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Molecular-Dynamics Simulation of the Interaction Processes of Pulsed Ion Beams with Metals

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Abstract—The molecular-dynamics method is used to model the interaction processes of pulsed ion beams with metal targets. The main parameters of a pulsed ion beam interacting with a target are the ion energy, pulse duration, and charge density per unit area of the target. Using averaged values of these parameters of ion beams published for various types of accelerators, a numerical study of the dependence of the dynamics of thermal and structural processes in irradiated targets upon a change in the size and heterogeneity of the structure is performed. Simulation of the irradiation processes and estimates of the distribution of beam ions in the volume are carried out in the range of beam ion energies of 1–2 keV using the concept of a shock wave. The results are important for developing the model of a pulsed ion beam and classifying the types of structural changes in the irradiated material depending on the model parameters.

Keywords: modeling, molecular-dynamics method, pulsed ion beams, target destruction, shock wave
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INTRODUCTION

Experimental and theoretical studies in such areas of radiation physics as the resistance of structural materials to exposure to radiation and a purposeful change in the properties of materials by irradiating them with particle beams have been carried out in Russia for more than 40 years. The use of high-power pulsed ion beams (HPIB) in experiments as sources of irradiation [1–5] can, despite differences in the mechanisms of interaction of materials with other sources, significantly reduce the time required to obtain the target outcomes of the research. This is possible with adequate theoretical description of the main mechanisms of interaction between a HPIB and a target and their dependence on the beam parameters. The main parameters of a pulsed ion beam interacting with a target are the ion energy, pulse duration, and charge density per unit target area. Using these parameters, it is possible to roughly estimate the number of ions incident on a unit of target surface area, depending on time, and this is important information for mathematical modeling. However, the distribution of beam ions in the volume is information that cannot be fully determined based on the parameters of the HPIB, which can affect the results of theoretical calculations. In the general case, the distribution of particles in space at the exit of the accelerator is understood as the number of particles per unit volume, depending on three coordinates: longitudinal Z coinciding with the direction of the beam, and two transverse X and Y [6–8]. Thus, it is necessary to more accurately estimate the number of ions in the pulse of the beam interacting with the target. We note that the theoretical and experimental characteristics of various materials sometimes differ by orders of magnitude. For example, the theoretical and experimental strength properties of metals and some alloys differ by two or three orders of magnitude [9, 10]. This is mainly due to the fact that theoretical calculations are based on the structure of ideal crystals, and real crystals may contain impurities and various defects. Consequently, theoretical studies should be carried out taking into account possible violations of the ideal structure of the target before its irradiation.

At present, in connection with the development of high-performance computing systems and parallel programming technologies, mathematical modeling based on the molecular dynamics (MD) method [11, 12] has become relevant in wide areas of science and technology, including for solving the problems discussed here. The aim of this work is to obtain information for the development of a model of a pulsed ion beam by means of MD simulation of the interaction of HPIB ions with energies of 1–2 keV with metal targets, depending on the beam distribution in the volume, as

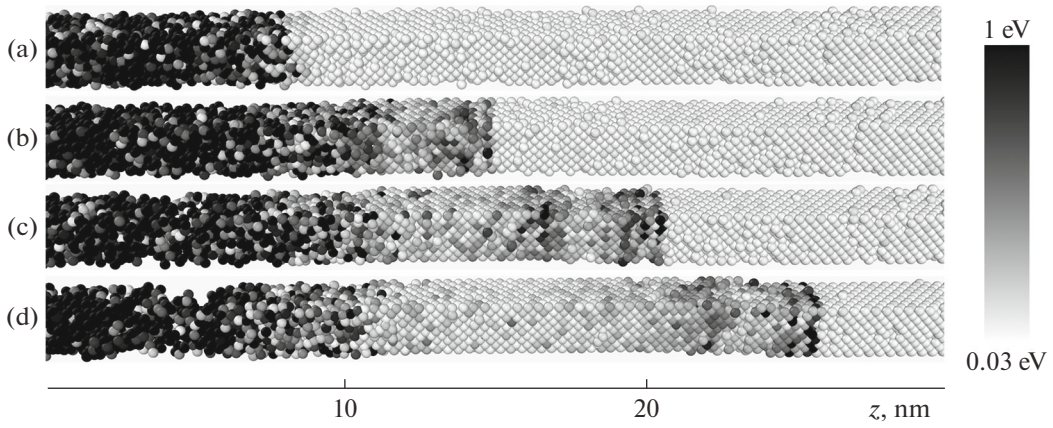

Fig. 1. Dynamics of thermal processes and a shock wave upon irradiation with four copper ions with an energy of 1 keV at the moments of time: 1 (a); 2 (b); 3 (c); 4 ps (d). The target size is 2 × 2 × 40 nm.

well as simulation of the irradiation of a target with a structural defect.

