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Elementary atomistic mechanism of crystal plasticity

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Abstract

The simulation of loaded crystal behavior under relaxation is carried out. Typical local structural distortions named protodefects, which give rise to conventional lattice defects, are discovered. The dynamics of atomic displacements that govern protodefect nucleation is studied in detail. A local expansion of atomic volume induces protodefect formation.

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The formation of lattice defects is one of the main plasticity mechanisms of crystalline materials. It is obvious that their generation in a stable crystal is related with the local loss of lattice stability [1], which can be due to thermal, mechanical, chemical or radiation actions, or their combinations. The search for a thermodynamic parameter whose variation would define local stability loss of the crystal is one of the key tasks in the modern physics of plasticity.

The influence of atomic density or, which is the same, atomic volume on the structural-phase state of solids has long been discussed [1–4]. As paper [4] demonstrates, atomic density is one of the thermodynamic variables that govern the phase state of condensed matter. The introduction of this parameter in an explicit form has allowed one for the first time to validate a new type of phase diagrams. The diagrams are plotted in the variables of temperature–concentration–atomic density. The use of the diagrams not only expands our notions about the conditions of phase coexistence at varying atomic density, but also explains instability of the lattice and its mechanical melting when a solid expands to a critical specific volume [4]. Molecular dynamics studies [5,6] also show that volume expansion is a cause of lattice instability; in so doing, as follows from [4], it is not important how the excess volume is achieved, whether due to heating or mechanically.

Notice that all the above-given results have been obtained on the assumption about homogeneous (uniform) expansion of the volume. It would natural to ask what effects can be induced by local volume change. First of all, whether the change will precede the formation of lattice defects and if yes, what defects exactly. Papers [7,8] show that under mechanical loading of fcc metals one can see the generation of specific local structural distortions that correspond to a local structural transition of fcc–hcp type. The local structural distortions may be considered as protodefects, because, as follows from [7,8], they give rise to defects of a higher level (partial dislocations, stacking faults, etc.). The formation mechanism of such local structural distortions is not understood. In view of the aforesaid, the question arises whether the formation of such protodefects is related with local volume expansion?

To study this question, in the present Letter we have performed molecular dynamics simulation of the behavior of a preloaded specimen at the relaxation stage, which allows excluding effects of dynamic nature.

The calculations were carried out at finite temperature ($T = 300$ K) for a 3D parallelepiped copper crystallite. The coordinate axes were oriented along the [110], [$1\bar{1}0$] and [001]

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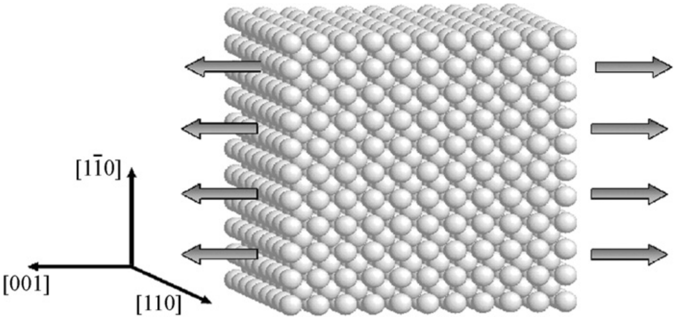

Fig. 1. Fragment of the simulated crystallite illustrating its crystallographic orientation.

crystallographic directions. Along the [110] crystallographic direction we simulated periodic boundary conditions, free surface were oriented normally to the [1$\bar{1}$0] direction. Preloading (tension at constant rate 50 m/s) was performed along the [001] direction (the loading scheme is given in Fig. 1). To simulate relaxation processes at a certain strain, the calculations were carried out with zero tension rate. Interatomic interaction was described in the framework of the embedded atom method [9–11]. Interatomic interaction potentials within this approach allow describing with rather high accuracy elastic characteristics of copper, its surface properties, energies of defect formation, etc. [12,13].

