Influence of deposited nanoparticles on the spall strength of metals under the action of picosecond pulses of shock compression

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Abstract. Molecular dynamic simulations of the generation and propagation of shock pulses of picosecond duration initiated by nanoscale impactors, and their interaction with the rear surface is carried out for aluminum and copper. It is shown that the presence of deposited nanoparticles on the rear surface increases the threshold value of the impact intensity leading to the rear spallation. The interaction of a shock wave with nanoparticles leads to severe plastic deformation in the surface layer of the metal including nanoparticles. A part of the compression pulse energy is expended on the plastic deformation, which suppresses the spall fracture. Spallation threshold substantially increases at large diameters of deposited nanoparticles, but instability develops on the rear surface of the target, which is accompanied by ejection of droplets. The instability disrupts the integrity of the rear surface, though the loss of integrity occurs through the ejection of mass, rather than a spallation.

1. Introduction

Reflection of a compression pulse from a free surface of a target leads to formation of a tension pulse propagating in the opposite direction, which can cause a rear spallation. Highest strain rates at spallation are experimentally attained by means of short and ultrashort powerful laser irradiation of thin metal foils [1–3]. The method of molecular dynamics (MD) is widely used in the theoretical study of the of spall fracture phenomenon by means of the modeling of generation and propagation of shock waves initiated by a piston or impactor [4–17].

Previously, we have shown [18] that, in a case the free surface is not a flat one, the interaction of the shock wave with nanorelief elements, for example in the form of nanoprojection, leads to severe plastic deformation in the surface layer, due to which a part of the energy of the compression pulse dissipates. This leads to a decrease in the amplitude of the reflected tension wave and, therefore, to an increase in the spallation threshold. The presence of large projections significantly increases the spallation threshold, but can lead to Richtmeyer–Meshkov instability and jet ejection [19–23], which is also a violation of the integrity of the rear surface. In this paper, a similar effect is investigated using molecular dynamic simulations for the case of a sell of deposited nanoparticles on a flat rear surface. Threshold amplitudes of the shock wave leading to spallation are determined for various nanoparticle diameters and number of layers. The investigations are carried out for aluminum and copper samples with nanoparticles of the same material.
2. MD problem statement for high-velocity impact
MD simulations are carried out using LAMMPS [24]. Calculations for Cu and Al are carried out using interatomic potentials [25] and [26], respectively. Both potentials are based on the embedded atom method. The visualization of atomic configurations is carried out using the OVITO program [27].

The MD systems considered are single crystals of copper or aluminum (fcc lattice) with crystallographic directions [100], [010] and [001] coinciding with the x, y and z coordinate axes. Figure 1 shows the schematic MD system. The size $D$ of the system along the y and z axes is taken equal to 30 lattice periods (10.8 nm for Cu) in all the calculations performed. After initial thermalization for 2 ps in a thermostat at 300 K and in a zero-pressure barostat, a flat surface layer (impactor) of thickness $H$ equal to 30 lattice periods (10.8 nm for Cu) acquire a velocity $V$, which is additional to the heat velocity and directed along the x axis (to the left in figure 1). The rest of the MD system plays the role of a target with a total thickness $L$, see figure 1(a), which is 120 lattice parameters (44 nm for Cu) in most calculations. The total number of atoms in the system of maximum dimensions reaches about half a million. Deposited nanoparticles with a total height of the shell $l$ and different diameters $d$ are situated on the rear surface of the target (see figure 1). The total height of the nanoparticle shell ranges from 0, which corresponds to a flat rear surface, to 90 lattice parameters (33 nm for Cu). The diameter $d$ of the deposited nanoparticles in the calculations varies from 14 lattice parameters (5 nm for Cu) to 30 lattice parameters (10.8 nm for Cu). The strengths of the samples with the same total thickness $L$ are compared, see figure 1(a).

The impact calculations are performed in the $NVE$ ensemble. Periodic boundary conditions are given along all axes. Along the direction of the x axis, the calculated region is chosen substantially larger than the size of the MD system, which ensures that the conditions of the free surface at the boundary of the impactor and the rear surface of the target are satisfied. A final-thickness impactor generates a compression pulse consisting of a shock wave and a following unloading wave. The maximum compressive stresses are determined by the impact velocity $V$.

