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Mechanism of crack healing at room temperature revealed by atomistic simulations

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ABSTRACT

Three dimensional molecular dynamics (MD) simulations are systematically carried out to reveal the mechanism of the crack healing at room temperature, in terms of the dislocation shielding and the atomic diffusion to control the crack closure, in a copper (Cu) plate suffering from a shear loading. The results show that the process of the crack healing is actualized through the dislocation emission at a crack tip accompanied with intrinsic stacking faults ribbon forming in the crack tip wake, the dislocation slipping in the matrix and the dislocation annihilation in the free surface. Dislocation included stress compressing the crack tip is examined from the MD simulations and the analytical models, and then the crack closes rapidly due to the assistance of the atomic diffusion induced by the thermal activation when the crack opening displacement is less than a threshold value. This phenomenon is very different from the previous results for the crack propagation under the external load applied because of the crack healing (advancing) largely dependent on the crystallographic orientations of crack and the directions of external loading. Furthermore, based on the energy characteristic and considering the crack size effect, a theoretical model is established to predict the relationships between the crack size and the shear stress which qualitatively agree well with that obtained in the MD simulations.

1. Introduction

Over the past few decades, nanocrystalline materials have been commonly used in various fields due to their outstanding mechanical and physical properties [1–6]. In most cases, nanocrystalline materials have superior strength, strong hardness and good wear resistance. Nevertheless, new failure modes are demonstrated for nanocrystalline materials due to their low tensile ductility and fracture toughness, limiting considerably the practical utility. At the same time, there are several examples of nanocrystalline materials with grain sizes below 100 nm failing before a significant plastic deformation occurs [7,8]. In order to further understanding the damage mechanism for nanocrystalline materials, considerable work has been investigated on this topic of intensive research for several decades [9–12].

Crack nucleation and propagation are driven due to various reasons, such as external loads [13], heat loads [14], and hydrogen effects [15,16]. For example, the three dimensional edge cracks in a single crystal Fe have been investigated under the loading of modes I, II and III considering different thicknesses and crystallographic orientations, showing the types of crack propagation dependence on loading mode and crystallographic orientation [17]. Crack evolution caused by hydrogen embrittlement is proposed using MD simulations, and the hydrogen accumulation around a crack tip suppresses the crack tip dislocation emission or absorption, preventing the crack tip blunting and the ductile fracture [18]. In fact, the fundamental reasons of fractures are due to the elastic interactions of cracks and dislocations undergoing a variety of stress fields which play an important role in the crack growth in a wide variety of engineering materials. Accordingly, a number of characteristic features of crack growth behaviors have been investigated using discrete dislocation (DD) modeling [19,20], MD simulations [21], experimental methods [22], and theoretical models [23].

Based on the above mentioned work, the relationships of cracks and dislocations are conducive to understand the crack closure for designing and predicting microstructure to improve damage tolerance. Early much work focuses on the crack healing caused by the heating in ceramics [24,25], polymers [26,27] and metal materials [28], because the heating reduces the atomic diffusion activation

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energy which in turn makes crack close through the volume diffusion or through the dislocation diffusion. Crack also can be healed through oxidation reaction which forms oxide film to prevent surface oxidation and fill of crack space with an oxidation product [29,30]. Recently, a new crack healing mechanism owning to disclination induced crack closure is observed by MD simulations [31]. Previous extensive literature largely concerns with the mechanisms for crack nucleation and expansion, while the great mass of past references have less work involving how to suppress fracture or repair crack for nanocrystalline materials. This case, that we cannot clearly grasp insight into the microscopic mechanism for crack healing, is extremely unfavorable to the development of nanocrystalline materials with self-healing ability. Hence, understanding how to eliminate crack or reduce crack size is of great scientific and technological interest as well as significant economic impact.

Building on previous studies above, this paper is aimed at revealing the mechanism of the crack healing in the Cu plate subjected to the shear loading, and it presents that the crack closure can be realized through the dislocation mechanism coordinating with the atom diffusion mechanism. A theoretical model which qualitatively agrees well with our MD simulation results is developed to explain the crack healing. Furthermore, the obtained model not only has been investigated the shear stress effect on the crack healing, but also provides the useful way to further enhance the sustainability and safety and lifetime of nanocrystalline materials. The paper is organized as follows. In Section 2, MD simulation method which has been proved a powerful approach to study the crack evolution is introduced briefly. In Section 3, we examine the crack healing at different inclined angles through analyzing crystal structure, stress, atomic displacement and atom number when the Cu plate experiences the shear stress. In Section 4, considering various crack sizes and shear stresses, we present a theoretical model and use it to calculate a change of elastic energy. Finally, in Section 5 we give a brief summary drawn from the present work.

