

On structural defect generation induced by thermal fluctuations in materials with a perfect lattice under dynamic loading

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Abstract

The possibility of structural defect generation induced by thermal fluctuations in single crystals under high-rate deformation is numerically investigated. It is shown that thermal fluctuations can be a reason for structural defect generation and there is a threshold strain value at which zones with local structural changes grow almost abruptly.

Keywords: Molecular dynamics simulations; Thermal fluctuations; Structural defects; Atomic structure; Deformation

The studying of the generation of structural defects such as point defects, dislocations, stacking faults, etc. under dynamic loading is important for understanding the mechanisms of plastic deformation initiation and evolution in materials [1–4]. In this case, one of the fundamental problems of solid state physics and materials science is the investigation of possible generation mechanisms of local structural distortions and transformations of the atomic structure, which can be related to the so-called precursor states [5]. The nucleation of various structural defects on the atomic level is rather difficult to investigate experimentally because of the need for high temporal (10^{-14} s) and spatial (10^{-9} m) resolution. Computer simulation is therefore an effective way to study both the mechanisms of structural defect generation and dynamics of their evolution. Note that for ease of result interpretation it is worthwhile to simulate deformation using a crystallite with a perfect structure because, in this case, first of all thermal fluctuations may be responsible for the generation of local structural changes.

The present Letter is aimed at the investigation of atomic mechanisms responsible for the generation of plastic deforma-

tion in a material with an initially perfect lattice in a wide temperature range (100–700 K) and for different crystallographic directions of loading.

Problems posed in the Letter are solved on the basis of molecular dynamics simulation using interatomic interaction potentials calculated in the framework of the embedded atom method. As is shown in papers [6–8] the potentials used allow describing with a high degree of accuracy structural, mechanical and energy properties in the material bulk, near-surface regions and directly on the free surface.

The simulated copper crystallite was a parallelepiped in shape. To eliminate the influence of surface effects, use was made of periodic boundary conditions along all three directions. The structure of the deformed crystal was analyzed with an algorithm proposed elsewhere [9], which allowed us to analyze the topology of structural bonds of each atom with its nearest neighbors. According to this algorithm, to each pair of atoms corresponds a set of four numbers. The first number characterizes the relationships between atoms. The number is 1 if the atoms are neighbors; otherwise it is 2. The second one is the number of common neighbors for the given pair of atoms. The third one is the number of bonds between common neighbors. The fourth one is the number of bonds in the longest continuous chain that includes neighbors of the given pair. For a perfect

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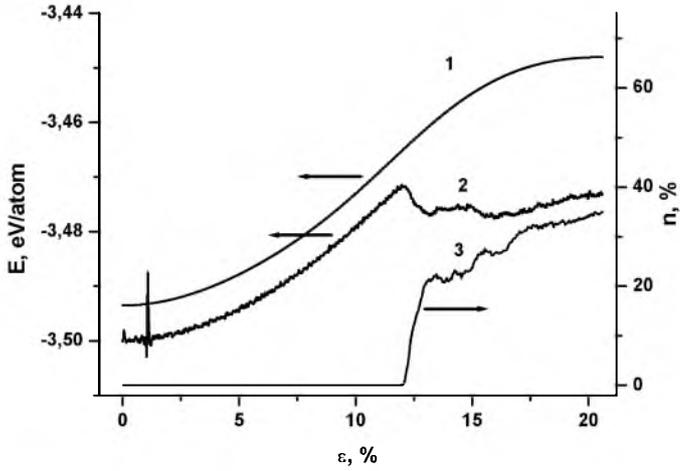


Fig. 1. Dependence of potential energy per one atom for 0 (1) and 300 K at a compression rate of 50 m/s (2); n —fraction of atoms with the topology of structural bonds, which corresponds to the HCP lattice (3).

FCC structure each atom is characterized by 12 sets of numbers $\{1/4/2/1\}$, for the HCP structure by 6 sets of $\{1/4/2/1\}$ and 6 sets of $\{1/4/2/2\}$, and for the BCC structure by 8 sets of $\{1/0/0/0\}$.

The simulated copper crystallite was oriented so that the X-axis was directed along the $[110]$ crystallographic direction, the Y-axis along $[1\bar{1}0]$, and the Z-axis along $[001]$. It is known that in uniform compression of an FCC crystal by $\sim 20\%$ along the $[001]$ direction and simultaneous tension by $\sim 12\%$ along the $[110]$ and $[1\bar{1}0]$ directions the initial structure is transformed into the BCC structure (scheme A). In this case, the change of potential energy per one atom comprises hundredth fractions of an electron volt (Fig. 1, curve 1). To account for the temperature effect, the initial crystallite was first relaxed at room temperature and then deformed in accordance with the scheme A.

