Plastic deformation nucleation in BCC crystallites under nanoindentation

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Citation: AIP Conference Proceedings **1683**, 020109 (2015); doi: 10.1063/1.4932799

View online: http://dx.doi.org/10.1063/1.4932799

View Table of Contents: http://aip.scitation.org/toc/apc/1683/1

Published by the American Institute of Physics

Plastic Deformation Nucleation in BCC Crystallites under Nanoindentation

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Abstract. Molecular dynamics investigation of metal crystallite with bcc lattice under nanoindentation was carried out. Potentials of interatomic interactions were calculated on the base of the approximation of the Finnis-Sinclair method. For clarity and simpler indentation data interpretation, an extended cylindrical indenter was used in the investigation. The features of the bcc iron structural response at nanoindentation of surfaces with different crystallographic orientations were revealed. Generation of structural defects in the contact zone always resulted in the decrease in the rate of growth of the reaction force.

INTRODUCTION

Micromechanical devices used in electronics incorporate small-sized components, which call for special-purpose methods for examination of their physical and mechanical parameters. It is common knowledge that the behavior exhibited by the solid on the macro- and mesoscale structural levels cannot be extrapolated to the nanostructural scale level. Nanoindentation incorporates a wide range of technical facilities for investigating the physical and mechanical properties of solids in the near-surface layers [1]. Therefore, this is an effective tool for examination of material strength properties on the nanostructural level. Due to the rapid development of computer engineering, computer simulation enjoys wide use alongside experimental approaches by addressing problems pertaining to material properties investigations on the micro-scale level.

Of particular interest are calculations performed in the frame of molecular dynamics [2–4]. This method affords detailed information on the dynamics of structural changes and on the stress fields in the atomic system of studied material [5]. A series of investigations were carried on using molecular dynamics method; the response to nanoindentation in metals having fcc lattice has been studied in sufficient detail [6–9]. To address the behavior of studied metals, many-particle interatomic interaction potentials were constructed. Metals having bcc lattice are insufficiently studied by numerical techniques. Therefore, the goal of the given study is investigation of metal response to nanoindentation. The study was made using metals having ideal bcc lattice with different loading surfaces.

The problem was addressed in the frame of molecular dynamics approach. The study was made for a bcc iron crystallite. The description of interatomic interaction was made using many-particle potential calculated on the base of Finnis-Sinclair approximation [10]. We have decided upon this kind of potential, since this permitted an accurate

Advanced Materials with Hierarchical Structure for New Technologies and Reliable Structures
AIP Conf. Proc. 1683, 020109-1–020109-4; doi: 10.1063/1.4932799

description of elastic characteristics, energy of formation and migration of point defects, lattice parameters, etc. [11, 12].

It should be noted that the results of simulation essentially depend on the crystallographic orientation of the studied crystallite as well as on the indenter shape, loading and boundary conditions, etc. [13, 14]. Indenters of spherical or pyramidal shape are in wide use in both numerical and natural experiments. However, such indenters will form a quasi-point contact area in the tested crystallite [9, 15]. The analysis of deformation origination and development for such a zone is problematic enough. In case of cylindrical indenter is used, the structural changes in the tested crystallite are amenable to examination. In deciding on this particular shape of indenter, we were guided by the following considerations: the indenter/specimen contact area is extended linearly from one side of the crystallite to the opposite side.

The origination and development of plastic deformation in the loaded specimen caused structural changes in its crystal lattice, which were identified on the base of analysis of relative atomic displacements. The magnitude of atomic displacements was assessed using reduced displacement vector [6].

LOADING CONDITIONS FOR SIMULATED CRYSTALLITES

The simulation was performed for crystallites having parallelepiped shape (Fig. 1). The simulated specimens had dimensions ~160 Å. Cylindrical indenter was constructed with iron atoms fixed in lattice sites. The loaded specimen face was a free surface, while for several atomic layers of the opposite crystallite side it was forbidden to shift in the direction of indentation. Other crystallite sides were simulated as free surfaces. In different calculations loading was performed along the [100], [110] and [111] crystallographic directions (axis *Z* in Fig. 1).

The indenter moved at a constant velocity of 5 m/s. The kinetic temperature of the specimens was 300 K. The molecular dynamics was simulated for short time intervals; indenter penetration occurred at a high rate; the specimen had ambient temperature—these factors taken together suggest that diffusion processes produce no appreciable effect on the structural response of the simulated specimen.