3. Interaction of compression pulse with flat surface
The picture of the compression pulse interaction with a flat surface of aluminum is illustrated in figure 2 for the impactor velocity of 1300 m/s and the target thickness of $L = 48.6$ nm. There is a pronounced separation of the surface layer (see figure 2). The spallation pattern is typical: after reflection of the compression pulse, a region of tensile stresses is formed in which plastic deformation begins, then formation of cavities takes place (16 ps) and the subsequent growth of the cavities with the formation of a main crack. The rear surface retains its flat shape.

4. Effect of deposited nanoparticles on spall strength
The interaction of the compression pulse with the rear surface of Al with the deposited Al nanoparticles (two layers) is illustrated in figure 3 for the impactor velocity of 1300 m/s and the total target thickness of $L = 48.6$ nm (the same parameters as for figure 2). In this case, the uniaxial deformed state typical for a plane shock wave changes to a more complex deformation state when interacting with nanoparticles. The shock wave flattens the protrusion from the deposited nanoparticles through plastic deformation. Part of the energy of the compression pulse is dissipated due to severe plastic deformation, which leads to a decrease in the amplitude of the tension wave and to an increase in the spallation threshold. As a result, for the impact velocity of 1300 m/s, which is the same as for the case of a plane surface considered earlier, no spallation occurs. The increase in the number of layers of nanoparticles does not qualitatively change the situation (figure 4), while the extreme nanoparticles remain undeformed, which indicates that the shock wave does not act on them. At a shock velocity of 1400 m/s, voids are formed in the calculated region (at times of (10–40 ps), but they do not grow further.
Figure 1. Configuration of the MD system at the beginning of the collision: (a) the schematic model and (b) the general view, the color shows the $x$ component of the atom velocity.

Figure 2. Reflection of the shock pulse from the flat rear surface: Al target and impactor; the target thickness is 120 lattice parameters; the impactor thickness is 30 lattice parameters; the impact velocity is 1300 m/s. Color corresponds to the longitudinal component of the atom velocity. The following stages are shown: the beginning of the collision (0 ps), the shock pulse reaches the rear surface and is reflected (8 ps), the nucleation and growth of the voids (16 ps), the formation of the main crack (24 ps) and the flight of the spalled layer (40 ps).
Figure 3. Reflection of the shock pulse from the rear surface with deposited nanoparticles: aluminum target, nanoparticle and impactor; total thickness of the target is 120 lattice parameters (including nanoparticles); the diameter of the nanoparticles is 20 lattice parameters; the thickness of the impactor is 30 lattice parameters; The impact velocity is 1300 m/s. Color corresponds to the longitudinal component of the atom velocity. The following steps are shown: the initial configuration (0 ps), the shock pulse reaches the rear surface and smooths out the nanoparticles (8–24 ps), and the flying target (40 ps).

A break with the formation of a main crack (figure 5) is observed at an impact velocity of 1450 m/s and more (in the presence of two or three layers of precipitated nanoparticles with a diameter of 20 lattice parameters or 8.1 nm). Thus, the deposited nanoparticles make the free surface more resistant to spall fracture initiated by the reflecting compression pulse. Figure 6 shows some configurations of the investigated MD systems with deposited nanoparticles. A complete list of the investigated MD systems and the obtained values of the threshold impact velocity leading to spallation or development of the instability are given in table 1 for Al or Cu, respectively. Analysis of the obtained data shows that the size of the first, the closest to the surface, layer of nanoparticles affects the increase in the spallation threshold most strongly. The greatest effect of hardening is observed when the diameter of nanoparticles is equal to the cross section of the MD system that is, taking into account the periodic boundary conditions, when adjacent columns of nanoparticles are in contact. In this case, the violation of integrity occurs mainly due to the development of instability (section 6).

