Molecular dynamic investigations of the shock pulses interaction with nanostructured free surface of a target

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Abstract. We performed the molecular dynamic simulations of the high-velocity impact of thin copper impactor with copper targets with both flat and nanostructured rear surface. It is shown that the spall fracture threshold can be increased due to the presence of nanostructures on the rear surface of target. Presence of protrusions changes the stress state and provokes an intensive plastic deformation. As a result, a part of the compression pulse energy dissipates due to the plastic deformation in this surface layer. It leads to decrease of the tensile wave amplitude and, consequently, an increase of the spallation threshold in terms of the incident shock wave intensity. The threshold increase is essential if the protrusion height is about the compression pulse width, which is controlled by the impactor thickness first of all.

1. Introduction

High-speed impact [1,2] or intensive irradiation [3–7] generates in material a compression pulse, which is a shock wave followed by an unloading wave. Reflection of the compression pulse from a free surface of material leads to formation of a tension wave propagating in the inverse direction. Action of tensile stresses can results in the spall fracture, which is commonly referred as a rear spallation. Molecular dynamic (MD) simulations are widely used for investigation of the shock wave propagation in metals and the rear spallation. The problem statements with both periodic [8–10] and free boundary [8] conditions along the directions perpendicular to the shock wave propagation direction are used in MD simulations. Free boundary conditions allow one to investigate the effect of side unloading on spallation. There are MD simulations of the jets ejection from the rear nanostructured surface of metals produced by strong enough shock waves [11, 12]. Meanwhile, we do not know any MD simulations investigating the rear surface nanorelief influence on the spallation threshold.

Deviation of the initial form of free rear surface from the plane one changes the stress state at the shock wave reflection in comparison with that is realized within the incident plane shock wave and, thus, influences the reflected wave amplitude. In this report, by an example of copper samples with thickness of tens of nanometers and by means of MD simulations, we investigated the influence of the surface nanorelief on the spallation threshold under the action of ultrashort compression pulses with duration of about a picosecond.
2. Molecular dynamic setup

MD simulations were done with using LAMMPS [13] and interatomic potential [14] for copper based on the embedded atom method [15]. Visualization of the atomic configurations were performed with the help of OVITO program [16]. The MD sample is a monocrystalline piece of copper (FCC lattice) with crystallographic directions \([100], [010] \) and \([001]\) coinciding with the \(x, y \) and \(z \) axes. The sample sizes along \(x \) and \(y \) axes were equal to 30 lattice parameters (about 11 nm) for all performed calculations. After initial thermalization during 2 ps in barostat at zero pressure and in thermostat at 300 K, a surface flat layer with the thickness of 15 lattice parameters (5.5 nm) obtains an additional velocity directed along \(x \) axis normally to the interface with the rest part of the sample. This surface layer plays the role of impactor, while the rest part of the sample is the target with flat (figure 1) or nanostructured (figure 2) rear surface.
Figure 2. Shock wave reflection from the rear surface of copper target with thickness of the continuous part of 27.5 nm and cylindrical protrusions with diameter of 7.3 nm and height of 5.5 nm: the total thickness of target with protrusions is 33 nm similar to the case of flat surface presented in figure 1. Impact is produced by copper impactor with the thickness of 5.5 nm, the impact velocity is 1500 m/s. Color corresponds to the centro-symmetry parameter in such a way that blue color corresponds to perfect lattice, green color corresponds to the traces of plastic deformation, yellow and red colors correspond to atoms on surfaces. Formation of voids without main crack and spallation is observed. Intensive plastic deformation takes place.
Calculations within the framework of NVE ensemble were performed after setting the impact velocity, which means conservation of the total energy of MD system. Periodic boundary conditions were set along all axes. Calculation domain was selected considerably larger than the MD system size along the direction of impact coinciding with $x$ axis, which provided the free boundary conditions on both ipmactor and target surfaces. The finite impactor generates a compression pulse propagating through the target; the compression pulse consists of the shock wave followed by the unloading wave. Along the $y$ and $z$ axes the MD system was periodically repeating with a period of 30 lattice parameters (about 11 nm). In the case of protrusions on the rear surface (figures 2), it is equivalent to the sample with the periodically situated protrusions.