The zones of local structural distortions were identified with the use of a technique based on the common neighbor analysis, which is proposed in [14] and used in [7,8]. According to the technique, to each pair of atoms there corresponds a set of four numbers. The first number defines the "relationship" between atoms ("1" – if the atoms are neighbors, "2" – in the contrary case). The second denotes the number of common neighbors for the given pair of atoms. The third is the number of bonds between the common neighbors. The fourth is the number of bonds in the longest chain that includes neighbors of the given pair. For a perfect fcc structure each atom is characterized by 12 sets of numbers {1/4/2/1}, for the hcp structure by 6 sets of numbers {1/4/2/1} and 6 sets {1/4/2/2}. As distinct from the methods that take into account only coordination numbers of atoms [15,16], the discussed method allows analyzing in more detail the topology of bonds and revealing local structural distortions.

As is shown in [7,8], there is a certain threshold strain value at which the growth of zones with local structural changes is almost avalanche-like. The calculations performed in the given papers suggest that the threshold value is in the range from 10–14% and depends on temperature and loading conditions. Note that increase in strain rate (load intensity) leads to the fact that relaxation processes have no time to provide the generation of local structural changes. As a consequence, the generation begins at higher strains. We may therefore expect that at long relaxation of the preloaded crystallite protodefect generation will start at lower strains. This is justified in the present study which demonstrates that really during relaxation local structural changes begin when the prestraining value achieves 8.5%. Notice that the loading conditions and temperature were assumed to be the same as in [7,8].

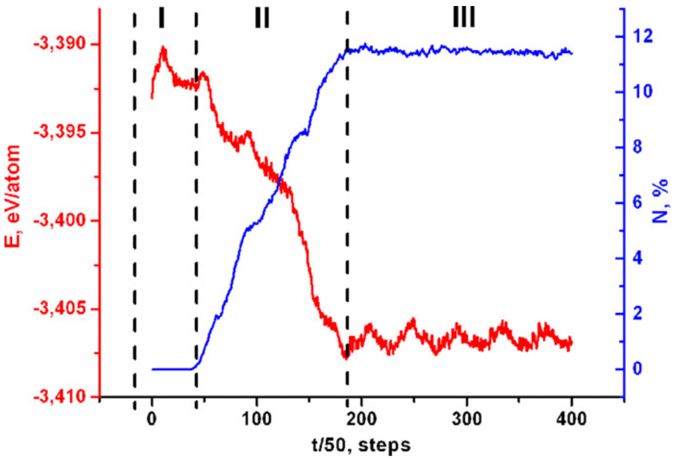

Fig. 2. Growth in the number of atoms (N) involved in local structural transformations and potential energy variation during relaxation of the crystallite prestrained to 8.8%.

The calculation results for the number of atoms involved in local structural transformations during relaxation of a tensile specimen prestrained by 8.8% are given in Fig. 2. The same figure illustrates respective changes in potential energy per one atom. Notice that the coordinated behavior of the both curves unambiguously points to the fact that the generation of local structural changes is one of the mechanisms of internal stress relaxation.

A detailed analysis of atomic displacements at the stage of nucleation of local structural distortions (protodefects) has revealed that their formation is related with specific rearrangement in the first and second coordination spheres of one of the atoms. Local structural distortion around the atom corresponds to the local topology of the hcp structure; hence in the subsequent discussion we will identify such atoms as centers of protodefects. Fig. 3 schematically illustrates the typical sequence of atomic displacements, which causes the formation of a protodefect in the vicinity of one of such atoms (green-colored and denoted by α). It is clearly seen that one of the atoms of the second coordination sphere (red-colored and denoted by β) is displaced to the first coordination sphere, while one of the atoms of the first coordination sphere (denoted by γ) leaves it.

To investigate the role of excess volume in protodefect formation during relaxation, we studied atomic volume variation for all atoms of the simulated system. The calculations have shown that for the atom α, which is in the state corresponding to that indicated in Fig. 3(a), the atomic volume is almost equal to equilibrium and the local structure corresponds to the fcc packing. When the environment of the atom α goes to the state illustrated in Fig. 3(b), the atomic volume grows by 5–6%. It is the atomic configuration that characterizes the local unstable state of the lattice. The calculations have also shown that this atomic configuration can either return to the initial fcc packing (Fig. 3(a)) or transform into the hcp packing (Fig. 3(c)). The latter leads to protodefect formation. In the both cases, the atomic volume reduces to the corresponding equilibrium value. Herein the deviation induced by thermal-fluctuation processes

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