2. Simulation methods

MD simulations are conducted at room temperature 300 K in a single crystal Cu plate containing a central nanocrack, as shown in Fig. 1. The orientations of the Cu plate are x-[1 1 0], y-[−1 1 0] and z-[0 0 1], which allow for dislocation emission from the crack tip. The shear stress σ is added to obtain the shear deformation of the Cu plate, and the reverse torque q is added to prevent its rotation. The sizes of the Cu plate are $6a \times 100a \times 120a$ ($L_x \times L_y \times L_z$) in where a = 3.61 Å is the lattice constant of a single crystal Cu. The sizes of crack by removing the corresponding atoms in the center of the Cu plate are $6a \times 25a \times 2a$ ($c_x \times c_y \times c_z$). There exist no interplaying forces between the atoms of the crack upper and lower surfaces, because the crack height $2a$ is larger than the potential cut-off distance 4.4 Å [32]. It should be noted that the crack is thermally stable at room temperature after an equilibration for the sufficient time without the external shear loading. Up to about 577,000 atoms are contained in the MD simulations. The periodic boundary conditions are applied in the x-direction and the free surfaces are used in the y- and z-directions. An embedded-atom method (EAM) potential [33] which has been proven to reliably describe the physical and mechanical properties of Cu materials [11] is chosen in the present MD simulations using LAMMPS code [34].

Prior to the plastic deformation, the Cu plate is first relaxed to their equilibrium configurations by the following procedure: The atoms are firstly relaxed to their minimum energy configurations. Then the plate is heated up to room temperature 300 K by the

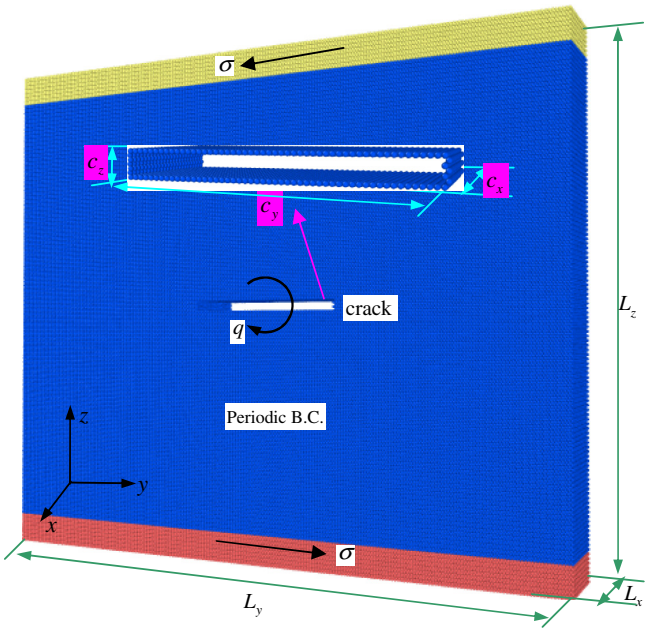

Fig. 1. MD simulation model of a Cu plate with a nanoscale crack at room temperature. Both the upper and lower boxes are setted the shear stress, and the plate applied the reverse torque.

dynamic MD simulation using the Nose–Hoover thermostat for 100 ps in the isothermal–isobaric NPT (constant number of atoms (N), constant pressure (P) and constant temperature (T)) ensemble. The atoms in the upper and lower slabs along the z direction are fixed in their perfect lattice positions to impose the inter-atomic forces on the neighboring dynamic atoms. During the plastic deformation, the shear loading is applied with an acceptable constant strain rate 1.0×10^9 s^{-1}. To minimize the stress fluctuations due to the incremental displacement, the atoms in the interior of the Cu plate are displaced such that the displacement fields vary linearly with a distance between the loading layers. The simulation results are visualized by OVITO [35] during the shear deformation. Three types of the atoms are colored according to the common neighbor analysis (CNA) values: red for atoms in stacking faults, green for atoms in face-centered cubic (FCC) atoms, and blue for atoms in the free surface or the dislocation cores [36].

3. Results and discussion

As a typical metal material, Cu is expected to test the physical and mechanical properties, such as elastic constant, melting point, lattice constant, thermal expansion and fracture strength at room temperature [2,6]. The fracture behavior for Cu has been extensively studied, while little work has focused on the crack healing, suggesting some unintelligible mechanisms for understanding the fracture and restoration behaviors. Indeed, the results of the subsequent MD simulations for the crack healing reveal that the dislocation shielding effect takes place around the crack tip, and then leads to compressing crack and ultimately driving crack full closure by means of atomic diffusion. In this section, MD simulations for the crack healing are presented including the resultant stress, potential energy, atomic number and atom displacement.

3.1. Horizontal crack closure

Fig. 2 and Movie S1 (see Supplementary material) show MD simulations of the crack closure when the Cu plate is subjected to the external shear stress. The elastic deformation only occurs