5. Influence of deposited nanoparticles on stress fields
The spatial distribution of longitudinal $\sigma_{xx}$ and transverse $(\sigma_{yy} + \sigma_{yy})/2$ stresses in an aluminum sample is considered for the case of a flat target surface and a surface with nanoparticles at a
Figure 4. Evolution of the MD system (Al) in the presence of deposited particles with a diameter of 20 lattice parameters (8.1 nm) with a total layer thickness of twice the impactor thickness ($l/H = 2$), at impact velocity of 1300 m/s and the total target thickness of 120 lattice parameters ($L = 48.6$ nm) including nanoparticles. The distribution of the centro-symmetry parameter (on the left) and the longitudinal component of the atom velocity (on the right) are shown. The reaching of the shock wave of the rear surface (10 ps); plastic deformation of the nanoparticles and the adjacent target region (10–20 ps); further movement of the target as a whole (30–40 ps)—no spallation occurs.

total thickness $L = 48.6$ nm at an impactor velocity of 1300 m/s (figures 7 and 8). In this case, the impactor forms a compression pulse with an amplitude of about 12 GPa (longitudinal stress) and a width of about 20 nm (duration of the order of a picosecond). The compression pulse moves deeper into the target, gradually broadening due to the fact that the unloading wave gradually overtakes the front of the shock wave. The transverse stresses in the incident wave are proportional to the longitudinal stresses, the relationship between them is determined by the elastic constants of the material [28]. In the case of a flat surface tensile stresses in the forming tension wave reach a maximum of about 10 GPa, which leads to a spall. After the spallation, the weakened tension pulse escapes in the depth of the target, and characteristic stress oscillations are observed in the spalled layer.

In the case of deposited nanoparticles, unloading on lateral surfaces of the target removes lateral stresses. The maximum tangential stress, which is equal to half the difference between the longitudinal and transverse stresses, exceeds the dynamic yield strength, which causes plastic deformation. Plastic deformation limits the longitudinal stresses in the region near the rear surface and, as a consequence, the amplitude of the reflected tension pulse, which is already insufficient for rear spallation, similar to the case of nano-projections [18, 29].

Calculations show that in the aluminum target in the presence of deposited nanoparticles on the rear surface, the maximum impact velocity, leading to a rear spall, can reach 1450 m/s (with total thickness of the target $L = 48.6$ nm). For a target of the same thickness with a flat surface, the corresponding limit is 1270 m/s.
Figure 5. Evolution of the MD system (Al) in the presence of deposited particles with a diameter of 20 lattice parameters (8.1 nm) with a total layer thickness of twice the impactor thickness ($l/H = 2$), at impact velocity of 1500 m/s and the total target thickness of 120 lattice parameters ($L = 48.6$ nm) including nanoparticles. The distribution of the centro-symmetry parameter (on the left) and the longitudinal component of the atom velocity (on the right) are shown. The reaching of the shock wave of the rear surface (10 ps); nucleation and growth of voids (6–16 ps); formation of a main crack (20 ps).

Figure 6. Examples of investigated MD systems with deposited nanoparticles with a diameter of 14 lattice parameters (5 nm for Al), 20 lattice parameters (7.3 nm) and 30 lattice parameters (10.8 nm). On the left, a impactor is coloured—a layer with a thickness $H$ equal to 30 lattice constants (10.8 nm), which receives an additional velocity $V$ directed normal to the surface. We note that samples with the same total thickness $L$, which includes the total height of the deposited particles, are investigated.
Table 1. Threshold impact velocities leading to spallation or instability in the cases of a flat rear surface (upper row) and layers of deposited nanoparticles: target, nanoparticles and impactor are made of Al or Cu; the total target thickness is 120 lattice parameters; the thickness of the striker is 30 lattice parameters.