MODEL PARAMETERS AND OBTAINED RESULTS

As indicated above, the main parameters of the HPIB for modeling the interaction of a beam with a target within the framework of the MD method are the ion energy, pulse duration, and charge density per unit target area. These parameters for various types of accelerators are given in [6–8]. The average values of the HPIB parameters in a pulse for modifying the target surface are as follows: beam power density of $R = 10^6$–10^{10} W/cm^2, ion energy of $E_0 = 100$–1000 keV, pulse duration of $\tau = 10^{-8}$–10^{-6} s, and an irradiation area of $S = 10$–50 cm^2 [5]. Using these data, in this work, we simulated the irradiation of a metal target by pulsed ion beams with an energy of 1–2 keV, since at this energy, mainly elastic energy losses of ions incident on the target occur, and inelastic energy losses can be neglected.

Earlier [13–15], the authors simulated the processes in a copper target under irradiation with copper nanoclusters; therefore, in this work, we used a copper target and copper ions, as well as a similar beam model. The simultaneous interactions of two to four copper-ion atoms in different regions of the target surface are simulated in a single beam pulse. The parameters of the pulsed ion beams during simulation: ion energy of 1–2 keV and particle density of 10^{13}–10^{14} atom/cm^2 (0.1–1 atom/nm^2). At an ion energy of 1–2 keV, their range in the target is several tens of nanometers, and the irradiation area is several square centimeters, and this makes it possible to use periodic boundary conditions in modeling. The use of periodic boundary conditions makes it possible to change the particle density when the target size changes along the axes x and y [16, 17]. In the simulation, the size of the parallelepiped-shaped target was selected from the range (2–10) × (2–10) × (40–80) nm with periodic boundary conditions in the directions x and y, irradiation was carried out in the direction z, where the target is adjacent to vacuum. Modeling was carried out using the LAMMPS package [18], and the EAM (Embedded Atom Model) [19], the potential for copper embedded in the LAMMPS package, was taken as the interatomic potential. The calculation results were visualized using the OVITO program [20]. They are presented as a visualization of the target structure, in which the color of the particle corresponds to its energy at different times. At the first stage, modeling was carried out for ideal crystal lattices. Figure 1 shows the results obtained by simulating the irradiation of a copper target by a pulsed beam consisting of four copper atoms with an energy of 1 keV. When irradiated, ions move along one line along the axis z, and the distance between them is 20 nm. The change in time of thermal processes and the structure of the target during the propagation of a shock wave in it, as well as structural changes near the surface, are shown.

Figure 2 shows the results obtained by simulating the irradiation of a copper target with a pulsed copper beam consisting of four copper atoms with an energy of 2 keV. The results reflect the dynamics of the destruction of the target edge under irradiation with a beam with a pulse of four ions with an energy of 2 keV. This occurs due to reflection of the shock wave from the edge of the sample; upon reflection, the shock wave—a compression wave—becomes an extension wave. When the amplitude of this wave exceeds the ultimate strength of the target, structural fracturing of the "spalling" type occurs at its edge (Fig. 2). This effect takes place for thin targets at a corresponding energy—in this case, at an energy of 2 keV. When a thin

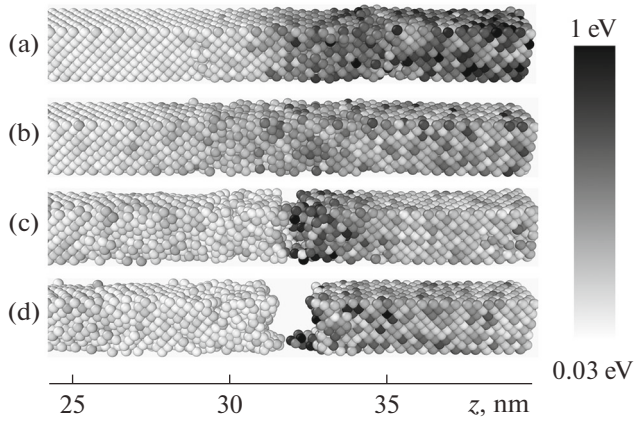

Fig. 2. Dynamics of the structural changes in the depth of the target under irradiation with four copper ions with an energy of 2 keV at the times: 8 (a); 9 (b); 10 (c); 11 ps (d). The target size is 2 × 2 × 40 nm.

target is irradiated with a beam of four ions with an energy of 1 keV, such damage does not occur. With increasing target thickness, in order to observe fracture of the "spalling" type, it is necessary to increase the energy and density of irradiation. In practice, the surfaces of bulk targets are irradiated, and the resulting shock wave goes deep into the target. If the target is an ideal crystal lattice, no structural changes occur in it. In practice, experiments are usually carried out with targets that are real crystal lattices containing various impurities, defects such as vacancies, dislocations, and pores. Since the shock wave is reflected from the edge of the target, simulation should be carried out for crystal lattices with pore-type defects. In this case, presumably, part of the shock wave can be reflected from a pore in the crystal lattice of the target or change the pore structure, which leads to subsequent disappearance of the pore itself, i.e., the properties of the target actually change. Therefore, the second stage of research was carried out for targets with different pore arrangements. Figure 3 shows the results obtained in the simulation of irradiation of the target containing a pore with a pulsed copper beam consisting of two copper atoms with an energy of 1.5 keV, in a cross section.

