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Molecular-Dynamics Study of Crystal Structure Defect Formation by the Thermal Fluctuation Mechanism during High-Rate Deformation

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Abstract—The possibility of structural defect generation in materials with the ideal crystal lattice under dynamic loading conditions in a broad temperature range has been studied by means of molecular dynamics using the embedded atom method with many-body interatomic interaction potentials. It is shown that thermal fluctuations can lead to a jumplike nucleation of defects in the ideal crystal under high-rate deformation conditions. Features of the defect nucleation via this mechanism are analyzed for various temperatures and loading regimes.

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One of the most important basic problems in solid state physics consists in the study of atomic mechanisms of the nucleation and development of structural defects, including those in crystalline materials with the ideal initial structure [1, 2]. Experimental investigations into the nucleation of structural defects in crystals encounter considerable difficulties, since both high temporal (10^{-14} s) and high spatial (10^{-9} m) resolution is required. Computer simulations based on molecular dynamics offer an effective means of studying both the generation of defects and the dynamics of their subsequent development.

This Letter presents the results of molecular dynamics investigation into the possibility of defect generation via the thermal fluctuation mechanism in an ideal crystal during high-rate deformation. The process was simulated in a broad temperature range (100–700 K) for a model crystal dynamically loaded in various crystallographic directions. The interatomic interactions were described using the embedded atom method developed by Daw and Baskes [3, 4]. The embedded atom potentials employed allow the structural, mechanical, and energy characteristics to be described with high precision both in the bulk and on the surface of a model crystal.

The model copper crystal had the shape of a parallelepiped, in which the boundary effects were excluded by formulating periodic boundary conditions in all directions. The structure of this crystal in a deformed state was analyzed using an algorithm proposed in [5], which took into account the topology of bonds between each atom and its nearest neighbors. According to this algorithm, each pair of atoms is assigned a set of four indices: the first index characterizes the "disposition" of atoms (1 for nearest neighbors and 2 otherwise); the second index shows the number of common neighbors for atoms of the given pair; the third index gives the number of bonds between common neighbors; and the fourth index shows the number of bonds in the longest continuous atomic chain passing through the neighbors of the given pair. In the ideal fcc structure, each atom is characterized by 12 sets {1/4/2/1}; atoms in the ideal hcp structure are characterized by six sets {1/4/2/1} and six sets {1/4/2/2}; in the ideal bcc structure is characterized by eight sets {1/0/0/0}

The single crystal in the initial state was oriented so that the crystallographic directions [110], $[1\bar{1}0]$, and [001] were parallel to the *X*, *Y*, and *Z* axes, respectively. As is known, a uniform 20% contraction of the crystal in the [001] direction and simultaneous uniform 12% extension in the [110] and $[1\bar{1}0]$ directions leads to the transformation of the initial fcc structure to the bcc lattice (scheme A). Upon this transformation, a change in the potential energy per atom is several hundredths of an electronvolt. The atomic volume per atom in the course of this deformation remains unchanged.

The dynamic loading was simulated using the following initial conditions. The rate of compression along the *Z* axis was about 50 m/s, while the rates of expansion in the lateral directions corresponded to the

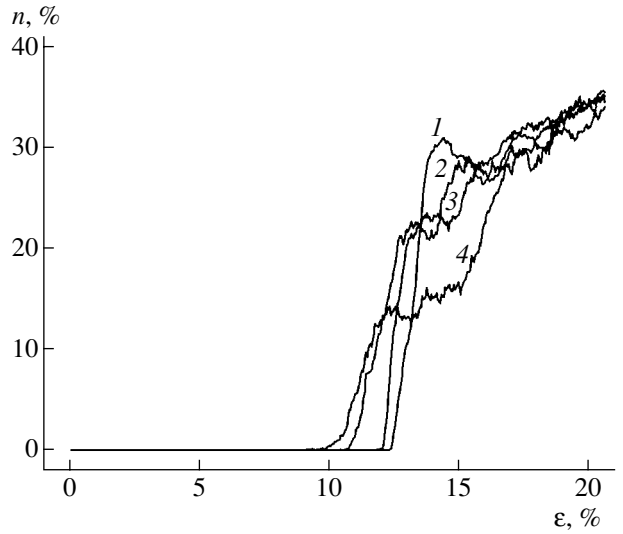

Fig. 1. Plots of the fraction n of atoms with a topology of bonds corresponding to the bcc lattice versus the degree of deformation ε of the initial fcc copper at various temperatures (K): (*1*) 100; (*2*) 300; (*3*) 500; (*4*) 700. The rate of sample compression along the Z axis ([001] direction) is 50 m/s.

