation and growth during the propagation of a nanoscale crack in an Al single crystal. Adnan and Sun [11] examined the crack formation process in nanostructured NaCl with nanoscale defects and evaluated the mode I fracture toughness. Cui and Beom [12,13] investigated the crack-size-dependent fracture behavior of Cu and Al single crystals, and Cu/Ag bimaterials with interface crack under mode I loading conditions. Nevertheless, these studies have been limited to cracks subjected to pure mode I loading; mixed-mode fractures have rarely been considered in previous works.

The purpose of the present study is to investigate the fracture toughness and kinking of a crack in a cubic single crystal under mixed-mode loads. The mixed-mode fracture toughness and favored crack propagation direction of a Cu single crystal are determined by atomistic simulations. The applied load is given by the *K*-field of a cubic symmetry material using LEFM calculations. For comparison, the kink angle and fracture toughness are also determined by solving an asymptotic problem on the basis of a proposed

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http://dx.doi.org/10.1016/j.commatsci.2017.05.011
0927-0256/

mixed-mode fracture criterion. A detailed comparison of results obtained by these different methods is made. The reasons for discrepancies among the results are discussed on the basis of the different fracture patterns observed in the atomistic simulations.

2. Computational model

Consider a crack of length c in a rectangular plate, as shown in Fig. 1. The plate has a width w, height h, and thickness t. The material is a Cu single crystal, which has a face-centered cubic (FCC) structure and cubic symmetry. The Cartesian coordinates x_1, x_2, and x_3 are coincident with the [100], [010], and [001] crystal directions, respectively. The crack lies on the (010) plane, and the crack front is along the [001] direction. Tractions vanish on the crack surface and periodic boundary conditions are imposed in the [001] direction. The K-field displacements for plane strain deformation are applied to the other directions.

Based on LEFM, the K-field displacements can be expressed as [14]

$$\begin{Bmatrix} u_1(r,\theta) \\ u_2(r,\theta) \end{Bmatrix} = -\sqrt{\frac{2r}{\pi}}\mathrm{Re}[i(\mathbf{L}+i\mathbf{M})\mathbf{B}\boldsymbol{\Theta}\mathbf{B}^{-1}]\begin{Bmatrix} K_{\mathrm{II}} \\ K_{\mathrm{I}} \end{Bmatrix}, \tag{1}$$

where

$$\mathbf{L} = \sqrt{2(\rho+1)}S_{11}^e\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad \mathbf{M} = (S_{11}^e + S_{12}^e)\begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}, \tag{2}$$

$$\mathbf{B} = \begin{bmatrix} -p_1 & -p_2 \\ 1 & 1 \end{bmatrix}, \quad \boldsymbol{\Theta} = \begin{bmatrix} \sqrt{\cos\theta + p_1\sin\theta} & 0 \\ 0 & \sqrt{\cos\theta + p_2\sin\theta} \end{bmatrix}, \tag{3}$$

$$p_1 = \frac{i}{\sqrt{2}}(\sqrt{\rho+1}+\sqrt{\rho-1}), \quad p_2 = \frac{i}{\sqrt{2}}(\sqrt{\rho+1}-\sqrt{\rho-1}), \tag{4}$$

$$\rho = \frac{2S_{12}^e + S_{44}^e}{2S_{11}^e}, \tag{5}$$

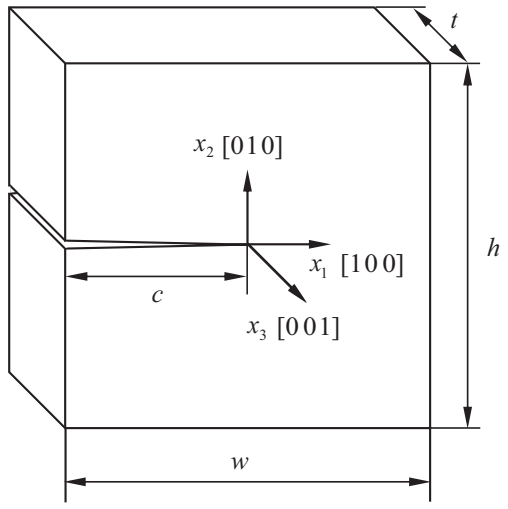

Fig. 1. Computational model for atomistic simulation of a crack in a rectangular plate. The plate has a width w, height h, thickness t, and crack length c.

$$S_{11}^e = \frac{C_{11}}{C_{11}^2 - C_{12}^2}, \quad S_{12}^e = -\frac{C_{12}}{C_{11}^2 - C_{12}^2}, \quad S_{44}^e = \frac{1}{C_{44}}. \tag{6}$$

Here, u_i is the displacement; Re denotes the real part; r and θ are the cylindrical coordinates centered at the crack tip; and K_{I} and K_{II} are the mode I and mode II stress intensity factors, respectively. Additionally, ρ is a dimensionless cubic parameter, S_{ij}^e is the plane strain compliance, and C_{ij} is the conventional stiffness.

For material fracture, there exists an unavoidable nonlinear or plastic zone near the crack tip, where the solution representation from the K-field fails. Furthermore, the continuum mechanics approach is invalid for the analysis of a small fracture process zone where the crack growth occurs. However, according to the LEFM, the K-field is valid in a K-dominated zone under small-scale, nonlinear conditions. Therefore, the stress intensity factors K_{I} and K_{II} can uniquely characterize the crack tip conditions if the nonlinear zone is sufficiently small. Even though the crack growth occurs in the nonlinear zone, the stress intensity factors control its onset with kinking under mixed-mode loads.

The J integral for a crack in a cubic material is given by [1,15]

$$J = \sqrt{\frac{\rho+1}{2}}S_{11}^e(K_{\mathrm{I}}^2 + K_{\mathrm{II}}^2). \tag{7}$$

The mode mixity (ψ) for a crack is defined as follows:

$$\psi = \tan^{-1}\frac{K_{\mathrm{II}}}{K_{\mathrm{I}}}. \tag{8}$$

Instead of the stress intensity factors, the J integral and mode mixity can also be used as crack tip parameters that can characterize the crack tip conditions. Since the J integral and mode mixity are related to the stress intensity factors as expressed in Eqs. (7) and (8), the fracture criterion for the onset of crack growth can be written in the form [1]

$$J = J_c(\psi), \tag{9}$$

$$J_c(\psi) = 2\gamma_s^0\Gamma(\psi), \tag{10}$$

where J_c is the mixed-mode fracture toughness, γ_s^0 is the surface energy for the (010) plane, and Γ is the normalized fracture toughness.

3. Atomistic simulations

We consider a Cu single crystal at a temperature of 0 K. The lattice constant of a unit cell for Cu is a = 0.3615 nm [16]. To obtain the mixed-mode fracture toughness of the Cu single crystal, atomistic simulations were performed using the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) code [17]. The embedded-atom-method (EAM) potential, developed from the density-functional theory [18], was employed to describe the potential energy of the system. The parameters used to define the EAM potential of a Cu single crystal were obtained from Mishin et al. [19]. The elastic stiffness constants are listed in Table 1.

Table 1
Elastic constants for a Cu single crystal [19].

C_{11} (GPa)	C_{12} (GPa)	C_{44} (GPa)
169.9	122.6	76.2