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Multiscale simulations on the reversible plasticity of Al (001) surface under a nano-sized indenter

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ABSTRACT

The incipient plasticity of Al (001) surface under a small cylindrical indenter is studied by using multiscale simulations. Results show that both reversible and irreversible plasticity occurs under the indenter. During the reversible stage, only a thin deformation twin is formed, and the plastically deformed surface will completely recover to undistorted state upon withdrawal of the indenter, otherwise, both a deformation twin and a few stacking fault ribbons are observed, and a permanent residual trace will remain on the surface, as a sign of the irreversible plasticity. Our findings suggest that the effects of some internal and external material parameters, such as indentation depth, lattice frictional force, and stacking fault energy, on the incipient surface plasticity are very important in some small contact issues. The contact force and pressure under the indenter are also analyzed. Results imply that the theoretical prediction of the critical force is suitable for estimating the beginning of reversible plastic deformation, not the onset of the irreversible plasticity.

1. Introduction

As the sizes of devices in electromechanical systems shrink to micro- and nano-scales, small mechanical contacts become significant for the performance of those tiny equipments [1]. Understanding the deformation mechanisms of surface atoms in the contact area is important to develop such systems. One of the main concerns about the mechanical behavior of material surfaces is the incipient plasticity, which is commonly studied by using nanoindentation tests [2,3]. Usually, the onset of surface plasticity is indicated by the appearance of the first pop-in [4,5] or abrupt drop [6–8] phenomenon in a F–δ curve, where F and δ represent contact force and indentation depth respectively. It is suggested that the discontinuity of contact force results from a few initial dislocation nucleation events under the indenter. However, recent experimental [9] and simulation [10] results imply that the contact force is not a reliable indicator of the beginning of the surface plasticity, when the indenter size is in the experimental range. They argue that discrete dislocation activities can precede the first dramatic force discontinuity, and the discontinuity events in a F–δ curve may correspond to much more profuse dislocation bursts that occur much later in a plastic stage. However, this controversial issue is still not well addressed.

Besides the indicator of the incipient surface plasticity, reversible plastic deformation of surface atoms is another intriguing issue. For an Au specimen with stepped surfaces, an intermediate state is identified, in which the F–δ curve departs from a theoretical prediction prior to the appearance of pop-ins [11]. It is suggested that the unique profile of the F–δ curve is associated with the dislocation activity under surface steps, most of which can retract and vanish upon withdrawal of the indenter. Similar reversible phenomena are also observed in nanoindentation simulations on stepped and atomically flat Cu surfaces [12]. A curiosity about reversible surface plasticity is inspired by these findings. Is it possible to learn more details about the self-healing processes of plastically deformed surface atoms?

The above concerns motivated the research described in this paper: Investigating the incipient plasticity of Al (001) surface by using the quasicontinuum (QC) method, which is a static multiscale simulation method [13]. The incipient plasticity of (001) surfaces of face-centered-cubic (FCC) metals has been studied by both experimental measurements [14,15] and molecular dynamics (MD) simulations [16,17]. Accompanying discontinuities in F–δ curves, dislocation loops nucleated by Shockley partial dislocations and stacking fault ribbons are often observed under an indenter. The reason we choose the QC method rather than MD simulations is that the QC simulations can break through the limitation of relatively small spatial sizes [18]. Thanks to this virtue, some nanoindentation simulations on large scales have been performed

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[19–21], since dislocation behavior in very thin films may not represent the situation in bulk. This paper is organized as follows: In Section 2, the basic principle of the QC method is briefly introduced and the details of the computational procedure are presented. In Section 3, the main results of the present work are displayed. Both reversible and irreversible plasticity are observed and identified. Finally, the simulation results are analyzed in Section 4. Our findings provide a further insight into the incipient surface plasticity of FCC metals contacted by small tips.

2. Computational method

2.1. The quasicontinuum method

The QC method, which can describe elastic and plastic deformations occurring on different length scales simultaneously, is a concurrent multi-scale method aiming at studying mechanical behaviors of solid materials. In 1996, the QC method was originally developed by Tadmor et al. [22,23], and then improved by Miller et al. [24,25]. The discrete defects carrying plastic deformation in a QC model are studied explicitly on atomic level, while the majority of the model experiencing elastic deformation is treated as a continuum. A key measure of the displacement field of a deformed body is the deformation gradient tensor $\boldsymbol{F}$ which is defined as follows:

$$\boldsymbol{F} \equiv \frac{\partial \boldsymbol{x}}{\partial \boldsymbol{X}} \equiv \boldsymbol{I} + \frac{\partial \boldsymbol{u}}{\partial \boldsymbol{X}} \tag{1}$$

where $\boldsymbol{X}$ and $\boldsymbol{x}$ describe the original and current states of the body respectively, $\boldsymbol{u} = \boldsymbol{x} - \boldsymbol{X}$ is the displacement field, $\boldsymbol{I}$ is the identity tensor. In the continuum region of the QC model, it is assumed that the deformation gradient changes gradually on the atomic scale. Thus, only the displacements of a small fraction of the atoms need to be treated explicitly, the displacements of other atoms can be approximately obtained through interpolation. Such an approach enables the QC method to model a large system without tracing every atom.

