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Identification of the Brownian Motion in Kinematics of the Dislocations for FCC Metals by Atomistic Simulations

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ABSTRACT

In the current context of a number of increasingly more controversial views on the mechanisms of deformation of nanocrystalline materials, it is increasingly recognized that severe plastic deformation of crystalline mediated by the crystalline grains play an important role in obtaining nanocrystalline materials with improved mechanical properties. Molecular dynamics simulations of dislocation motion in crystalline grain boundaries offer new perspectives on the emergence of sources of dislocations in nanocrystalline materials. They are used to describe dislocation motion and acceleration to extreme speeds. Kinematics description of these dislocations helps improving the mechanical properties of materials. This paper presents identification of Brownian motion in the kinematics of dislocations in terms of face-centred-cubic material (FCC) material.

KEYWORDS: severe plastic deformation, nanocrystalline materials, molecular dynamics, dislocations

1. Introduction

Recent surveys have shown that ultra-fine grain materials, which show improved mechanical properties, have drawn attention to the use of large-strain plastic deformation to obtain fine microstructures in metals. Homogeneous formation of these structures were first applied by [Valiev et al.] in the equal-channel angular pressing technique (ECAP) with the grain sizes of nano level.

In nanocrystalline and in ultra-fine grain materials irreversible plastic deformation appears immediately after a recoverable plastic deformation regime and is governed by nucleation and motion of defects in the crystalline lattice. To investigate the mechanisms of deformation less than 50nm scale, researchers have conducted investigations with TEM and HRTEM. In case of ductile copper, the twinning mechanism was discovered [11].

Many material properties (strength, ductility) are directly related to the structure and motion of the dislocation line. It is well known that grain boundaries have an important role on mechanical properties of material resulting in relatively well-known Hall-Petch relationship:

$$\sigma = \sigma_0 + kD^{-\frac{1}{2}}, \qquad (1)$$

where σ is the yield stress σ_0 is the "friction stress" needed to move an individual dislocation during deformation, k is the constant called the Hall-Patch slope and is material dependent, and D is the average size of grain. This relationship is no longer valid for values of smaller grains of 10-30nm.

Investigations on the deformation mechanisms and material properties in nanocrystalline materials with grain size less than 200 nm are based on indirect techniques of analysis, which may reflect the emergence and interaction of defects in the crystalline network. One of these indirect techniques used to achieve a description in terms of atomic dislocations is molecular dynamics modelling technique. This method takes into account a small number of dislocations and refers to specific deformation mechanisms such as cross slip, dislocation cutting process or dislocation from cracks [14].

This paper aims to identify the emergence of Brownian motion in kinematics of dislocations in FCC metals using atomic simulations.

2. Experimental Conditions for Generating the Model

Nanocrystalline materials and ultra-fine grain materials processed by severe plastic deformation have been the subject of intense research over many years. Among the most well known severe plastic deformation methods is the equal channel angular pressing because it has the advantage of producing large samples. Deformation mechanisms leading to emergence of strains are mainly twinning and grain boundary sliding.

3. Creating the Molecular Dynamic Model

Molecular dynamics simulations were used to study atomic-scale processes that occur during plastic deformation in nanocrystalline materials, because no model at this scale can capture the actual state of the deformation mechanism. Simulations suggest that nanocrystalline materials adjust to the external applied forces by grains boundaries slipping and the emission of partial dislocations that run along grains. Molecular dynamics simulations also suggest the fact that grains sliding and partial dislocations emission is due to atomic shuffling and free migration of grain volume [2,3,5,7].

Recent TEM surveys have shown that ductile copper contains irregularly shaped grains with random orientations. Grains size is between 100 nm and 1 mm. To create the model we use copper crystal lattice, which is a face-centred-cubic material (FCC). FCC materials have much larger interstitial spaces, being able to retain other atoms with atomic radius r = 0.146a, where a is the lattice constant.

Based on representations made by [Buehler et al., 2005] we have built our own molecular model shown in Figure 1.

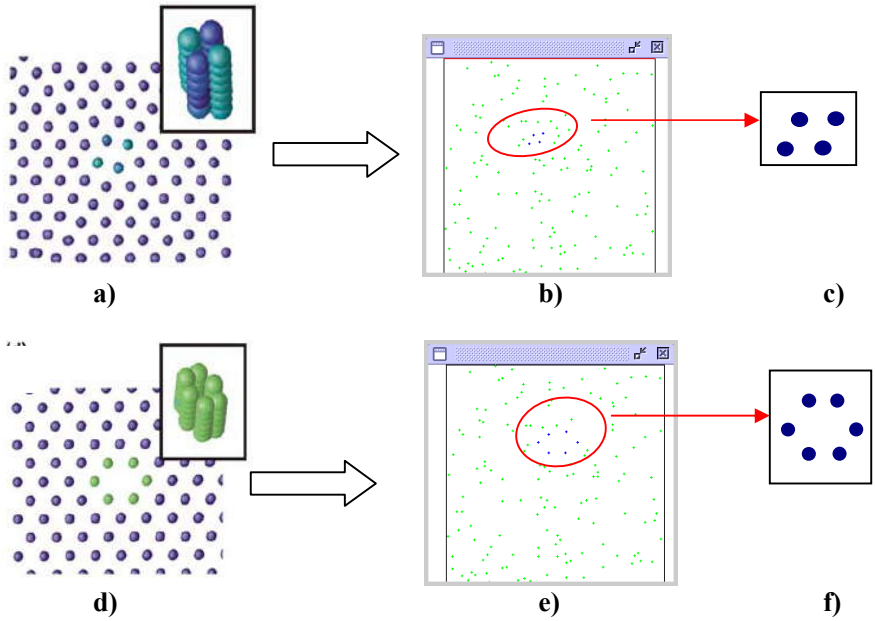

Fig. 1. *Schematic model of two dislocation process: a) trail of partial point defects, d) vacancy tube [Buehler et al., 2005], b) trail of partial point defects, e) vacancy tube, our generated models, c) and f) 2D section through the dimensional elastic field for both cases.*

