THE ROLE OF THE EXCESS VOLUME AT THE NUCLEATION OF PLASTIC DEFORMATION IN METALS

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Abstract. The computer simulation results on the atomic structure of the copper crystallite and its behavior in nanoindentation demonstrate the key role of local structural transformations in nucleation of plasticity. The generation of local structural transformations can be considered as an elementary event during the formation of higher scale defects, including partial dislocations and stacking faults. The cause for local structural transformations, both direct fcc-hcp and reverse hcp-fcc, is an abrupt local increase in atomic volume. A characteristic feature is that the values of local volume jumps in direct and reverse structural transformations are comparable with that in melting and lie in the range 5-7 %.

1 INTRODUCTION

The last decades the study of plastic deformation is subjected to close attention. However, issues related to the peculiarities of the plastic deformation nucleation in metals at the lowest, atomic, level still remain poorly understood. It is known that different types of external action with attendant thermal fluctuations can give rise to local regions of excess volume in a material. In this context, the question arises: What are the conditions under which a local volume change will lead to a local structural change? The possibility of such structural changes is supported by studies showing that mechanically loaded fcc metals experience specific local structural distortions which correspond to a local structural transition of the fcc-
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hcp type. It is demonstrated that these distortions are preceded by the generation of excess volume. Effect of the atomic density, or, equivalently, the atomic volume is discussed for a long time [1-4]. As shown in [4] atomic density is an important thermodynamic variable that determines the phase state of the system. The introduction of this parameter allowed substantiating a new type of phase diagrams. This improved the understanding of the conditions of coexistence of phases at changing the atomic density, and also explained the instability of the crystal lattice and its melting, when the solid expands up to a critical specific volume. Molecular dynamics simulations [5-9] revealed the atomic mechanisms of this process. For example, in [5] it was shown that the increase in volume is the cause of the lattice instability, and, as follows from [1] no matter how the excess volume is achieved either by heating or by mechanical loading. These studies and the results obtained in [3] illustrate the validity of the conclusions made in [10,11] for case of homogeneous increase of the whole sample volume. In [10, 12] it was shown that local structural changes (LSCs) generated under mechanical loading may be considered as some protodefects.

In this connection, it is vital to answer the question, how the formation of the local structural changes is connected with the local increase in volume. The aim of the present study is molecular dynamics simulation to elucidate the role of local excess volume in nucleation of plasticity in metals. Based on the calculations performed, it will be concluded that the local increase in volume is necessary condition for local structural transformations of different types and responsible for nucleation of plasticity in loaded materials.

2 FORMALISM

Nanoindentation is one of the most visual and effective methods for the study of physical and mechanical properties of materials in contact interaction. It enables to influence the origin and evolution of the source of plastic deformation by changing indentation parameters [13-16]. As a rule, the purpose of the investigations related to computer simulation of material behavior during indentation, is the study of the mechanisms of plastic deformation of the material in the vicinity of the indenter, the analysis of defect structures and interpretation of nanoindentation force-displacement curves [17-20]. Despite the informative value of such studies, it is difficult to analyse the obtained results due to the complexity of deformation picture.

An indenter of extended cylindrical shape was used in simulations for simplifying the interpretation of the indentation results. The loading was realized by its side surface. The indenter had the atomic structure of copper with atoms fixed in lattice sites. The objects of the simulation are copper single crystals of the parallelepiped shape (Fig. 1). The size of their edges is 160 Å, the initial temperature is 300°K. The simulated specimens contain about 400 thousand atoms. Loaded crystallite faces simulated as free surfaces. Crystallographic indexes of loaded surfaces in different calculations were next ones: (01̅1), (001) and (111). Periodic boundary conditions were used in the direction parallel to the indenter axis. The rest of the faces perpendicular to the direction of the indentation are simulated as free surfaces. Three atomic planes of the face opposite to loading one were fixed for eliminating movement of crystallite as a whole. The indenter is moved with a speed of 25 m/s.
Interatomic interaction was described in the frame of the embedded atom method [21]. In the framework of this approach the potentials of interatomic interaction allow to describe with high degree of accuracy the elastic properties of copper, its surface properties, as well as the energy of defect formation, the effects of contraction of the near-surface atomic planes, etc.

