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The influence of the surface on the fracture process of nanostructures under dynamic loads

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ABSTRACT

In this paper, the authors conducted a study of the free surface effect on the process of damage, deformation and fracture of metallic nanoclusters. In particular, a detailed study of the dynamic processes in systems of surface and bulk atoms in a metallic copper crystal caused by the movement of one of the external borders of the crystal at a constant velocity was conducted.

1. Introduction

The present work aims to address the fundamental problem of determining the role of free surfaces in the processes of nucleation and transfer of transfer defects, the development of plastic deformation, crack initiation, and further fracture of materials at the microscopic level. The detailed study of this problem will justify the theoretical basis of three basic principles of physical mesomechanics [1]: (a) surface layers of solids act as an independent mesoscale level of deformation, which defines the primary nucleation of deformation defects; (b) stress concentrators that formed on the internal interfaces determine the prevalence of plastic shear and crack nucleation in the bulk layer of deformable solids; and (c) surface layers and internal interfaces control the development of mass transfer processes in a loaded solid.

In particular, a detailed study of dynamic processes in systems of surface and bulk atoms in the metal nanostructure caused by movement of one of the boundaries at a constant velocity was conducted. In this case, the surface layers were considered as independent subsystems of atoms [2] in accordance with the basic statements of physical mesomechanics. The studies were conducted on metal solid structures with dimensions in the nanometer range, at which these effects are particularly evident. In this case, the characteristics of the spatial and temporal scales of the processes were approximately 10^{-9} cm and 10^{-12} s, respectively. It is known that the experimental study of such processes is currently impossible. As a result, the molecular dynamics method based on first principles was used in this study.

To date, there are many works devoted to research regarding the response of nanostructures to external mechanical loads, including the material fracture evolution. In this study, the role of the surface in this response is investigated. Thus, following the works of [3–6], an initial central crack is introduced by removing the corresponding atoms, and then its evolution under the external dynamic loads is investigated.

A comprehensive review of the studies of fatigue-crack growth is found in the work of [7]. However, in the presented works, the nanocrack was created beforehand, and the processes in the surface atoms system were not simulated in detail.

Studies of the fracture process under dynamic loading can be found in [8,9]. However, three-dimensional periodic boundary conditions were imposed in [8], and two-dimensional periodic boundary conditions along the Y and Z axes were applied at the impact loading in [9], which initially excludes the study of processes in the surface atom subsystem.

The problem statements of the works [10,11] are similar to that of the present paper. The strain rate, temperature and size-dependent effects on the mechanical properties of diamond nanowires were studied in the work of [10]. Similar research studies were conducted for FCC nickel nanowires in the work of [11]. However, in these works, no detailed study was performed of processes in the bulk and in the surface layer and of the fracture evolution in these subsystems.

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A thorough investigation of processes in the surface and subsurface layers was realized in the work of [12], but the processes were examined at high speed grinding, in contrast to the present work, where the fracture process was investigated for the motion of one edge at constant velocity.

In the work of [13], a study was performed of the ability of Continuum mechanics to predict the material response at the atomic scale on the example of a graphene sheet; however, in this work, the investigation of processes in the surface and bulk atom subsystems was not conducted.

The work most similar to the present work is the research of [14] involving the study of the influence of the surface on nanostructure properties. The authors of [14] particularly studied the surface properties of silicon nanoplates and their effect on the mechanical characteristics of silicon nanoplates. In spite of that report, the direction of our research does not coincide with the work of [14] for a number of reasons. The primary reason is that our work involves a different material and the approximation of elastic deformation of the material in which the processes strongly differ from the processes at the structure fracture. The second reason is the use of quasistatic deformation assumption in the work of [14]. The expressions (2)–(4) and (6) are true only in the frame of this assumption. As a result, the authors of [14] should execute the system mesoanalysis in the future and demonstrate that the strain is indeed constant along the full length of the nanostructure in the realized molecular dynamics calculations.

As demonstrated in the present paper, the local strain at dynamic loading, and especially before fracture, can differ by an order of magnitude from the strain of the total system. This difference stipulated the use of another approach for the determination of the properties of the surface atoms and the bulk atoms. Thus, the analysis of dynamic processes in the subsystems of the surface and bulk atoms is required to address the absence of such research studies in the literature.

2. Description of the physical and mathematical model

The illustration of fracture in the solid nanostructures is provided for a copper cluster of cuboid shape, with dimensions of 50, 5, and 5 crystal cells along the X, Y, and Z axes, respectively. The crystal orientation (1,0,0) was selected for clarity of the results. To describe the interatomic interactions, Voter's many-body potential was used [15].

