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Molecular dynamics simulations of edge cracks in copper and aluminum single crystals

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ABSTRACT

Edge cracks in Cu and Al single crystals under mode I loading conditions are investigated using molecular dynamics simulations. Calculations are carried out at 0 K and the embedded atom method potentials are adopted for (100)[011] edge crack systems. Five different crack lengths are employed to examine the effects of crack length on the fracture behavior of each material. The results show that Cu and Al exhibit different fracture mechanisms. The overall failure feature of Cu is brittle except for the shortest crack, for which the emission of dislocations preceded crack propagation. All the edge cracks in Al are extended through void nucleation and coalescence, and a zigzag fracture pattern is observed for each crack. Detailed analysis shows that the strikingly different fracture behavior of the two materials is the result of their different vacancy-formation energies and surface energies.

1. Introduction

Face-centered cubic (FCC) materials such as Cu and Al are broadly used in various industries as structural materials. Thus, in order to improve safety and reliability, it is crucial to understand how such materials fail. Even with the same FCC structure, different materials exhibit diverse failure patterns because of their dissimilar material properties. The fracture of a material is intrinsically a multiscale phenomenon, which originates at the atomic scale as a result of the breaking of the bonds between atoms. The fracture behavior of materials is, therefore, strongly dependent on the local atomic environment, such as the atomistic structure, lattice orientation, and the discrete nature of matter distribution. Accordingly, it is unsuitable to analyze fracture at the atomic scale using a traditional continuum mechanics-based approach; atomic scale modeling and simulation are required. Molecular dynamics (MD) is one of the most widely used numerical simulation techniques for investigating the fracture behavior of materials at the atomic scale [1–7].

To understand mode I fracture—the most common failure pattern—many studies of cracks in FCC materials on an atomic scale have been performed and various crack orientations have been examined. Becquart et al. [1] studied the fracture behavior of (010)[001] and (1$\bar{1}$0)[001] cracks in Al using the embedded atom method (EAM) potentials. Here, the crack system is presented by the crack plane and the direction of the crack front. The results showed that the crack did not propagate and that it was always blunted by copious dislocation emissions at some specific temperatures. Zhang et al. [2] studied a family of cracks in Cu single crystals with crack fronts all along the [112] direction at 0 K by using an N-body potential. The reference model was considered as a crack with crack surfaces on the {111} plane, and the other models were obtained by rotation of the reference model about the crack front by an inclined angle of θ. They found that for inclined angles of $0^\circ < \theta < 16^\circ$, brittle cleavage occurred along the slip direction on the slip plane, whereas for inclined angles of $16^\circ < \theta < 90^\circ$, dislocation emission occurred before the cleavage. Cleri et al. [3] used the Lennard–Jones (LJ) potential to study the (221)[1$\bar{1}$0]cracks in FCC materials at approximately 0 K. They concluded that dislocation emissions increase the material toughness and that crack blunting is intimately connected with the formation of a step in the fracture surface immediately at the crack tip. Abraham and Gao [4] used a hyperelasticity model to illuminate the anomalous ductile–brittle fracture behavior in FCC crystals. They found that because of the higher cohesive stress on the {111} plane than on the {110} plane, a system with crack surfaces on the {110} plane is brittle, whereas that on the {111} plane is ductile. Kimizuka et al. [5] investigated the dynamic behavior of dislocations near a crack tip in two FCC lattices. The (110)[001] crack system was considered, and the results obtained for Cu and Al showed multiple emissions of dislocation loops from the crack tip and incipient evolution of plastic deformation during crack extension. Recently, Xu and Deng [6] and Wu and Yao [7] used similar methods to investigate nanoscale void nucleation and

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growth and crack tip stress evolution ahead of a growing (010)[001] crack in single-crystal Al and Ni, respectively. In such studies, the {100}⟨011⟩ crack system has rarely been investigated, though under mode I loading conditions, this crack system is suitable for studying the competition between brittle crack extension and dislocation nucleation.

In this paper, the different fracture behaviors of Cu and Al with edge cracks under mode I loading conditions are elucidated by using MD simulations. The (100)[011] edge crack system is considered and the EAM potentials are adopted. To examine the effect of crack length on the fracture behavior of these two materials, five different initial crack lengths are chosen for each material and the failure strains are obtained through MD calculations. Using the results obtained by these calculations, the critical energy-release rates are calculated by the continuum counterpart of the MD model with the finite element method. The results are then compared to the energy-release rates obtained by the Griffith fracture criterion. The different fracture mechanisms of the two materials are discussed in terms of their different material properties.