The calculation of the atomic volume was carried out by the following formula:

$$V_i = \left( \frac{\sum |\vec{r}_i - \vec{r}_j|}{N_s} \right)^3,$$

where $N_s$ is the number of nearest neighbors of the $i$-th atom, $\vec{r}_i$ and $\vec{r}_j$ are corresponding radius vectors.

Analysis of changes in the simulated structure and classification of generated defects was carried out on the base of common neighbor analysis, taking into account the mutual arrangement of the nearest neighbors for each of the atoms [22]. Force–displacement curves were calculated in order to evaluate the system response on nanoindentation. The indentation force ($F$) was defined as the total force acting on the indenter from crystallite atoms. Indentation depth ($d$) calculated as the distance from the lower boundary surface of the indenter to a level corresponding to the surface of the crystallite in the initial state (before loading).

2 RESULTS AND DISCUSSION

The simulation results showed that LSCs similar to those found in [7] are nucleated in the specimen at the mechanical loading. The analysis revealed that they are the result of specific rearrangements in the first and second coordination spheres of atoms—centers of these changes. The initial local fcc structure of these atoms is transformed into a hcp structure (Fig. 2). They are realized when one of the atoms $\beta$ leaves the first coordination sphere while another atom $\alpha$ from the second coordination sphere comes into it. Further loading of specimen leads to the formation of planar defects by LSCs. Analysis of alternating atomic planes showed that the LSCs form the intrinsic stacking faults as well as extrinsic ones. They are bounded by partial dislocations which move in $\{111\}$ glide planes from contact area to lateral free surfaces. The
simulation results showed that local excess of the atomic volume always precedes formation of LSCs in the crystal lattice. The magnitude of the jump in the volume of direct local fcc-hcp and inverse hcp-fcc structural transformations is 6-8 % (Fig. 3).

![Figure 2: The scheme of fcc-hcp structural rearrangements in the first coordination sphere: a) the initial fcc configuration of atoms in the first coordination sphere; b) an intermediate stage; c) the stage at which the environment of the central atom (red coloured) already has hcp topology. The dashed lines indicate the position of the central atom’s first coordination sphere](image)

![Figure 3: The dependence of the relative change in the local volume for one of the atoms, which nearest neighbours undergo direct and reverse transformation. Colour of curves indicates the type of the local structure: blue – fcc local environment, red – hcp local environment](image)

The resulting indentation force-displacement curve for the loaded crystal surface orientation (011) is shown in Fig. 4. Note that the interaction between the indenter and the crystallite occurs as soon as the distance between them becomes smaller cutoff radius of the interatomic interaction. As in [15], initially between the indenter and load surface an attraction takes place (Fig. 4, this corresponds to the negative value indentation force). This effect is called “jump-to-contact” [23]. After further motion of the indenter the attraction is replaced by repulsion. Accordingly, the indentation force in Fig. 4 has a pronounced...
minimum. The dependence between indentation force and penetration depth calculated for the given conditions can be divided into four stages.

The first stage is characterized by a linear dependence of the indentation force from the indentation depth and corresponds to the elastic response of the material. Generation of LSCs takes place at the beginning of the second stage in the zone of contact between the indenter and crystallite (Fig. 5a). Generation of LSCs in a perfect crystal leads to a partial relaxation of excess stresses and reducing the curve slope in Fig. 4 to the zero value. Although at this stage the classic structure defects such as dislocations and stacking faults are not yet formed the stress relaxation is already carried out by generation of LSCs. It should be noted that change in the behaviour of the indentation force directly during the transition from the first to the second stage is also related to structural features of the indenter. In particular, as it moves next atomic layers of indenter start interacting with the crystallite free surface. Initially this interaction is attractive thus the value of indentation force is reduced. The number of defects in the contact zone in the second stage quickly reaches saturation and after that their number in the third stage do not changes significantly. This leads to the exhausting of this stress relaxation mechanism, resulting in an increase of the loading curve slope at the third stage.

