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Plastic Deformation Nucleation in Elastically Loaded CuNi Alloy during Nanoindentation

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Abstract. The molecular dynamics simulation of the behavior of elastically loaded CuNi alloy at nanoindentation is carried out. It is shown that the stoichiometric composition and the preliminary elastic deformation influence characteristics of the nucleation of plastic deformation. Under tension of specimens with a low concentration of nickel, the nucleation of plastic deformation is determined by the formation of stacking faults. The formation of nanotwins makes a significant contribution to the nucleation of plasticity at high concentrations of nickel. The increase of the degree of preliminary elastic deformation of the crystallites leads to a decrease in the depth of indentation at which structural defects start to form.

INTRODUCTION

Nowadays the production of different micro- and nanoelectromechanical systems is being actively developed. Many components of such systems while in operation are in mechanical contact with each other. Understanding of the mechanisms of their interaction on the atomic scale is important for the improvement of mechanical properties of available systems and for the development of new ones. Research of properties and the behavior of nanosized objects requires reliable and precise techniques. One of the most efficient and widely used methods for studying mechanical properties of nanostructured materials and thin films is nanoindentation [1–3]. The method is based on local loading of the material and simultaneous recording of its deformation response. Along with experimental research, computer simulation of the behavior of the materials during nanoindentation has been actively developed in the last decades [4–7]. One of the significant advantages of computer simulation is the possibility of a real time research of atomic structures and special features of microscale processes in materials [8–12]. It should be noted that prior to indentation, the specimens are in equilibrium state. Deviations from the equilibrium state, which can be caused by various external influences, including mechanical deformation, will change the response of the material during indentation. In the context of the foregoing, the objective of the present work is to study features of the nucleation and development of plastic deformation in previously elastically deformed CuNi crystallites during nanoindentation.

MATERIALS AND METHODS

The simulation was performed for fcc CuNi crystallites having a parallelepiped shape and containing approximately 50 000 atoms. The nickel concentration varied from 0 to 100%. Edges of the crystallite were oriented along directions $[1\bar{1}0]$, $[110]$ and $[001]$. Surfaces (110) were set free. Two atomic layers of the face opposite to loaded surface (110) were forbidden to move along the direction of indentation. Periodic boundary conditions were used in other directions. The initial temperature was set to 300 K.
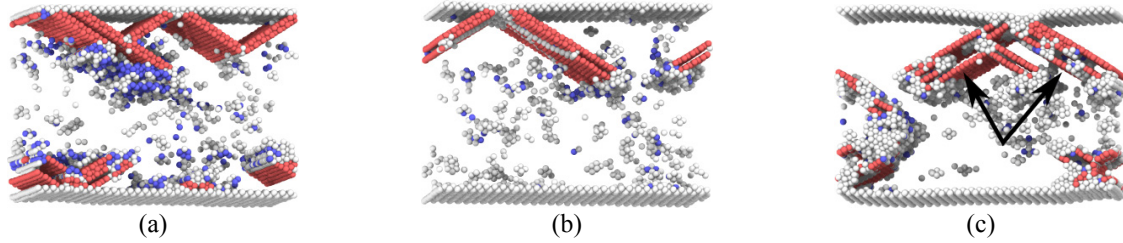
FIGURE 1. Structure of the simulated crystallites with the concentration of nickel 0 (a), 50 (b), and 100% (c) deformed at 8.36, 9.65, and 11.61%, correspondingly. Atoms with the hcp, bcc, and unknown local symmetry are marked in red, blue and grey colors, correspondingly. Atoms with the fcc local symmetry are not shown. Twins are indicated by arrows

Uniaxial tension was carried out along direction [001]. The tension rate was equal to 3.5 m/s. The perfectly rigid indenter had a shape of a half-cylinder. It consisted of copper atoms arranged in the fcc lattice. The rate of indentation was equal to 5 m/s.

The many-body potential in the approximation of the embedded atom method was used to describe interatomic interactions in the simulated specimens [13]. Calculations were performed using the LAMMPS package [14]. Identification of structural defects was conducted by common neighbor analysis [15]. Indentation depth was calculated as the difference between the average position of the unloaded surface and the coordinate of the tip of the indenter. Note that interaction between the indenter and the crystallite starts before its penetration, which corresponds to negative values of the penetration depth.