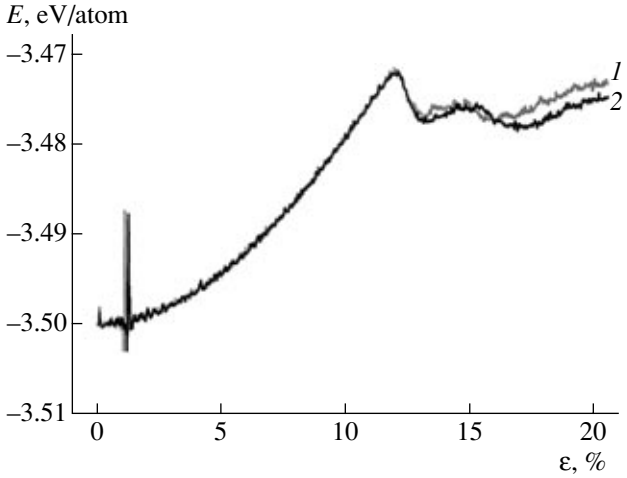

Fig. 2. Plots of the potential energy E per atom as versus the degree of deformation ε at 300 K at a rate of 50 m/s according to (*1*) scheme A and (*2*) the Bain scheme.

aforementioned algorithm (scheme A) of the crystal structure transformation from the fcc to bcc lattice. The influence of temperature on the structural response of the model crystal was studied by simulating the process at 100, 300, 500, and 700 K.

Figure 1 shows the results of simulations illustrating the effect of the sample temperature on the nucleation and development of structural defects in the model crystal under high-rate deformation conditions. As can be seen, the deformation at low temperatures is accompanied by a virtually jumplike growth in the number of defects. As the temperature is increased, the generation of regions featuring local changes in the lattice structure begins at lower degrees of deformation and is described by less steep curves. This behavior is evidence for the thermal fluctuation mechanism of the generation of regions with local structural changes (higher temperatures favor the earlier nucleation of structural defects). Note that the fraction of structural defects increases at lower temperatures, which is related to a higher level of pumped elastic energy.

It should also be noted that there are alternative geometric schemes of loading by which an fcc structure can be transformed into a bcc lattice. One well-known pathway is via the Bain scheme [6], according to which the initial fcc lattice ($c/a = 1$) is contracted in the [100] direction and simultaneously expanded to an equal extent in the [010] and [001] directions so that the volume per atom remains unchanged. On reaching $c/a = 1/\sqrt{2}$, the lattice transforms from fcc to bcc. Calculations showed that the course of variation of the potential energy in the case of crystal deformation according to this scheme is qualitatively analogous to the case described above, since the passage from fcc to bcc lattice in both cases does not involve the surmounting of an energy barrier and, hence, the sample response is much alike. This conclusion was confirmed both by the curves showing the fraction of regions with local structural changes and by the coinciding shapes of the potential energy variation as a function of the degree of deformation (Fig. 2). An analysis of these results showed that the jump in the potential energy at low deformations (~2%) is related to the fact that the characteristic rates of structural changes necessary for relaxation of the model crystal in this interval of ε values are significantly lower than the loading rate employed.

Thus, the results of our molecular dynamics investigation lead to a conclusion that the thermal fluctuations of atoms may cause the nucleation of structural defects in materials with the initially perfect crystalline structure subjected to a high-rate mechanical loading. In the cases studied, the character of nucleation and development of such structural defects is determined to a considerable extent by the sample temperature and is less dependent on the scheme of loading.

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