

# Nucleation of Structural Defects in Materials with a Perfect Crystal Lattice by Thermal Fluctuations under Dynamic Loading

S. G. Psakh'e,<sup>1</sup> K. P. Zol'nikov,<sup>1</sup>  
D. S. Kryzhevich,<sup>1</sup> and A. G. Lipnitskii<sup>1</sup>

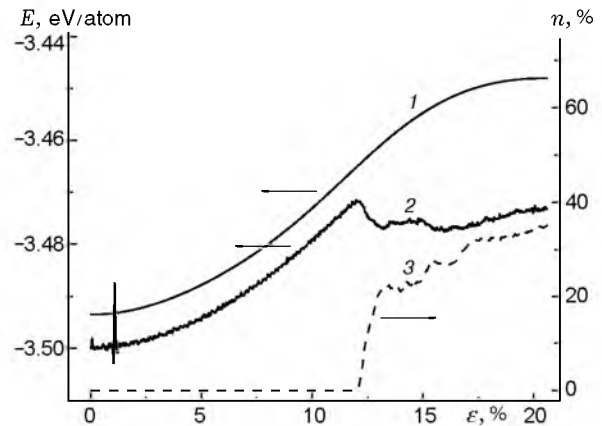
UDC 539.63

**A molecular-dynamic study of nucleation of structural defects in materials with an initially perfect crystal lattice by thermal fluctuations under high strain rates is performed. It is shown that thermal fluctuations can generate structural defects. There exists some threshold value of strain at which abrupt growth of regions with local structural changes is observed.**

**Key words:** crystal lattice, molecular dynamics, thermal fluctuations.

An important aspect in studying the material behavior under dynamic loading at the microscopic level is simulation of nucleation and formation of structural imperfections, which include point defects, dislocations, packing defects, microcracks, etc. In addition, a comprehensive study of atomic mechanisms giving rise to local structural rearrangements, which can be classified as the so-called precursor states [1], is undoubtedly a fundamental problem in solid-state physics and material science. It has been widely recognized (see [2–6]) that the nature of such processes is largely determined by the fact that the deformable material is a hierarchically organized sophisticated system whose atomic subsystem is inevitably involved into the macroscopic response of the material to external actions.

The investigation into the mechanisms of defect nucleation as applied to materials with an initially perfect structure under conditions of high-velocity mechanical actions is a topical problem of fundamental significance in revealing general features of plastic deformation processes. As no stress concentrators are present in materials with a perfect crystal structure, it can be anticipated that thermal fluctuations could be responsible for nucleation of local structural rearrangements and plastic deformation in such materials.

