MOLECULAR DYNAMICS SIMULATION OF CRACK-TIP PROCESSES IN COPPER*

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ABSTRACT: The crack tip processes in copper under mode II loading have been simulated by a molecular dynamics method. The nucleation, emission, dislocation free zone (DFZ) and pile-up of the dislocations are analyzed by using a suitable atom lattice configuration and Finnis & Sinclair potential. The simulated results show that the dislocation emitted always exhibits a dissociated fashion. The stress intensity factor for dislocation nucleation, DFZ and dissociated width of partial dislocations are strongly dependent on the loading rate. The stress distributions are in agreement with the elasticity solution before the dislocation emission, but are not in agreement after the emission. The dislocation can move at subsonic wave speed (less than the shear wave speed) or at transonic speed (greater than the shear wave speed but less than the longitudinal wave speed), but at the longitudinal wave speed the atom lattice breaks down.

KEY WORDS: molecular dynamics, crack tip, dislocation, loading rate

I. INTRODUCTION

In the study of fracture of crystal solids, the dislocation nucleation from the crack tip remains an important problem requiring further insight[1-4]. Rice and Thomson[2] used linear elasticity to establish the criterion of nucleation of a discrete dislocation and the transition of ductile and brittle fracture. More recently, Rice[3] used Peierls concept to reanalyze the dislocation nucleation from a crack tip and proposed a new solid state parameter $\gamma_{us}$, the unstable stacking energy, to evaluate the critical external loading which corresponds to the dislocation nucleation. The above analysis was unsatisfactory because of its use of the continuum elasticity for crack tip stress field. When a dislocation is very near the crack tip where the nonlinear and atomic lattice effects are great, the atomic force law needs to be considered.

Using the Embedded-Atom Method (EAM)[5], Baskes, Daw and Foiles[6] investigated the dislocation mobility in nickel. Tan and Yang[7,8] used EAM to calculate the nucleation and emission of dislocations at and near crack tip. Cheung, Argon and Yip[9] also used EAM to analyze the dislocation nucleation from crack tips in $\alpha$-iron.

Here we use the "N-body" potential proposed by Finnis and Sinclair[10] and constructed by Ackland, Tichy, Vitek and Finnis[11] to simulate the crack tip processes in the ground...
II. CALCULATION PROCEDURE

1. Interatomic potential

The interatomic potential used here is the "N-body" potential proposed by Finnis and Sinclair. The equation they used is

$$E_{\text{tot}} = -\sum_i \rho_i^{1/2} + \frac{1}{2} \sum_i \sum_{i \neq j} V_{ij}$$

(1)

$\rho_i$ is the second moment of the density of states, and

$$\rho_i = \sum_{j(i \neq j)} \Phi_{ij}$$

(2)

$V_{ij}$ and $\Phi_{ij}$ are functions depending only on the interatomic distance, and can be obtained by assuming some function forms and then fitting with the experimental data.

2. Method of solution

The mode II isotropic elastic displacement field is used to prescribe the displacement of the border discrete atoms. The loading rate $K_{II}$ is used as the loading control parameter. The inner atoms follow the law of Newton

$$F_i = -\frac{\partial U_{\text{tot}}}{\partial r_i} = m_i \cdot a_i$$

(3)

In the present paper, the Leapfrog Algorithm is used, which provides an update formulation. The time step in the present calculation is taken to be $1.18 \times 10^{-14}$ s.

The atomic level stress associated with an atom is calculated by using the potential of Finnis and Sinclair

$$\sigma_{\alpha\beta} = \frac{1}{2\Omega_i} \left[ \sum_j \phi^{'}(r_{ij}) - \rho_i^{-1/2} \sum_j \Phi^{'}(r_{ij}) \right] \frac{r_{ij}^\alpha r_{ij}^\beta}{r_{ij}}$$

(4)

3. The atom lattice geometry

The \{110\}, \{111\} and \{112\} crystallographic planes of the parallelepiped with a slit are used in the present calculations. The $x$, $y$ and $z$ axes of the coordinate system are selected to be along \{110\}, \{112\} and \{111\} directions, respectively. In FCC crystal, dislocation moves in \{110\} direction on \{111\} plane. So, in the present model as shown in Fig.1, crack plane is taken to be \{111\} plane, crack front is along \{112\} direction. Under mode II loading, the dislocations shall move along \{110\} direction. The periodicity along \{111\} is 3 layers, along \{110\} is 2 layers and along \{112\} is 6 layers. Since a long extension in slip direction is particularly important, here the \{110\} slip direction is made as extensive as is feasible in the computation.

A full dislocation in copper will be dissociated into two partial dislocations, between the two partial dislocations, there is a faulted plane. As for the periodicity condition is used along \{112\} direction, the nucleation and motion of partial dislocations can be described with the present lattice configuration.