Features of structural rearrangements at onset of plasticity in bcc iron with free surfaces of different orientation

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Abstract. The features of structural rearrangements in nanosized body-centered cubic single crystals of iron with different crystallographic orientation under uniaxial tension, which lead to formation and propagation of structural defects, were investigated on the basis of the molecular dynamics method. It is shown that, when the elastic limit is reached, either twins or dislocations arise in the crystals. The mechanisms of their formation and motion differ substantially for the considered orientations of the crystals. At stretching along the $X$ [$11\overline{2}0$] direction, the evolution of plastic deformation is determined by the nucleation and growth of one twin. Dislocations originate and slide only in the twin body. When the crystal is stretched along the $Z$ [$1\overline{1}00$] direction, a number of twins nucleate, at the front of which representative regions with face-centered cubic and hexagonal close packed lattices are formed. The nucleation of plasticity upon stretching a crystal along $Y$ [111] is dislocation nature.

1. Introduction

Interest in the investigation of nanocrystalline materials is determined primarily by their unique physical-mechanical properties: high strength, hardness, wear resistance, etc. The grain sizes of such materials have a significant effect on the mechanisms of plasticity initiation and determine the formation of special properties for this class of materials [1]. Experimental data, atomistic simulation, and theoretical models for different nanocrystalline systems have revealed a wide variety of mechanisms of plasticity initiation due to interface boundaries [2–5]. At the same time, studies focused more on nanocrystalline materials with the face-centered cubic (fcc) lattice. Atomic mechanisms of nucleation and development of plasticity in nanocrystalline materials with a body-centered cubic (bcc) structure are much less studied [3]. It is known that the most important mechanisms of plastic deformation in bcc materials are dislocation sliding and twinning. Along with them at high rates of deformation, the material with a bcc structure can flow like a viscous liquid, while retaining its crystal lattice, remaining a strong and stiff metal [6].

Experimental studies show that at room temperature and low deformation rates plasticity in bulk single crystals of the bcc iron with different orientations is realized on the basis of dislocation sliding [7]. In this case, an increase in the rate of deformation of a single crystal or a decrease in its temperature leads to an increase in the role of twinning. It was found that at high rates of deformation and low temperatures, the degree of deformation twinning depends significantly on the orientation of the single crystal relative to the loading [7]. In particular, at
room temperature and high tensile rates in directions close to the crystallographic [001] axis, the single crystal of iron is deformed on the basis of twinning. In the case of stretching along the directions close to the [110] and [111] axes, twinning is less pronounced.

Note that the nature of the nucleation of plastic deformation in nanocrystalline and nanosized crystals of iron can qualitatively differ from bulk single crystals. This is primarily due to the increased influence of the surface on the physical-mechanical properties of such samples, characterized by a high density of interfaces. The results of experimental studies and computer simulations show that the mechanisms of nucleation of plasticity in nanocrystalline materials and nanocrystals are similar in many respects. So the nucleation of defects of the crystal structure in them occurs when the stresses comparable to the theoretical strength of these materials are reached [8, 9]. This makes it possible to extend the results of calculations of the deformation behavior of nanocrystals with an ideal lattice to nanocrystalline materials.

In view of the smallness of the space-time scale of the processes that determine the structural changes in materials, experimental studies encounter significant difficulties. In turn, atomistic simulation of structural rearrangements at nucleation and development of plastic deformation in nanosized samples is a promising approach to solving this problem [10–12]. In connection with the rapid development of computer capability and the construction of reliable interatomic potentials, the molecular dynamics simulation has become widely used to study nanocrystalline materials and nanosized samples. It should be noted that this approach allows us to describe in detail the features of nucleation of structural defects and to reveal mechanisms of plastic deformation development in materials [13, 14].

In this work, a molecular-dynamics study of the influence of the crystallographic orientation on the mechanisms of the plastic deformation nucleation in nanosized crystals of iron with a bcc lattice under uniaxial tension is carried out.