2. Interatomic potential and definition of stress

2.1. Interatomic potential

The interatomic potential, which controls the force field of the simulation system, is of great importance in MD calculations. For metallic materials, EAM potentials are widely used. The EAM potential considers the local electron density and can effectively describe the bonding in a metallic system. Many studies have shown that the EAM potential can closely approximate the roles of the local environment in terms of surfaces and defects, and hence it is suitable for modeling the fracture of metallic materials.

The total potential energy U of a system for EAM potential is defined as [8]

$$U=\sum_i F^i(\rho^i)+\frac{1}{2}\sum_{ij}\phi(r^{ij}), \tag{1}$$

$$\rho^i=\sum_{j\neq i}\rho^j(r^{ij}), \tag{2}$$

where F^i is the embedding energy, which is a function of the atomic electron density ρ^i, and the superscripts i and j indicate the atom indexes. Here, ρ^i is induced by all the other atoms in the system at the site of atom i, as shown in Eq. (2). The symbol ϕ represents a pair potential, and r^{ij} is the relative position from atom j to atom i. For Cu and Al, the potentials developed by Mishin et al. [9,10] were employed, which were parameterized from various experimental and *ab initio* data. Various structural and mechanical properties can thus be accurately reproduced, including elastic constant, vacancy-formation energy, surface energy, stacking fault energy, and so on. The stiffness and surface energies calculated from the EAM potentials are illustrated in Tables 1 and 2, respectively; these values agree well with the results obtained by Mishin et al. [9,10].

Table 1
Stiffness components of Cu and Al.

Materials	c_{11}(GPa)	c_{12}(GPa)	c_{44}(GPa)
Cu	169.9	122.6	76.2
Al	113.8	61.6	31.6

Table 2
Surface energies of Cu and Al. Superscripts in parentheses indicate specific surface planes.

Materials	$\gamma_s^{(100)}$ (mJ/m)	$\gamma_s^{(110)}$ (mJ/m)	$\gamma_s^{(111)}$ (mJ/m)
Cu	1345	1475	1239
Al	943	1006	871

2.2. Definition of stress

The definition of stress for an atomic simulation is different from the continuum stress concept. In this study, the well-known and commonly used definition of virial stress [11] is used. Atomic scale virial stresses are equivalent to the continuum Cauchy stresses [12]. This stress consists of two parts, the potential energy part and the kinetic energy part, and is defined as

$$\sigma_{\alpha\beta}=\frac{1}{V}\sum_i\left[\frac{1}{2}\sum_{j=1}^{N}(r_\alpha^j-r_\alpha^i)f_\beta^{ij}-m^i v_\alpha^i v_\beta^i\right] \tag{3}$$

where the subscripts α and β indicate the Cartesian components and V is the total volume of the system. Here, atom i has N neighbors of atom j; r_α^i and r_α^j are, respectively, the α component of the position of atom i and atom j; f_β^{ij} is the β direction force on atom i induced by atom j; m^i is the mass of atom i; and v_α^i and v_β^i are the velocities of atom i along the α and β directions, respectively. To roughly calculate the local stress field of the system, the 'atomic stress' for each atom in the model is used to render the snapshots of the results obtained by MD calculations. Here, the 'atomic stress' corresponds to the term in the square brackets of Eq. (3) and has the units of stress × volume.

3. Modeling details

The quasi-static crack propagation processes of edge cracks in Cu and Al single crystals were simulated using the MD method. The open source MD code Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) [13] was adopted for the computations and the atomic configuration of the MD simulation results were visualized by using AtomEye [14].

The simulation cell is illustrated in Fig. 1, where the x, y, and z axes are oriented along the [01$\bar{1}$], [100], and [011] lattice directions, respectively, with a periodic boundary condition in the z direction and non-periodic conditions in the remaining directions. For both Cu and Al FCC single crystals, the dimensions of the simulation cells were chosen as $L_x=60\sqrt{2}a$, $L_y=60a$, and $L_z=4\sqrt{2}a$, where a is the lattice constant (a=3.615 Å for Cu and 4.05 Å for Al) of the materials. Approximately 120,000 atoms were used in each simulation. The thickness of the simulation cells

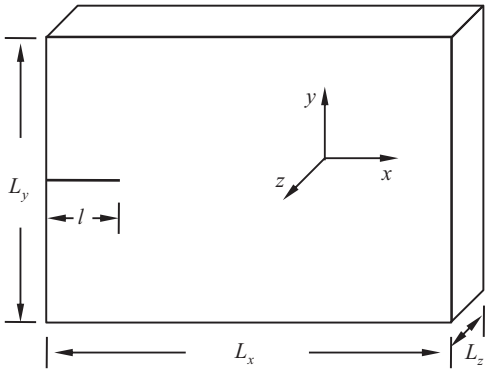

Fig. 1. Geometry of simulated system of a single crystal with edge crack. The crack plane is on the y plane ((100)plane) and the crack front is along the z direction ([011]direction).