The calculation results for the dependence of the potential energy falling to one atom on the strain value of the crystal at 300 K are presented in Fig. 1 (curve 2) for a compression rate of 50 m/s along the Z-axis. It is clearly seen that an account for

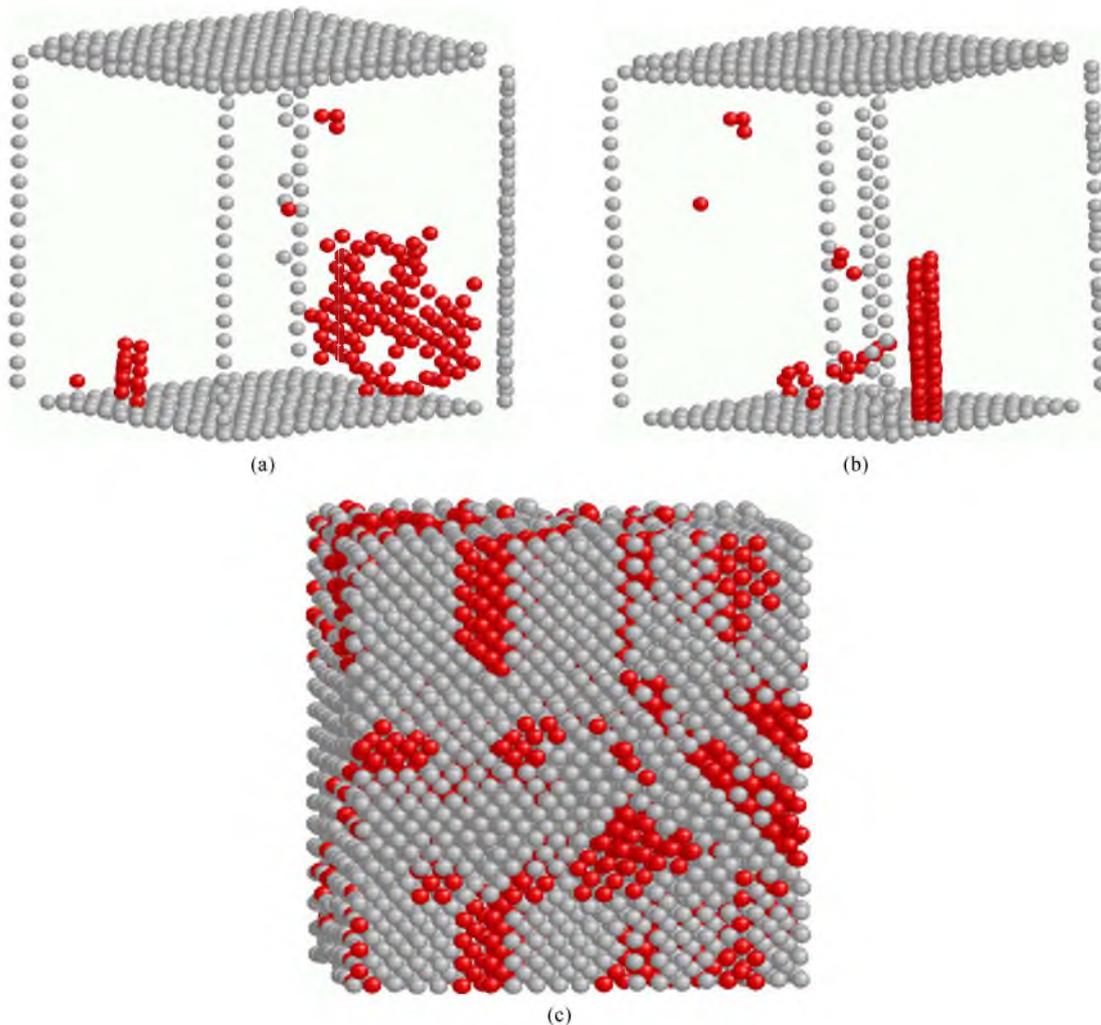


Fig. 2. Atomic structure at different view angles for the zone with local structural changes in compression by 11.3% along the Z-axis (a), (b). General view of the simulated crystallite in compression by 18% along the Z-axis (c); red spheres denote atoms belonging to the zone with local structural changes. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

temperature leads to considerable changes in the curve path. To analyze the potential energy behavior depending on the strain degree curve 2 can be arbitrarily divided into two portions. In the first portion the potential energy increases (is accumulated). In the second one it decreases for a while and further starts growing again, but much more slowly.

Analysis of the simulation results has shown that the beginning of the second stage is related directly to the formation of zones with local structural changes, which consist of atoms with a set of numbers typical for the HCP structure. This is clearly demonstrated in the correlation of curves 2 and 3 (the latter depicts the fraction of atoms belonging to the zones with local structural changes). As an example Figs. 2(a) and (b) illustrate (at different angles of view) atoms belonging to these zones at 11.3% deformation. Analysis of the positional relationship between atoms has shown that the internal structure of these zones corresponds to the stacking fault structure. The general (three-dimensional) view of the crystallite for a later stage of deformation (18%) is represented in Fig. 2(c). The considered zones are seen to orient along certain crystallographic directions. It should be noted that during deformation together with the zones of local structural changes we see the formation of zones with lattice distortions; the latter are not associated with the HCP structure. The investigations have revealed that their formation has a fluctuation character. Some of them are later transformed into zones with the HCP geometry, which is manifested in a saw-tooth shape of curve 2 in Fig. 1.

