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# REFLECTION OF A SHOCK PULSE FROM A FREE SURFACE OF AL AND CU WITH NANORELIEF OR DEPOSITED NANOPARTICLES: MOLECULAR DYNAMICS INVESTIGATION

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**Key words:** Shock Waves; Spall Fracture, Nanorelief; Deposited Nanoparticles; Plastic Deformation; Molecular Dynamic Simulations.

**Summary.** We investigate the effect of the spallation threshold increase due to the presence of the deposited nanoparticles or nonorelief on the rear surface. The increase is substantial on the condition of comparability between the compression pulse width and the protrusion height or the deposited nanoparticles layer thickness; it is observed for ultra-short shock pulses.

## 1 INTRODUCTION

A high-speed impact [1] or an intensive irradiation [2] generates a compression pulse in material; the compression pulse is a shock wave followed by a rarefaction wave. Using of femtosecond laser pulses allows one to obtain compression pulses with duration of about a hundred of picosecons [3]. 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. Using the molecular dynamic (MD) simulations, we tried to investigate the conditions of nanoparticles removal from a free surface of metal by means of interaction of an ultra-short compression pulse with the surface with the deposited nanoparticles. A spallation threshold increase was revealed instead of removal. The increase means that the minimal (threshold) pressure jump in the shock wave leading to spallation for the free surface with the deposited nanoparticles is higher than that for an ideally plane surface. The effect is also valid for free surface with a nanorelief. In our presentation we consider the results of MD investigations of this effect for both cases of the deposited nanoparticles and the cylindrical nanoprotrusions.

## 2 PROBLEM STATEMENT

MD simulations are performed with the help of LAMMPS [4]. We use interatomic potentials [5] and [6] for copper and aluminum, respectively; both potentials are based on the embedded atom method. Atom configurations are visualized with the help of OVITO [7].

Layers of deposited nanoparticles or cylindrical protrusions are introduced in such a manner that the total thickness of the sample with nanorelief is the same as for the sample with an ideally plane rear surface. A plate impactor with a thickness ranging from 15 to 30 lattice parameters strikes the front surface of the sample generating a plane shock wave. The periodic boundary conditions are used in the transverse directions, which is equivalent to the periodically situated protrusions or particles. The threshold impact velocity and the corresponding pressure jump in the shock wave are compared.

## 3 RESULTS AND DISCUSSION

Figures 1 and 2 show the spall fracture in the case of flat rear surface and the absence of spallation in the case of deposited nanoparticles; the impact velocity and, consequently, the pressure jump in the shock wave are the same in both cases. As one can see from Figure 2, there is an intensive plastic deformation of the nanoparticles initiated by the shock wave, instead of spallation. Tabel 1 collects the threshold velocities obtained for various number of nanoparticle layers and radii of nanoparticles. In the case of cylindrical protrusions, the general behavior is the same, while the effect is even more pronounced. The case of protrusions is described in [8] in details.

| Number of layers | Diameter of particles (lattice constants) | Threshold velocity (m/s) |
|---|---|---|
| Flat surface | - | 1270 |
| 1 | 14 | 1340 |
| 1 | 20 | 1440 |
| 2 | 14 | 1350 |
| 2 | 20 | 1450 |
| 3 | 14 | 1370 |
| 3 | 20 | 1460 |

Table 1 : Threshold impact velocities in the cases of flat rear surface (upper row) and layers of deposited nanoparticles; aluminum target, nanoparticles and impactor; total target thickness is 120 lattice parameters; impactor thickness is 30 lattice parameters.

The revealed regularities are the following. In the case when the free surface is not a flat one and has some deposited nanoparticles, protrusions or troughs, which are comparable in size with the compression pulse thickness, the uniaxial strain state typical for a plane shock wave is changed on a more complex strain state during the interaction with these surface relief elements. As a result, a part of the compression pulse energy dissipates due to an intensive plastic deformation in this surface layer (Figure 2). It leads to a decrease in the tensile wave amplitude and, consequently, an increase in the spallation threshold in terms of the incident shock wave intensity. The increase is substantial on the condition of comparability between the compression pulse width and the protrusion height or the deposited nanoparticles layer thickness. Another condition is the ratio of the protrusion or the deposited nanoparticle cross-section to the total surface area, which should be neither small nor large– about 0.3-0.4 in the best case. At the nanorelief height higher than the compression pulse width or at large cross section, instability develops on the rear surface of target that is accompanied by the mass ejection and violation of the target integrity.