Targets of different thicknesses—from 30 lattice parameters (11 nm) up to 120 lattice parameters (44 nm)—were investigated. Targets with flat rear surface and nanostructured rear surface of the same total thickness were compared. In the case of nanostructured rear surface, the total thickness is equal to the distance from the impactor boundary to the protrusion outer edge (compare figures 1 and 2). Cylindrical protrusions with diameter of 20 lattice parameters (about 7.2 nm) and various heights—from 5 lattice parameters (1.8 nm) to 40 lattice parameters (14.7 nm) were investigated in the main bulk of calculations. Several additional calculations were performed for the case of conical protrusions, which reveal that the investigated effect is more pronounced for cylindrical ones.

3. Results and discussion
Features of the compression pulse interaction with the flat and nanostructured rear surfaces are illustrated in figures 1 and 2, respectively. In the case of flat rear surface of target (figure 1), the picture is very typical. The initial discontinuity of velocity leads to formation and propagation of a compression pulse (5 ps). The substance velocity within this pulse is about half the impact velocity, which is expected due to the fact that both impactor and target are made of the same metal. Reflection of the compression pulse from the free surface increases velocity up to the value of impact velocity and leads to the rear surface motion (10 ps). Tension of substance near the rear surface leads to the plastic deformation, the initiation (10 ps) and development (15–20 ps) of the rear spallation. Distinct voids and formation of a main crack are observed for the considered impact velocity of 1500 m/s in the case of flat rear surface.

In the case of protrusions (figure 2), the compression pulse reflection becomes more complex. The shock wave cannot simply enter the protrusion because a uniaxial stress state should be realized inside such cylindrical element as opposed to the uniaxial strain state realized within a flat shock wave. Transition between the uniaxial strain and uniaxial stress states leads to the fact that both positive and negative pressures in protrusion are restricted by the plastic flow. Therefore, interaction of the compression pulse with the rear surface leads to an intensive plastic deformation of the protrusion and adjoined material (8–10 ps). The shock wave wrinkles the protrusion by means of plastic deformation; a considerable part of the shock wave energy is dissipated during this process. As a result, the impact velocity of 1500 m/s does not lead to formation of the main crack in the considered case of cylindrical protrusions. Voids are formed (10–20 ps), but thereafter are healed (40 ps) due to the action of stress waves propagating across the sample.

The compression pulse propagation and reflection from the rear surface is shown in figure 3 for the cases of flat (a) and nanostructured (b) samples. A steady compression pulse with the maximal stress of about 40 GPa is formed at the impact velocity of 1500 m/s. Reflection of this pulse from the flat rear surface results in formation of the tension wave (figure 3a), which is strong enough to lead to the spallation; the maximal tensile stress reaches 15 GPa at 3.2 ps from the impact beginning. In the case of nanostructured surface, the plastic deformation of protrusions restricts the tension wave amplitude by the value of about 12.5 GPa (figure 3b), which is not enough for spallation.
Figure 3. Spatial distributions over $x$ axis of the longitudinal stress in targets with flat rear surface (a) and rear surface with cylindrical protrusions (b) in consequent time moments. Total target thickness is 22 nm, impactor thickness is 5.5 nm, impact velocity is 1500 m/s. In the case of cylindrical protrusions, they have diameter of 7.3 nm and height of 5.5 nm. Stresses are averaged over $y$ and $z$ directions.

The effect of the spallation threshold increase in terms of the incident shock wave intensity was revealed in all considered cases: the threshold impact velocity for flat surface is always lower than that for the nanostructured surface. The maximal difference reaches about 600 m/s (about 20 GPa in terms of stresses in the incident shock wave). The threshold increase is essential if the protrusion height is about the compression pulse width, which is controlled by the impactor thickness first of all.

4. Conclusions
MD simulations for ultrathin copper targets show that the spall fracture threshold can be increased due to the presence of nanostructures on the rear surface of target. Presence of protrusions changes the stress state and provokes an intensive plastic deformation. As a result, a part of the compression pulse energy dissipates due to the plastic deformation in this surface layer. It leads to decrease of the tensile wave amplitude and, consequently, an increase of the spallation threshold in terms of the incident shock wave intensity. The threshold increase is essential if the protrusion height is about the compression pulse width, which is controlled by the impactor thickness first of all.

Interaction of moderate shock wave with the structured surface of solid metal, which has a significant strength relative to the form change, is qualitatively different from that is observed in the case of liquids, where the Richtmyer–Meshkov instability leads to the mass ejection from the surface [17–19], and in the case of strong shock waves [11, 12], at which the metal behaves itself as a liquid. We did not observe detachments of drops or dust from the rear surface. The absence of ejection is connected with both the elastic-plastic properties of the target material and with the comparability of the compression pulse width with the length of protrusions.

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