DISCUSSION OF COMPUTATION RESULTS

The specimen reaction force as a function of penetration depth in the case of loading (100) surface is presented in Fig. 2a. The elastic response of the crystallite corresponds to the linear portion of the curve. At reaching the indentation depth of 4.6 Å the dislocation arises in contact zone and then it moves toward the free surface. Dislocation path of movement can be traced by the atoms whose reduced slip vector is more than 20% in Figs. 2b and 2c. Resize of computational cell here and in following figures is connected with the movement of the indenter. The nucleation of plastic deformation can be also defined by a sharp decrease in the reaction force.

At the indentation depth of 5.6 Å the dislocation emerges at a free surface forming a step on it. After this the reaction force starts to grow. At the indentation depth of 8.7 Å another dislocation is formed in the contact zone which leads to a decrease of the slope of the curve in Fig. 2a. Next significant slope reduction of the reaction force curve occurs at the indentation depth of 10.5 Å which is associated with the formation of new dislocation. Dislocations in the process of their movement to the free surface could change their direction of motion.

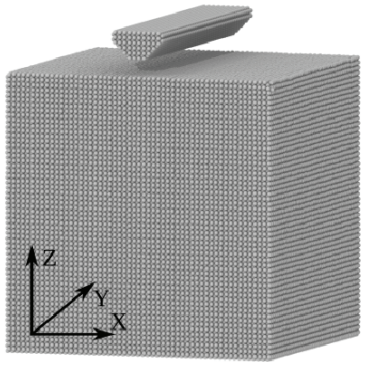
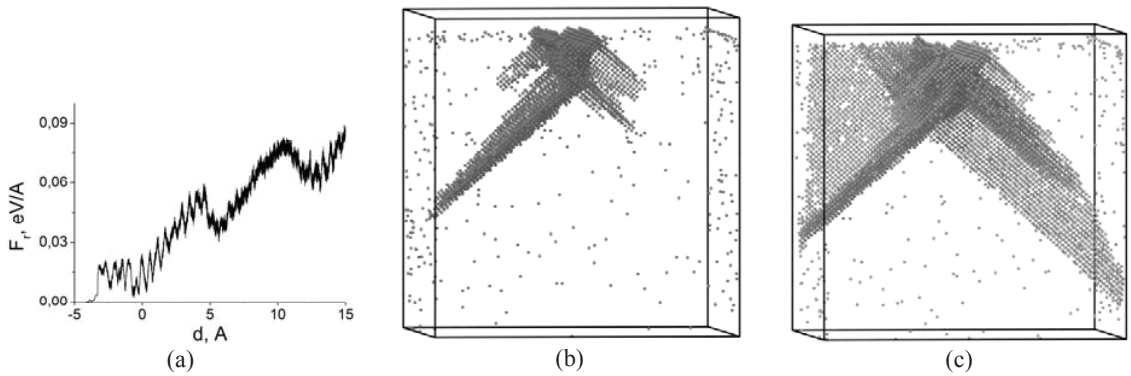


FIGURE 1. Simulated specimen



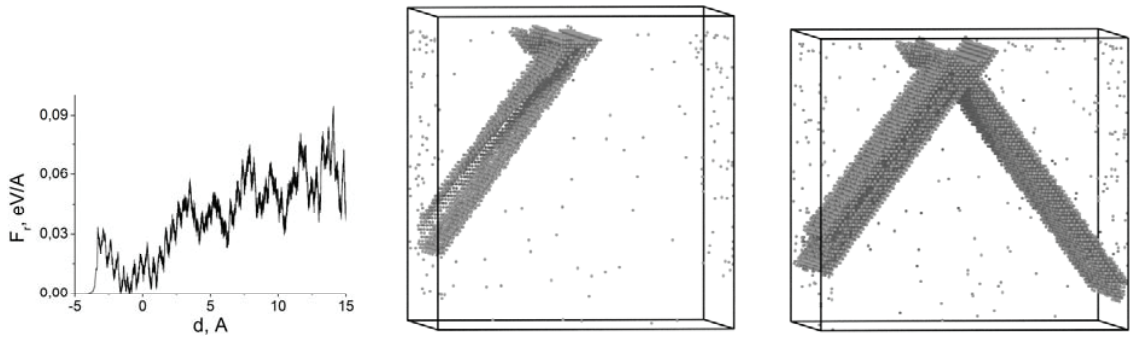
(a) (b) (c)