2. Formalism
Simulation of uniaxial stretching of iron crystals was carried out with the use of the LAMMPS computational package [15]. To describe the interatomic interactions in iron, the potential was used [16], calculated in the Finnis–Sinclair approximation. The simulated crystals were nanowhiskers in the form of parallelepipeds 45 nm in length with a square cross section of 30×30 nm and contained about 3.5 million atoms. Along the “long” direction, periodic boundary conditions were used, and along the other two free ones were simulated. Along the “long” direction, the crystals uniformly stretched at a rate of $10^9$ s$^{-1}$. The simulation was carried out for crystals with 3 different directions of stretching: $X$—[112]; $Y$—[111]; $Z$—[110]. The temperature of the crystals was 300 K. The integration step was chosen equal to 5 fs. Identification of the structure of the nearest environment of atoms was carried out using the common neighbor analysis [17] and the dislocation extraction algorithm [18]. To visualize the structure of crystals, the OVITO package [19] was used.

3. Results and discussion
Analysis of simulation results shows that in the case of stretching along the $X$ direction at reaching the elastic limit a lot of atoms with the fcc lattice of the environment are formed in the sample. They are uniformly distributed throughout the sample. The physical nature of their formation is due to the thermal oscillations of the atoms of the crystal lattice. When the elastic limit is reached, a twin appears on the edge of the sample. An analysis of the structure shows that local regions with the fcc lattice can form at the propagation front of twinning dislocations, figure 1(a). In this case, the twin growth is accompanied by the generation of dislocations inside it with the $1/2$ [111] Burgers vector. When the twin approaches the free surface $Z = 30$ nm in its body (in the region adjacent to the twinning dislocations), sections with the fcc and hexagonal close packed (hcp) crystal lattice are formed, figure 1(b). Their formation is due to the fact that
Figure 1. Defect structure of the crystal stretched along the $X$ direction at different instant times: 750 (a), 765 (b), 785 (c), 850 ps (d). Transparent green color shows free surfaces and twin borders. Light green and red spheres correspond to atoms with the fcc and hcp symmetry of the nearest environment. For clarity, the fcc atoms caused by thermal fluctuations are not shown. The blue lines show dislocations with the $1/2 \langle 111 \rangle$ Burgers vector.

As the approach to the free surface $Z = 30$ nm, the stresses in the neighborhood of the front of the twin propagation increase.

Subsequently, dislocations with the $1/2 \langle 111 \rangle$ Burgers vector are formed in these regions, figure 1(c). It should be noted that dislocations are generated only inside the twin. Along with the growth of the first twin, twins of smaller sizes are generated in its vicinity, which practically do not grow during deformation. When the first twin reaches the free surface $Z = 30$ nm, it begins to increase its width, see figure 1(b, c), to the sizes which are shown in figure 1(d). At the same time, an intense glide of dislocations occurs inside the twin, which then escapes to a free surface or to twin boundaries.

When stretching along $Z$ direction, the structure of the nearest environment of some atoms is randomly rearranged to the hcp or fcc lattice, and then again takes the initial bcc configuration. Such local structural rearrangements have a thermofluctuational nature and their number increases at the approach of tension to the elastic limit. In the process of uniaxial stretching,
the sample is substantially compressed along one of the diagonals of its square section and the cross section becomes diamond-shaped one. This is due to the large anisotropy of the elastic properties of the material in the (1\overline{1}0) plane which is perpendicular to the tension direction. On opposite edges, which correspond to sharp corners, the twinning occurs. One of them is shown in figure 2(a). These twins are significantly different from the twin formed when the sample is stretched along the $X$ direction. Firstly, they have a smaller thickness and a higher growth rate of their area. Secondly, they are formed in large numbers. Thirdly, the nucleation and motion of twins are accompanied by the formation of much larger in size regions in which the crystal lattice has the fcc and hcp symmetry, figure 2(b). During the subsequent deformation, the thickness of approximately 50% of the twins decreases. In this case, the regions with the fcc and hcp lattice symmetry almost completely disappear, and the material plasticity in this deformation interval is realized by dislocation sliding at practically constant dislocation density, figure 2(c).
Figure 3. Dislocation structure of the sample under tension along Y direction at different instant times: 162.5 (a), 163.4 (b), 164.4 (c), 165.2 ps (d). Green color shows free surfaces. Light green and red spheres correspond to atoms with the fcc and hcp of the relative positions of their neighbors, respectively.