The model used for molecular dynamics simulations was performed in copper. Simulations used a total of 149 atoms in a square cell of 6.9x6.9 mm with a time step of 0.5-0.6ns with the shear stress τ_{max} = 10.7GPa in the conditions of the diffusion process.

Our MD simulations used periodic boundary conditions with reflecting walls with the temperature between 0.2-2.5º K and the internal pressure between 0.5 and 2 MPa.

During the simulations, once we increase the temperature and the internal pressure is constant, the kinetic energy also increases. When we decrease the pressure and the temperature is constant, the kinetic energy decreases, below the average value. For the second type of dislocation, when we decrease the pressure and the temperature is constant, the kinetic energy does not decrease so much, being still above the average value. The total energy depends both on the temperature and the pressure. When both

parameters increase, the total energy also increases. In both cases, when the temperature was constant and we increased the external pressure, the pressure inside the simulation cell increased significantly. The velocity distribution increased once with the temperature, lost part of its intensity.

4. Brownian Model of Dislocation Motion

Due to the fact that at 50 nm the classic deformation mechanisms are not available any more, researchers as [Van Swygenhoven, 2006] and others have done TEM and HRTEM investigations in order to observe the physical phenomena that determine the plastic deformation. On this scale, sliding between grains boundaries, dislocation density and atomic diffusion in the grain borders are the main components of the deformation mechanisms.

In case of ductile copper, it has been observed the twining mechanism. Deformation twinning is a mechanism that accommodates plastic deformation in copper and is considered to be directly related to the particular nanostructures, which has not been observed in their coarse-grained parts. Plastic deformation of materials appears immediately after an elastic springback state has been governed by the appearance of defects in the crystal lattice.

In order to try to understand better the deformation mechanisms that appear in ultra-fine grain materials with grain size smaller that 50nm, we have tried to identify the Brownian motion in kinematics of the dislocation.

Dislocation motion controlled by kink processes can be treated as a Brownian motion of a linear extended object. We assume that a dislocation is made up of unit elements and the length of each element is equal to the lattice period along the Peierls barrier. The position of a n-th element from the dislocation can be determined by an integer number J(n), which describes the unit element, and by h, the Peierls area period. Further, we know that:

a) Each area can pass through three states: I (n) = J (n +1)-J) n) = 1 (node positive), 0 (no node) or 1 (node negative).

b) The interaction energies between nodes can be neglected.

From the assumed issues above, there are only 3 elementary states for dislocation movement: R_m (migration), R_f (pair of nodes formation) and R_a (pair of nodes annihilation) (Fig. 3). Each state for a different area is self independent so the probability that an area has a node can be expressed as:

$$p = \frac{2x}{1+2x}, \quad x = \exp^{-\frac{F}{kBt}}, \qquad (2)$$

where F is the free energy necessary for the formation of a pair of nodes, k is the Boltzmann constant, t, period of time.

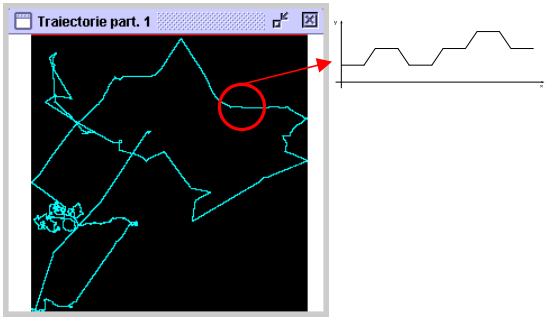

Fig. 2. *Trajectories for the partial point defects for one atom of the trail and the kink model of the dislocation lattice*

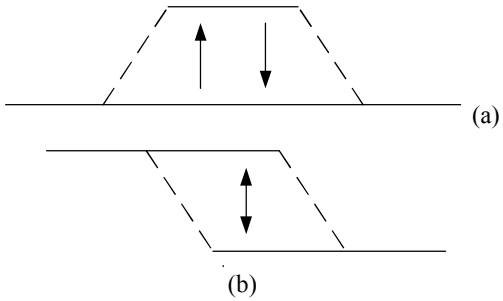

Fig. 3. *The elementary states for the dislocation movement: a) migration and pair of nodes formation, (b) pair of nodes annihilation*

Brownian motion is the apparently random movement of particles from a metal, a move which is due to forces exerted by collision with much smaller molecules. As the temperature is higher the more the molecules move faster and hit with much more difficulty anything they meet. As can be seen in fig. 2, during simulations copper particles had a random motion, passing quickly from one state to another, due to thermal activation.

5. Conclusions

We performed a molecular dynamics simulation to study the kinematics of dislocations in a 2D model that mimics crystalline copper network, under a simple shear. The kink model can be applied for the covalent crystals, in which the structure of the chemical bonds is essential in order to specify a state for a dislocation lattice. During the diffusion process, the value of the n element changes randomly in time and it is difficult to identify a certain state of the dislocation lattice.

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