In the molecular dynamics calculations, Verlet's velocity modification was used as a numerical scheme with a time step $\tau = 10^{-16}$ s, enabling an accuracy of the energy at the end of the calculation (N_t = 500,000 of 10^{-5}%.

Atoms were initially placed in the sites of the perfect crystal fcc-lattice. Next, using the method of artificial viscosity [16], the coordinates and momenta of the system in the state of the global minimum potential energy (“cooling” system) were found. Finally, the obtained values of the coordinates and momenta were used as the initial data.

The boundary conditions were simulated as follows. Atoms of extreme faces, perpendicular to the X axis, were placed in a harmonic potential:

$$V(\vec{r}_i) = \frac{k}{2}\left(x_i - x_i^0 - v_0 t\right)^2$$

Here, x_i^0 is the coordinate of the i-th atom face after cooling. On the left side, the velocity v_0 is assumed to be zero, and on the right side, it was the controlled external parameter. This enabled the simulation of fixed and moving clamps using a generalized non-steady potential. The lateral boundaries were free.

The velocity of movement of the free (right) boundary varied from 10 m/s to 500 m/s, which allowed for the simulation of the velocity of the unit elongation in the range from 10^{+8} to 10^{+10} s^{-1} for the selected size range of the structure.

3. Calculation of the system mesocharacteristics

The system mesocharacteristics are defined as the characteristics related to certain subsystems of atoms. The selection of crystal orientation (1,0,0) provided the simplest orientation of atomic planes in the space – they are perpendicular to the X axis. In this regard, the entire crystal was divided into mesovolumes of rectangular parallelepiped shapes and one atomic plane. Along the X axis, the mesovolume size was determined by the following formula:

$$\Delta L_i = \frac{(x_{i+1} + x_i)}{2} - \frac{(x_i + x_{i-1})}{2}$$

where x_i is the average value of x-coordinates of atoms in the i-th plane. Knowing the array of mesovolume lengths at the initial and arbitrary points of time allowed for determination of the spatial distribution of local elongations ε_x at any time.

The mesovolume transverse sizes are based on the average values of y- and z-coordinates of the extreme atoms in the i-th plane.

Such a detailed approach enables the calculation of the density, the velocity of the centers of masses, the temperature in the mesovolumes and the binding energy between the atomic planes at the desired times.

The mesoanalysis of the potential energy was based on the following characteristics. The potential energy of the atomic planes U_b was a common definition of the relations between the two subsystems A and B: $U_b = U_{A+B} - U_A - U_B$. Here, U_{A+B} is the total energy; U_A is the energy of the subsystem A, as if there were no subsystem B; and U_B is the subsystem of the subsystem B, as if there were no subsystem A. Physically, the energy U_b equals in its modulo the work required for complete separation of the system into independent subsystems A and B separated by an infinite distance.

Throughout the paper, the system of bulk atoms refers to the atoms with the coordination number 12, as in the perfect infinite fcc lattice. If the number of the nearest neighbors is less than 12, then the atoms are called surface atoms by the construction. Having the feature of surface or bulk atom, all characteristics listed above were calculated for the subsystems of the surface and the bulk atoms lying in one atomic plane.

The problem of choosing the system boundaries of bulk and surface atoms was solved in the following way. To select the boundary between bulk and surface atoms, the geometric equivalence principle was used for the volumes of these atoms. The border in the YZ plane was drawn midway between the atoms of these types. To determine surface boundaries, the condition of coincidence of the experimental and calculated density of the substance (in this case, of copper) was used. The external border should be shifted to 0.25 Å from the coordinates of the surface atoms (or more precisely, the nuclei of atoms). Therefore, the algorithm for calculating the cross-sectional area was as follows. The average values of the y- and z-coordinates of the extreme volume and the surface atoms were determined. The coordinates of the separating surfaces were a half-sum of these coordinates. This algorithm allowed for determination of the cross-sectional area of the system of bulk atoms. The full cross-sectional area of the structure was based on the knowledge of the coordinates of the surface (the average values of the coordinates of the atoms in the surface plane and the added padding). The sectional area of the surface atoms was determined as the difference between the total cross-section and the section of bulk atoms.

The analysis of the forces acting in the atoms of the subsystems was performed as follows. The x-coordinate x_{pi} was determined between two successive atomic planes i_p and $i_p + 1$, and based on the known Voter's potential, the forces acting on atoms with the x-coordinate less than x_{pi} from the atoms with the x-coordinate