Figure 4 shows the results obtained in the simulation of the irradiation of a target containing a pore with a pulsed copper beam consisting of four copper atoms with an energy of 1 keV, in a cross section, at different times. This figure clearly shows the effect of the shock wave on the disappearance of the pore in the target. Similar results can be obtained for pores of other sizes, depending on the energy and density of the beam. Another possible change in the irradiation parameters is a change in the distance between beam ions. This leads to a change in the irradiation intensity (changes in the irradiation power per unit time). One of the

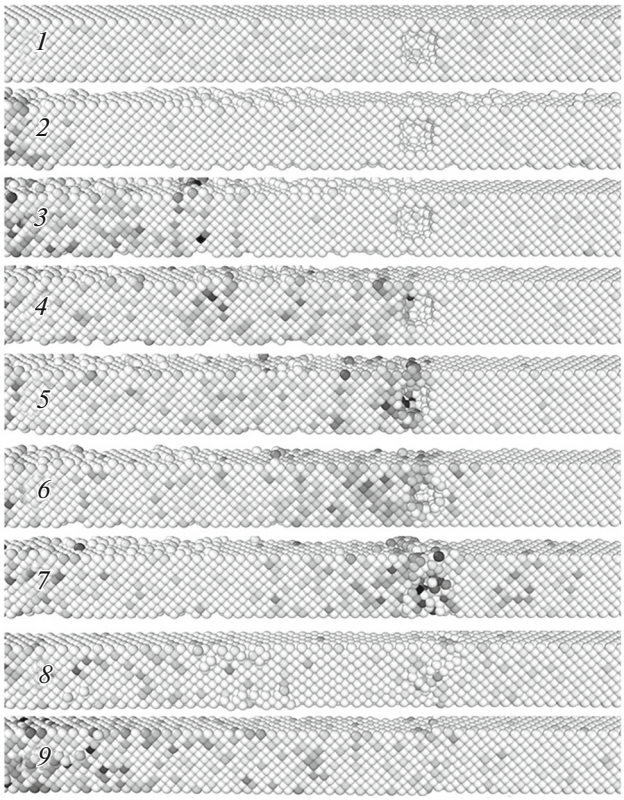

Fig. 3. Dynamics of the shock wave and its effect on a pore with a size of 1 nm at a target depth of 20 nm under irradiation with two copper ions with an energy of 1.5 keV at different times: 0 (*1*); 1 (*2*); 2 (*3*); 3 (*4*); 3.2 (*5*); 3.4 (*6*); 4 (*7*); 8 (*8*); 12 ps (*9*). The target size is 2 × 2 × 40 nm.

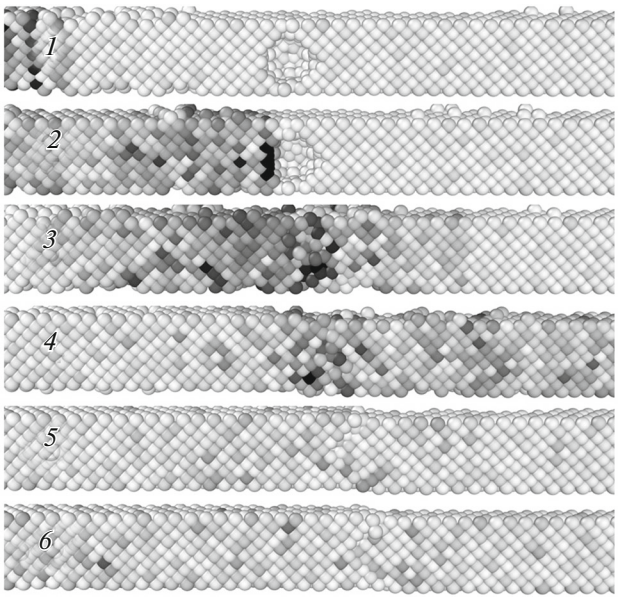

Fig. 4. Dynamics of a shock wave and its effect on a pore with a size of 1 nm at a target depth of 25 nm under irradiation with four copper ions with an energy of 1 keV at different times: 3 (*1*); 4 (*2*); 5 (*3*); 6 (*4*); 10 (*5*); 20 ps (*6*). The target size is 1.8 × 1.8 × 72 nm.

important results in these studies is determination of the values of the threshold energy and power density of the beam at which the pore disappears. Thus, by varying the beam parameters, various interesting results can be obtained.

CONCLUSIONS

The results of modeling the irradiation of metal targets with a pulsed ion beam are obtained as a function of the ion energy and target size. Thermal processes, the formation of shock waves and their effect on the structure of the target are investigated. Irradiation of the target with a beam of four ions with an energy of 1 keV and a beam of two ions with an energy of 1.5 keV leads to disappearance of the pore. The results obtained show that, by increasing the energy and power density of the irradiation (the number of particles), it is possible to change the defect structures at different depths of the target. These results can be used for further development of the pulsed ion-beam model. An important step in these studies is also classification of the results depending on the various parameters of the HPIB, which is planned in future studies.

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