To study the temperature effect on the structural response of the simulated crystallite, the calculations were performed at 100, 300, 500, and 700 K. Fig. 3 demonstrates the integral effect of temperature on the nucleation and evolution of structural defects at high-rate specimen deformation. As is seen from the figure, at low temperatures structural defects grow almost abruptly, while at increasing temperature the zones with local structural changes are generated more smoothly and at smaller strain degrees. This substantiates the fact that the generation of the zones with local structural changes is induced by thermal fluctuations (at higher temperatures structural defects nucleate earlier). It is significant that the fraction of structural defects at low temperatures is larger, which is related to a higher level of stored elastic energy.

Notice that there are also other geometrical paths of loading when the HCP structure can be transformed into the BCC structure. A well-known path of lattice transformation is that by the Bain scheme [10–12]. It consists in the following: the initial FCC lattice ($c/a = 1$) is compressed along the [100] direction and simultaneously elongated by identical values in the [010] and [001] directions so that the initial atomic volume remains constant. At the ratio $c/a = 1/\sqrt{2}$ the lattice is transformed into the BCC one.

The calculations have shown that the change of potential energy under deformation along directions corresponding to the Bain scheme is qualitatively similar to the above-considered case (scheme A) (Fig. 1), because the HCP to BCC transformation in both cases is not related with overcoming the energy barrier. Therefore it could be expected beforehand that the response of specimens would be similar as well. It has been sub-

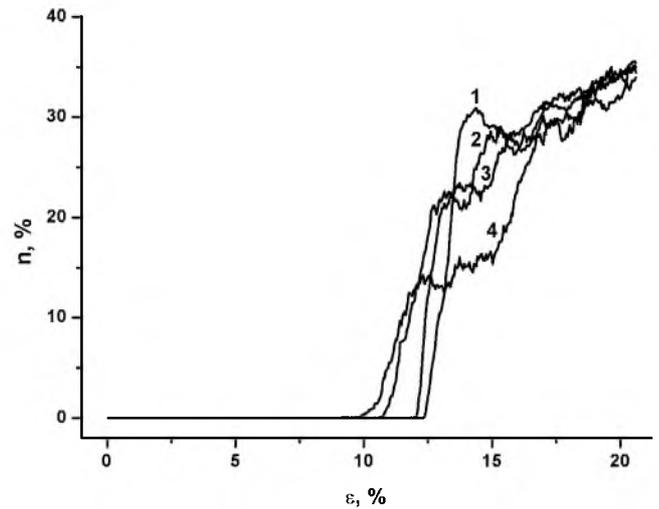


Fig. 3. Fraction of atoms (n) with the topology of structural bonds, which corresponds to the HCP lattice, versus strain degree for different temperatures of the crystal: 100 (1); 300 (2); 500 (3); 700 K (4). The compression rate along the Z-axis is 50 m/s.

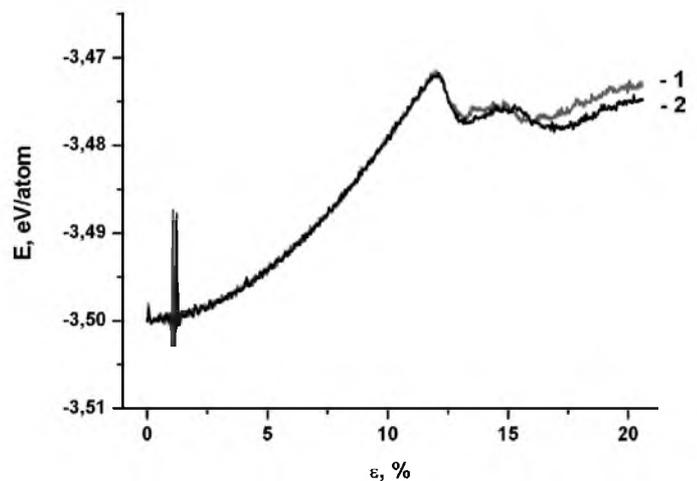


Fig. 4. Potential energy per one atom versus strain degree at 300 K for a compression rate of 50 m/s; scheme A (1) and Bain scheme (2).

stantiated both by the obtained dependences of the fraction of the zones with local structural changes and by the shape of the strain degree dependence of potential energy (see Fig. 4). Note that, according to the result analysis, the abrupt change of potential energy at low strain degrees ($\sim 2\%$) is related to the fact that characteristic rates of structural transformations necessary for the simulated crystal to relax in this strain interval are much lower than the loading rate.

Thus, it has been first demonstrated with the direct molecular dynamics simulation that the generation of structural defects induced by thermal fluctuations is possible under dynamic loading in materials with an initially perfect lattice. Notice that there is a certain threshold value of strain at which zones with local structural changes grow almost abruptly. In the cases considered, the character of structural defect nucleation and evolution depends to a greater extent on the specimen temperature and to a lesser extent on the loading scheme. Though the loading system was deliberately chosen for directional symmetry changing

that corresponds to the BCC transition, the topology of these regions corresponded to the HCP structure. Such a behavior is evidently related to relatively close values of energy for the FCC and HCP structural states.

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