We note that an increase in the number of stochastically located atoms with the fcc and hcp of the relative positions with their neighbor atoms at the elastic interval indicates a decrease in the potential barriers of such lattice rearrangements. After overcoming the elastic limit, the largest stresses are realized for atoms which form the fcc and hcp lattice with their neighbor atoms. Therefore, on the front of the propagation of twins and dislocations, there are always regions with the fcc or hcp phase, which are an intermediate state (or mechanism of rearrangement) for the growth of the defective system.

When the sample is stretched along Y direction, the nucleation and development of plasticity is controlled by screw dislocations with the $1/2 \langle 111 \rangle$ Burgers vector. The nucleation of the first dislocations is shown in figure 3. The first screw dislocation arises on the edge of the crystallite ($X = 0, Z = 30$ nm) and an atom cluster with the fcc lattice is formed on one of its sections, see figure 3(a). As the dislocation moves, this cluster increases in its size and a dislocation loop (the second dislocation) is formed on its boundaries, see figure 3(b), which by one of its edge goes to the screw dislocation. Later, the dislocation loop increases in diameter, and its edge segments move much faster than the screw segments and reach the free surfaces, see figure 3(c). As a result, there are already two screw dislocations in the crystals. Further, as the length of screw dislocations increases, the formation of loops on them takes place more and more actively. For example, one new loop is formed during one thousand steps on the first dislocation and three loops on the second one, see figure 3(c, d).

As the plasticity develops, the process of multiplication of dislocations becomes avalanche-like character. New loops are formed on moving screw dislocations. When the first screw dislocations begin to escape to the surface $X = 30$ nm of the sample, figure 4(a), in the lower half of the sample ($Z = 0–15$ nm), new (secondary) screw dislocations with the same $1/2 \langle 111 \rangle$ Burgers vector are generated on moving screw dislocations as in the old primary one, but in the adjacent direction at an angle of 72.8 degrees. This leads to the beginning of the formation of a dislocation grid. After 895 ps on the back surface $X = 0$ and the upper surface $Z = 30$ nm, a large step begins to form, figure 4(b). The total length of dislocations reaches a maximum value. In the interval 940–1000 ps more mobile screw dislocations leave the sample. After 1000 ps the formation of a cellular dislocation structure ends, figure 4(c). Further deformation of the sample is achieved by the escape of almost all dislocations on the free surface. A large
Figure 4. The structure of the sample at different instant times of stretching along Y direction: 865 (a), 895 (b), 1000 (c), 1250 ps (d). The green, red and gray spheres correspond to atoms with the fcc, hcp and undefined of the relative positions of their neighbors, respectively. Atoms with the bcc symmetry of neighbor positions are not shown.

number of vacancies remain in the sample as a result of the multiple intersections of dislocations from different slip planes, figure 4(d).

Our results are in good agreement with the data obtained elsewhere [7], and reveal the dynamics of nucleation and development of plasticity in bcc iron. The realization of the plasticity mechanisms in the simulated samples depends on the misorientation angle between the direction of tension and the basic slip planes.

4. Conclusions
The results of the molecular dynamics simulation have shown that the nucleation of the plastic deformation under uniform stretching essentially depends on the crystallographic orientation of the single crystal of iron. Local structural rearrangements corresponding to the fcc and bcc lattice begin to appear and disappear in the elastic interval of sample stretching along the X and Z directions as a result of atom thermal fluctuations. The number of such rearrangements increases as we approach the elastic limit.

When stretching along X direction exceeding the elastic limit, the nucleation and development of plasticity is determined by the generation and growth of one twin, at the front of which the
bcc lattice is rearranged into the fcc one. Generation of dislocations occurs only in the body of the twin, causing its growth until it reaches to the opposite surface.

Regions with the fcc and hcp phases are formed at the front of the propagation of numerous twins which are nucleated when the sample is stretched along the Z direction. Twins are characterized by a high growth rate and a small thickness. The thickness of almost 50% of twins with time becomes smaller and they are transformed into dislocations.

The nucleation of plasticity when the sample is stretched along the Y direction has dislocation nature. First, screw dislocations begin to generate on which loops appear during their motion. This process has an avalanche-like character. Over time, all dislocations escape to free surfaces and numerous vacancies formed by the intersection of dislocations remain in the deformed sample.

Acknowledgments
The work was carried out with financial support from the Russian Science Foundation (project No. 17-19-01374).

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