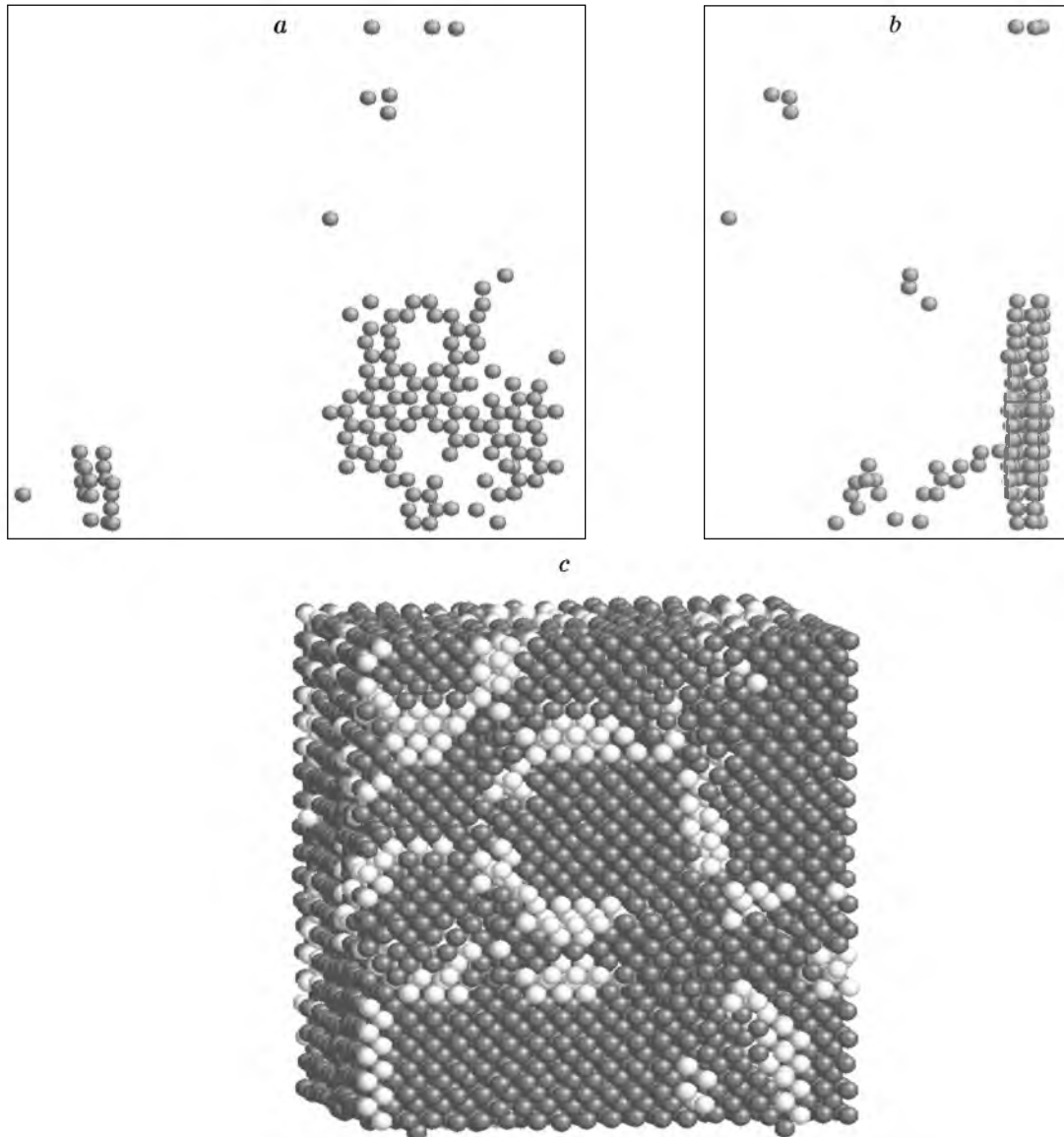


**Fig. 1.** Potential energy per one atom at 0 (1) and 300 K (2) in a material under the rate of compression of 50 m/sec; fraction of atoms with the topology of structural bonds typical of the hexagonal close-packed lattice (3).

In connection with the aforesaid, the purpose of the present study was to investigate the atomic mechanisms responsible for nucleation of plastic strains in a material with an initially perfect structure at finite temperatures.

<sup>1</sup>Institute of Strength Physics and Material Science,  
Siberian Division, Russian Academy of Sciences,  
Tomsk 634021; root@ispms.tomsk.ru.

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**Fig. 2.** Atomic structure in a region with local structural changes under 11.3-% compression along the  $Z$  axis, as viewed from two different angles (a, b); general view of the simulated crystallite under 18-% compression along the  $Z$  axis (c) (light spheres are atoms that belong to regions with local structural changes).

The posed problems were solved using the molecular-dynamic modeling with interatomic interaction potentials constructed within the framework of the embedded-atom method [7–9]. Such potentials make it possible to accurately predict the structural, mechanical, and energetic properties not only inside the bulk of the materials but also on their free surfaces and in near-surface regions [10].

The simulated copper crystal was shaped as a parallelepiped. To avoid surface effects, we used periodic boundary conditions in all directions. The structure of

the deformed material was analyzed using the algorithm developed in [11], which takes into account the topology of structural bonds of each atom with its neighbors. In this algorithm, a set of four numbers corresponds to each pair of atoms. The first number shows the “relation” between the atoms (1 for neighboring atoms and 2 otherwise), the second number gives the total amount of common neighbors for a given pair of atoms, the third number is the number of bonds between the common neighbors, and the fourth number is the total number of bonds in the longest continuous chain passing through

the neighbors for a given pair. Each atom is characterized by 12 sets of numbers  $\{1/4/2/1\}$  in the perfect face-centered cubic (FCC) structure, 6 sets  $\{1/4/2/1\}$  and 6 sets  $\{1/4/2/2\}$  in the hexagonal close-packed (HCP) structure, and 8 sets  $\{1/0/0/0\}$  in the body-centered cubic (BCC) structure.

The copper crystallite used in the simulations was oriented as follows: the  $X$  axis was directed along the crystallographic direction  $[110]$ , the  $Y$  axis was aligned in the direction  $[1\bar{1}0]$ , and the  $Z$  axis was set in the direction  $[001]$ . It is well known that uniform compression of a FCC crystal by  $\approx 20\%$  along the direction  $[001]$  with simultaneous extension of this crystal by  $\approx 12\%$  along the directions  $[110]$  and  $[1\bar{1}0]$  transform the initial structure into a BCC structure. As an example, curve 1 in Fig. 1 shows the potential energy per one atom versus strain for a crystal temperature  $T = 0$  K. To allow for temperature-induced effects, the initial crystallite was first let relax at room temperature to be then deformed in the directions indicated above.