The regions described on atomic and continuum levels can be seamlessly coupled by energy calculation based on empirical interatomic potentials. Within the embedded atom method (EAM) potential function [26], the total energy in the atomistic region can be written as:

$$E_1 = \sum_{a=1} E_a \tag{2}$$

$$E_a = \frac{1}{2}\sum_{b\neq a} \varphi_{ab}(r_{ab}) + F_a(\bar{\rho}_a) \tag{3}$$

where E_{ab} is the energy of atom a, F_a can be interpreted as the embedding energy of atom a, φ_{ab} and r_{ab} are the pair potential and distance between atom a and its neighboring atom b. $\bar{\rho}_a = \sum_{b\neq a}\rho_b(r_{ab})$ is the superposition of electron density contributions from each of the neighbors. In the continuum region, the Cauchy–Born rule [27], which indicates that every atom in a region subject to a uniform deformation gradient will be energetically equivalent, is applied. Consequently, the energy calculation can be approximately expressed as:

$$E_2 = \sum_{c=1} n_c E_c \tag{4}$$

where E_c is the energy of the selected representative atom and takes the same form as formula (3), n_c can be interpreted as the number of atoms represented by atom c. The equilibrium configuration of the overall system can be established through minimization of the total energy $(E_1 + E_2)$ with respect to atomic positions. As the defects proceed, the QC method is able to automatically adjust the distributions of the two different regions. Detailed information about the theory and application of the QC method can be found in the review article written by Miller and Tadmor [28].

Some special traits of the present QC code should be mentioned here. First, the QC simulation is suitable for studying phenomena at low temperature, because thermal effect on the mechanical behavior of a material system is ignored. Second, periodic boundary condition is applied along the out-of-plane direction, i.e. the QC model is quasi-two-dimensional (quasi-2D) and the QC simulation is performed in columnar grain geometry. Some constraints to the overall mechanical behavior of the system might be introduced by the columnar grain structure. However, it is easier to analyze various deformation mechanisms of surface atoms, due to the quasi-2D constraint.

2.2. Model and parameters

The QC model for nanoindentation on Al (001) surface is schematically presented in Fig. 1. The semi-empirical EAM potential developed by Voter and Chen [29] was used to describe the Al single crystal, whose in-plane size was 200 × 100 nm. A cylindrical indenter oriented along the [1 −1 0] out-of-plane direction was placed on the top surface. The local structures of atoms under the indenter were visualized by the software 'Atomeye' [30] combined with the common neighbor analysis method [31]. The interaction between indenter and surface atoms was simulated by an external repulsive potential [32]:

$$\Psi = AH(R-r)(R-r)^3 \tag{5}$$

where A is a force constant, R is the radius of the indenter, and $H(R-r)$ is the step function. In the present simulations, $A = 1.602\ \mu N/nm^2$, and $R = 2.5$ nm. During the indentation processes, the indenter proceeds in displacement-control in the step of 0.02 nm, meanwhile the atoms in the lateral and bottom surfaces were kept fixed. After each loading step, the total energy was minimized until the sum of out-of-balance forces over the entire system is less than 1.602×10^{-3} nN. The maximum indentation depth is 3.38 nm. The contact force applied by an indenter was calculated by using the formula:

$$P = \sum_{i\in Z} P_i \tag{6}$$

where Z represents all atoms belonging to the contact zone and P_i is the out-of-balance force on the ith atom in this zone, projected along the indentation direction. The contact zone was computed after each loading step by only including atoms directly touched by the indenter. According to the applied force P, The contact pressure was determined at each step as: [33]:

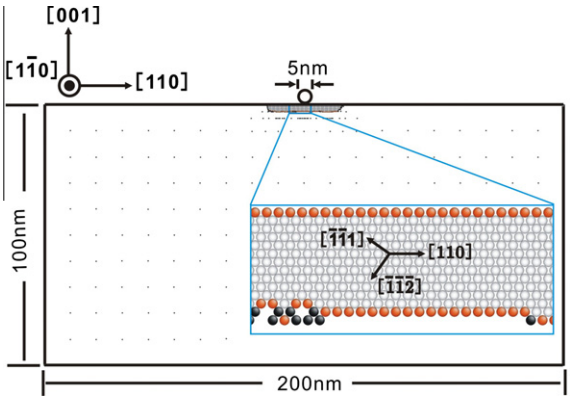

Fig. 1. QC model for nanoindentation on the (001) surface of an Al crystal.