RESULTS AND DISCUSSION

Uniaxial Tension

The simulation shows that plastic deformation under uniaxial tension of crystallites begins to nucleate at the free surface. The specific region of the plasticity nucleation on the free surface is determined by stochastic temperature fluctuations of atoms. It is found that the character of nucleation of plastic deformation depends on the stoichiometric composition. Therefore, extrinsic and intrinsic stacking faults are formed at the nucleation of plastic deformation in the crystallites with small concentrations of nickel (Figs. 1a, 1b). The twinning mechanism starts to make a sufficient contribution to plasticity at high concentrations of nickel (Fig. 1c).

The state of the simulated system can be characterized by a change in potential energy [16, 17]. It is seen in Fig. 2a that potential energy initially increases monotonically. The simulated crystallite has a fcc lattice on this strain interval. When strain reaches some threshold value, potential energy of the crystallite decreases abruptly. The analysis of the structure shows that the potential energy decrease is connected with the generation of structural defects in the simulated crystallite. Their generation and evolution was the way of elastic stress relaxation of the loaded lattice.

Threshold values of strain for pure copper and nickel are significantly different. Since CuNi alloy is a solid solution, it can be expected that the threshold strain will change in proportion to the concentration of elements. Indeed, it is clearly seen in Fig. 2b that the threshold strain is almost linearly dependent on the concentration of the second element.
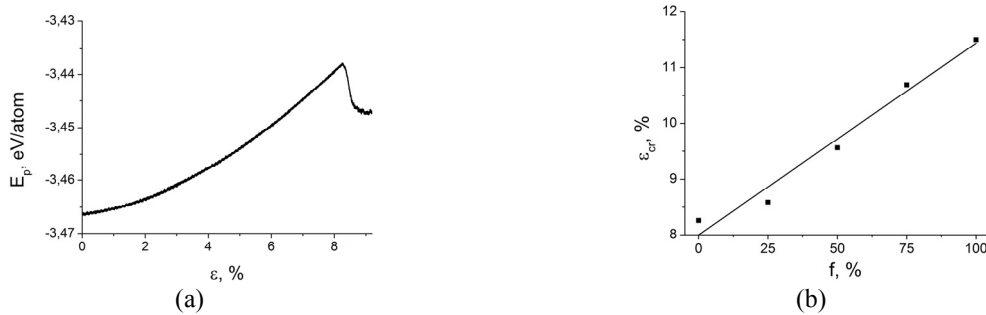
FIGURE 2. Dependence of potential energy per atom on strain for pure copper (a).
Threshold strain versus nickel concentration (b)
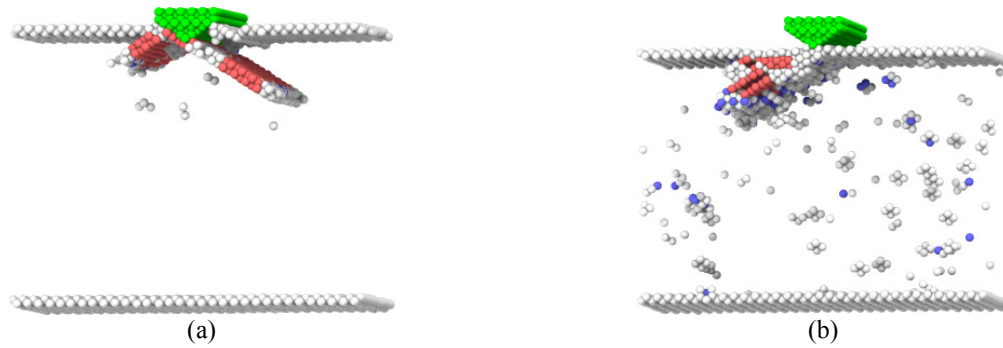
FIGURE 3. Structure of the simulated crystallites of pure copper during nanoindentation with different value of pre-tension: 0 (a) and 7% (b). The depth of the indenter penetration is 3.77 and 2.24 Å, respectively. Red, blue and grey colors mark atoms with the hcp, bcc and uncertain local symmetry of neighbors, respectively. The indenter is marked in green color. Atoms with the local fcc symmetry are not shown
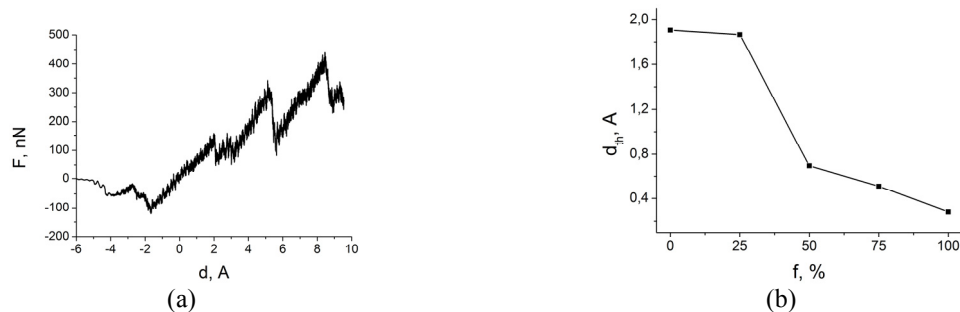
Nanoindentation