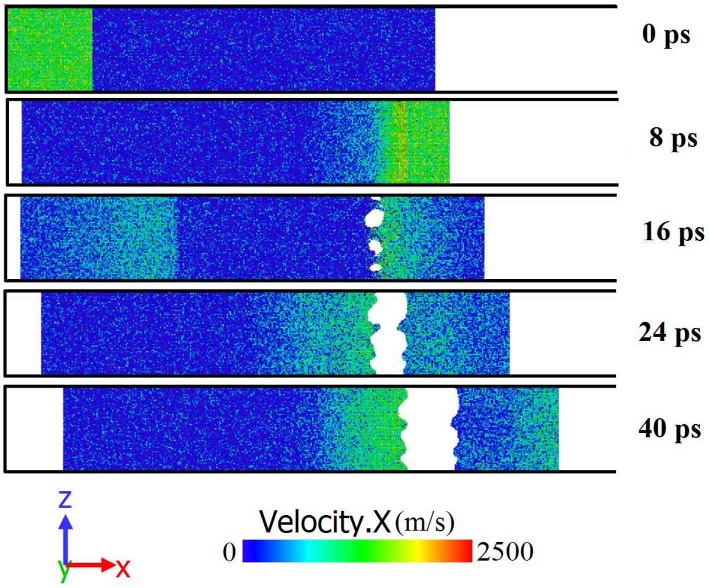


Figure 1: Reflection of the shock pulse from the plane rear surface: aluminum target and impactor; target thickness is 120 lattice parameters; impactor thickness is 30 lattice parameters; impact velocity is 1300 m/s. Color corresponds to the longitudinal component of the atom velocity. The following stages are shown: begining of the impact (0 ps), the shock pulse reaches the rear surface and reflects (8 ps), the nucleation and growth of voids near the rear surface (16 ps), the formation of a main crack (24 ps), and flying away of the spalled layer (40 ps).

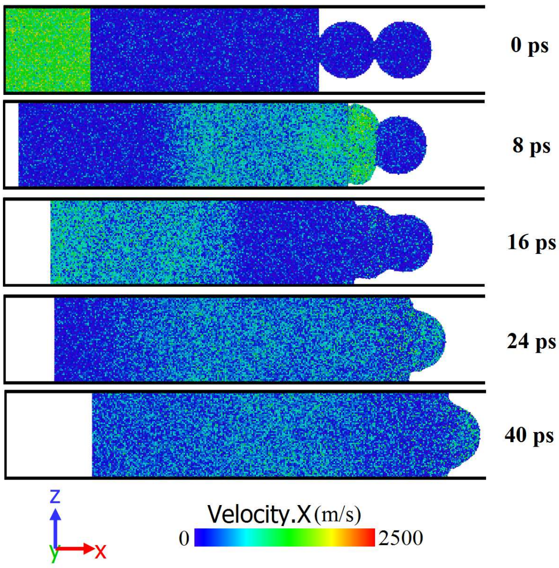


Figure 2: Reflection of the shock pulse from the rear surface with the deposited nanoparticles: aluminum target, nanoparticles and impactor; total target thickness is 120 lattice parameters (including nanoparticles); diameter of nanoparticles is 20 lattice parameters; impactor thickness is 30 lattice parameters; impact velocity is 1300 m/s. Color corresponds to the longitudinal component of the atom velocity. The following stages are shown: begining of the impact (0 ps), the shock pulse reaches the rear surface and flattens the nanoparticles (8-24 ps), and flying of the unfractured target (40 ps).

## 4 CONCLUSIONS

- Deposited nanoparticles or nanorelief make a free surface more persistent with respect to the spall fracture initiated by a reflecting compression pulse.
- The spallation threshold increase is due to the intensive plastic deformation of nanoparticles or nanorelief elements during the compression pulse reflection, which dissipates a part of the shock wave energy.
- Main regularities of this effect are investigated by means of molecular dynamic simulations.

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