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Figure 4: Indentation force versus penetration depth for loaded surface (01\(\bar{1}\))

Figure 5: Fragment of the simulated crystallite at different indentation depths: a) -1.0 Å, b) 8.7 Å. Atoms having nearest neighbours with fcc symmetry are not shown. Indenter atoms are marked as red spheres, atoms with hcp symmetry of the nearest neighbours are blue, atoms with broken symmetry of nearest neighbours are green
Analysis of the simulation results shows that the further indentation (the beginning of the fourth stage) leads to the intensive growth of the number of LSTs (Fig. 5b) and, as a consequence, loading curve not only slows its growing, but also experiences drops. At this stage generation of LSCs leads to the formation and development of structural defects of a higher rank, in particular partial dislocations and stacking faults. Note that structural defects are generated in the contact zone in {111} atomic planes. Formed partial dislocations and stacking faults may move in gliding planes and reach the free surface. This leads to the change in shape of the crystallite – formation of surface steps.

Calculations showed that the crystallite behaves differently at loading of (001) surface. At the indenter position -3.4 Å attraction force between it and the surface reaches a maximum value. The number of defects increases due to the bending of the free surface of the sample. The indentation force and the number of atoms involved in LSCs start to grow upon further loading. When the indentation depth becomes -0.8 Å a defective area of a size comparable to the size of the indenter forms in contact zone. After that the size of defect region grows with the penetration depth of the indenter. It should be noted that a more intense increase in the number of defects at indentation depth of 7.0 Å reduces the indentation force. Simulation results showed that, after stopping the indenter at a depth of 10.0 Å dislocation loops are emitted to the lateral sides of specimen from the bottom of defect region (Figure 6a-d). They escape at the free surfaces and form surface steps. Note that after that the percentage of LSCs is reduced from 2.0 to 0.3 %. Development of defect structures in copper crystals with the loaded surface (111) is presented in Figures 6e-h. Calculations have shown that the LSCs are nucleated in the sample at the indenter penetration depth of -3.0 Å. At the indentation depth of 0.8 Å stacking fault starts to grow in the (011̅) plane, and the indentation force slightly changes. During sample loading a group of partial dislocations a/6 <112> {111} is generated and starts moving in the adjacent atomic planes (011̅). As a result a twin bounded by twin boundaries, which are recognized as hcp atoms is formed in the specimen (Fig. 6h). Note that a fragmented region consisting of hcp atoms is formed in the contact zone. This region develops in a direction toward the right side edge of the specimen.

12 CONCLUSIONS

The results of the simulations showed that LSCs are formed during nanoindentation of the copper crystallites. Their nucleation is always preceded by a local increase of the atomic volume by 6-8 %. Generation and evolution of LSCs leads to the formation of structural defects of a higher level: dislocations, stacking faults, etc. It is noted that the indentation force and the number of atoms involved in the LSCs are well correlated. This behaviour is due to the fact that the generation of structural defects is a mechanism of elastic relaxation.

It was found that the crystallographic orientation of the loaded specimen surface substantially affects nanoindentation response of copper. For example, when loading surface oriented in (011) plane, stacking faults are generated and move towards lateral free surfaces. During indentation of (001) surface all LSCs are formed in the contact zone, and after stopping the indenter they escape at lateral free surfaces of specimen. The loading of (111) surface leads to the formation of twin bounded by LSCs.
Figure 6: Projection of crystallite structure with loaded surface (001) at different moments of time at the indenter penetration depth of 10.0 Å: a) 0 ps, b) 25 ps, c) 50 ps, d) 120 ps. Projection of crystallite structure with loaded surface (111) at different indenter penetration depths: e) -1.4 Å, f) 1.4 Å, g) 5 Å, h) 10 Å.
REFERENCES