Nanoindention was conducted for elastically stretched crystallites. Based on the obtained threshold strain, four values are chosen for each concentration of nickel, including zero and close to the threshold. The simulations show that the degree of pre-tension and the concentration of the second element (nickel) affect the characteristics of the nucleation of plastic deformation in the crystallite during nanoindentation.

The simulation results show that the threshold value of indentation, at which plastic deformation begins to nucleate, decreases with increasing elastic pre-tension of copper specimens. This behavior during nanoindentation is also characteristic for CuNi alloys and pure nickel. As in the case of uniaxial tension, stacking faults are formed in the indented crystallites. It should be noted that at small values of elastic pre-tension the defect nucleation occurs in the region where the indenter contacts the crystallite (Fig. 3a). However, in the case of elastic pre-tension close to the threshold value the region of the defect nucleation is shifted (Fig. 3b). This may be due to the so called "jump to contact" effect: the attraction of surface atoms to the indenter initially appears as it approaches the specimen. The attraction of the contact zone to the indenter results in distortion of a neighboring region and leads to the appearance of excess stresses. As a result, structural defects begin to nucleate in the distorted region. In this case, the formed defect structure is more complex than for small elastic pre-tension.

The dynamics of the defect structure is well correlated with features of changes of the reaction force acting on the indenter versus the penetration depth. As an example, the dependence of the reaction force on the indenter penetration depth for the crystallite containing 75% nickel without pre-tension is shown in Fig. 4a. The surface of the crystallite is attracted to the indenter to the depth of indentation approximately –4 Å, and structural defects are not generated in the simulated specimen. Upon further indentation, the local symmetry of some atoms begins to change and however the crystallite restores its initial fcc symmetry at the indentation depth –1.5 Å. At this depth, the curve of the reaction force has a minimum. Dislocation loops begin to form in the specimen at the indentation depth of 0.5 Å. As it has been shown for uniaxial tension, this is the way of relaxation of the specimen. This event is reflected in the decreasing slope of the curve in Fig. 4a. In general, for any stoichiometric composition and degree of elastic pre-tension, each act of generation of structural defects leads to the appearance of special features of dependences of the reaction force on the indentation depth in the form of breaks or bursts.

The calculations show that, in contrast to uniaxial tension, in the nanoindentation of crystallites containing over 50% nickel with small elastic pre-tension twins are not formed at a small indentation depth. Only partial dislocations and stacking faults are nucleated in this case. Note that the twinning structure begins to generate at sufficiently large values of the indentation depth.

It is found that in the case of small elastic pre-tension, an increase in the concentration of nickel leads to a decrease in the threshold value of the indentation depth (Fig. 4b). The change in the nickel concentration also leads to the appearance of singularities in the dependence of the reaction force on the depth of indentation corresponding to the nucleation of dislocation loops. So for pure copper and crystallites with a nickel concentration of up to 50% the nucleation of plastic deformation leads to an abrupt decrease in the magnitude of the reaction force. For crystallites with the nickel concentration more than 50%, the nucleation of plastic deformation leads to the appearance of a break in the curve of the reaction force (Fig. 4a at the indentation depth of 0.5 Å).

FIGURE 4. Dependence of the reaction force on the indentation depth for the crystallite with 75% nickel (a). Dependence of the threshold indentation depth on the concentration of nickel (b). Crystallites without pre-tension

SUMMARY

Molecular dynamics simulation of the behavior of elastically deformed CuNi alloys under nanoindentation showed that the degree of elastic pre-tension and the stoichiometric composition have a significant influence on the nucleation of plastic deformation. So the increase in the elastic pre-tension of the crystallite decreases the threshold indentation depth at which structural defects begin to generate in the material. The nucleation of structural defects during nanoindentation is shifted away from the contact zone for large values of elastic pre-tension of the material. The increase of the nickel concentration in the alloy reduces the threshold value of the indentation depth.

ACKNOWLEDGMENTS

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