FIGURE 2. Loaded surface orientation is (100). The dependence of the reaction force vs the indentation depth (a). The structure of the simulated specimen at various indentation depths: 5.5 (b), 9.5 Å (c). Only atoms with the value of a reduced slip vector more than 20% are shown

The interval of the elastic region is much less in the case of loading the (110) surface than for (100) surface. The first dislocation is generated at the indentation depth of 0.5 Å and then it moves to the free surface. Further, the reaction force increases almost linearly upto the indentation depth of 3.4 Å (Fig. 3a). At this depth another dislocation is formed in the specimen (Fig. 3b). Each subsequent reduction of the slope of the reaction force curve is also associated with the generation of dislocations in the indenter-specimen contact region.

Note that during indentation of the surface (110) the dislocations are formed much more frequently than in the case of the (100) surface. Besides, the dislocations do not change the direction of their motion. In Fig. 3c it is possible to trace the trajectory of several dislocations in the specimen.

During indentation of the surface (111) the first dislocation is formed at the indentation depth of 0.3 Å. Subsequent linear interval of reaction force curve in Fig. 4a ends at the indentation depth of 4.0 Å. At that the accommodation is due to the extrusion of the surface layer in the contact zone (Fig. 4b). This process ends at the indentation depth of 4.6 Å. Further until the indentation depth of 6.6 Å no significant structural changes in the specimen occur. The subsequent decrease in the slope of the reaction force curve is associated with the dislocation formation and its movement towards the free surface. Unlike the previously discussed cases an area in the contact zone is formed where the atoms with substantial displacement are present. However the local environment of those atoms corresponds to a bcc lattice. It is possible to trace the trajectory of several dislocations in the specimen at the final indentation depth in Fig. 4c.



(a) (b) (c)

FIGURE 3. Loaded surface orientation is (110). The dependence of the reaction force vs the indentation depth (a). The structure of the simulated specimen at various indentation depths: 3.5 (b), 13.8 Å (c). Only atoms with the value of a reduced slip vector more than 20% are shown

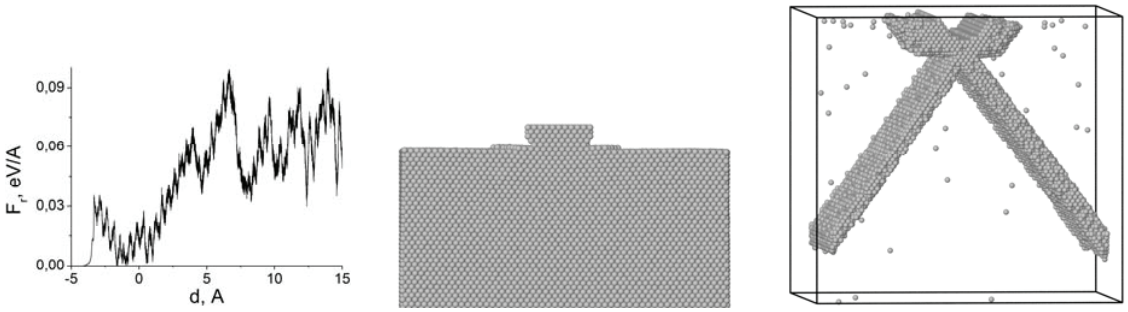


FIGURE 4. Loaded surface orientation is (111). The dependence of the reaction force vs the indentation depth (a). The structure of the simulated specimen at various indentation depths: (b) 4.6 Å (fragment); (c) 15.0 Å (only atoms with the value of a reduced slip vector more than 20% are shown)

SUMMARY

The calculations show that the structural response of the bcc iron during nanoindentation depends on the crystallographic orientation of the loaded surface. In the case of loading the (100) surface the dislocations can change slip plane to an adjacent one during their motion. The nucleation of plastic deformation during loading the (111) surface occurs at the lowest value of the indentation depth. Generation of structural defects in the contact zone always resulted in the decrease in the rate of growth of the reaction force.

ACKNOWLEDGMENTS

The work is done in the framework of the Programme of fundamental research of state academies of Sciences for 2013–2020 and with a partial financial support of the Tomsk State University Competitiveness Improvement Program.

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