Figure 1 also shows the calculated potential energy per one atom versus strain in the crystal at a temperature of 300 K under the rate of compression of 50 m/sec along the  $Z$  axis (curve 2). It is clearly seen that allowance for temperature substantially modifies the curve behavior. In analyzing the potential energy as a function of strain, curve 2 can be conventionally divided into two segments: the first segment is characterized by an increase in potential energy, and the second segment describes the temporary decrease in potential energy and its subsequent (much slower) increase.

An analysis of the simulation data showed that the beginning of the second stage is directly related to formation of regions with local structural changes (involving atoms with sets of numbers typical of the HCP structure). This can be clearly seen by comparing curves 2 and 3, the latter curve presenting the fraction of atoms ( $n$ ) that belong to regions with local structural changes. Atoms from these regions are shown in Fig. 2a and b, as viewed from different angles, in the crystal with a strain of 11.3%. As it follows from the inspection of the mutual arrangement of atoms, the inner structure in these regions resembles the structure of the packing defect. The general (three-dimensional) form of the crystallite under subsequent (18%) strain is plotted in Fig. 2c; these regions are seen to be oriented along certain crystallographic directions. It should be noted that zones of distortions in the crystal lattice not associated with the HCP structure are formed during the deformation process in addition to regions with local structural changes. Origination of these regions is of the fluctuation nature. Some of these regions subsequently transform into structural imperfections with

the HCP symmetry manifested as a saw-like shape of curve 2 in Fig. 1.

Thus, a direct molecular-dynamic simulation was performed for the first time to show that structural defects in materials with a perfect crystal lattice under dynamic loading can be generated by the mechanism with thermal fluctuations. It is found that there exists some threshold strain at which an abrupt growth of regions with local structural changes begins. Though the loading system in the present study was deliberately chosen to provide for a directional change in symmetry toward the BCC structure, the topology of these regions corresponded to the HCP lattice. Apparently, such a behavior is a consequence of comparatively close values of energy of the FCC and HCP structural states.

## REFERENCES

1. V. A. Polukhin, *Modeling of the Nanostructure and Precursor States* [in Russian], Izd. Ural. Otd. Akad. Nauk, Ekaterinburg (2004).
2. V. E. Panin, "Foundations of physical mesomechanics," *Fiz. Mezomekh.*, **1**, No. 1, 5–22 (1998).
3. V. A. Likhachev, V. E. Panin, E. E. Zasimchuk, et al., *Cooperative Deformation Processes and Deformation Localization* [in Russian], Naukova Dumka, Kiev (1989).
4. V. A. Likhachev, A. E. Volkov, and V. E. Shudegov, *Continual Theory of Defects* [in Russian], Izd. Leningrad. Univ., Leningrad (1986).
5. V. E. Panin, "Sinergetic principles in physical mesomechanics," *Fiz. Mezomekh.*, **3**, No. 6, 5–36 (2000).
6. S. G. Psakh'e and K. P. Zol'nikov, "Possibility of a vortex mechanism of displacement of the grain boundaries under high-rate shear loading," *Combust., Expl., Shock Waves*, **34**, No. 3, 367–368 (1998).
7. M. S. Daw and M. I. Baskes, "Embedded-atom method: Derivation and application to impurities, surfaces, and other defects in metals," *Phys. Rev.*, **B29**, No. 12, 6443–6453 (1984).
8. Y. Mishin, "Structural stability and lattice defects in copper: Ab initio, tight-binding, and embedded-atom calculations," *Phys. Rev.*, **B63**, 224106 (2001).
9. S. M. Foiles, M. I. Baskes, and M. S. Daw, "Embedded-atom method for the fcc metals Cu, Ag, Au, Ni, Pd, Pt, and their alloys," *Phys. Rev.*, **B33**, No. 12, 7983–7991 (1986).
10. S. G. Psakh'e, K. P. Zol'nikov, and T. Yu. Uvarov, "New approach to the application of multilayer superthin coatings: Effects of mixing," *Combust., Expl., Shock Waves*, **36**, No. 4, 543–545 (2000).
11. H. Van Swygenhoven, D. Farkas, and A. Caro, "Grain-boundary structures in polycrystalline metals at the nanoscale," *Phys. Rev.*, **B62**, No. 2, 831–838 (2000).