| Number of layers | $d_1$, lattice parameters | $d_2$, lattice parameters | $d_3$, lattice parameters | $v_{Al}$ (m/s) | $v_{Cu}$ (m/s) |
|------------------|--------------------------|---------------------------|---------------------------|----------------|----------------|
| Flat surface     |                          |                           |                           | 1270           | 1230           |
| 1                | 14                       | —                         | —                         | 1340           | 1350           |
| 1                | 20                       | —                         | —                         | 1440           | 1570           |
| 1                | 30                       | —                         | —                         | 1630*          | 1200*          |
| 2                | 14                       | 14                       | —                         | 1350*          | 1350           |
| 2                | 14                       | 20                       | —                         | 1380*          | 1410           |
| 2                | 20                       | 14                       | —                         | 1460           | 1570           |
| 2                | 20                       | 20                       | —                         | 1450           | 1540           |
| 2                | 20                       | 30                       | —                         | 1450           | 1470*          |
| 2                | 30                       | 14                       | —                         | 1660*          | 1210*          |
| 2                | 30                       | 20                       | —                         | 1670*          | 1200*          |
| 2                | 30                       | 30                       | —                         | 1660*          | 1230*          |
| 3                | 14                       | 14                       | 14                        | 1370           | 1370           |
| 3                | 14                       | 14                       | 20                        | 1360           | 1360           |
| 3                | 14                       | 14                       | 30                        | 1370           | 1380           |
| 3                | 14                       | 20                       | 14                        | 1360           | 1370           |
| 3                | 14                       | 20                       | 20                        | 1370           | 1360           |
| 3                | 14                       | 20                       | 30                        | 1400           | 1390           |
| 3                | 14                       | 30                       | 14                        | 1390           | 1420           |
| 3                | 14                       | 30                       | 20                        | 1410           | 1410           |
| 3                | 14                       | 30                       | 30                        | 1430           | 1450           |
| 3                | 20                       | 14                       | 14                        | 1440           | 1530           |
| 3                | 20                       | 14                       | 20                        | 1440           | 1540           |
| 3                | 20                       | 14                       | 30                        | 1450           | 1550           |
| 3                | 20                       | 20                       | 14                        | 1460           | 1540           |
| 3                | 20                       | 20                       | 20                        | 1450           | 1520           |
| 3                | 20                       | 20                       | 30                        | 1480           | 1550           |
| 3                | 20                       | 30                       | 14                        | 1480           | 1540           |
| 3                | 20                       | 30                       | 20                        | 1490           | 1570           |
| 3                | 20                       | 30                       | 30                        | 1560           | 1550*          |
| 3                | 30                       | 14                       | 14                        | 1670*          | 1220*          |
| 3                | 30                       | 14                       | 20                        | 1740*          | 1230*          |
| 3                | 30                       | 14                       | 30                        | 1730*          | 1200*          |
| 3                | 30                       | 20                       | 14                        | 1710*          | 1210*          |
| 3                | 30                       | 20                       | 20                        | 1720*          | 1270*          |
| 3                | 30                       | 20                       | 30                        | 1760*          | 1260*          |
| 3                | 30                       | 30                       | 14                        | 1780*          | 1270*          |
| 3                | 30                       | 30                       | 20                        | 1750*          | 1270*          |
| 3                | 30                       | 30                       | 30                        | 1800*          | 1290*          |

* Restriction due to development of instability.
Figure 7. Spatial distribution along the direction of propagation of the shock wave (along the \( x \) coordinate) of the stresses: longitudinal (left) and transverse (right). Aluminum target and impactor: drummer velocity is 1270 m/s, target thickness is \( L = 48.6 \) nm; flat rear surface.

Figure 8. Spatial distribution of stresses along the direction of the shock wave propagation (along the coordinate \( x \)): longitudinal \( \sigma_{xx} \) (left) and transverse \( \frac{\sigma_{yy} + \sigma_{yy}}{2} \) (right) stresses. Aluminum target and impactor: impactor velocity is 1300 m/s, total target thickness is \( L = 48.6 \) nm. Target with the deposited particles of diameter 8.1 nm with the particle layer thickness twice the thickness of the impactor \( (l/H = 2) \).

The compression wave amplitude increases together with an increase in the impact velocity within this range, while the amplitude of the reflected tension pulse remains unchanged and insufficient for spallation. This mechanism ceases to work when the shock wave completely flattens the nanoparticle layers nearest to the surface, after which the amplitude of the reflected wave begins to grow together with the amplitude of the incident wave.
Figure 9. Evolution of the MD system (Al) in the presence of deposited particles of diameter 8.1 nm with a shell height twice that of the striker ($l/H = 2$), at an impactor velocity of 1800 m/s and a target total thickness $L = 48.6$ nm; The distribution of the centrally symmetric parameter (on the left) and the longitudinal component of the atom velocity (on the right) is given. The formation of jets on the surface and cavities in the near-surface layer is observed.

6. Development of Richtmeyer–Meshkov instability

Analysis of calculation results (see section 4) shows that the greatest effect of strengthening is observed when the neighboring columns of nanoparticles come into contact. The limitation of the safe impact velocity in this case is related to the effect of mass ejection from the rear surface in the form of jets (figure 9). Plastic deformation translates the substance of the surface layer into a state with a completely disordered crystal lattice at an elevated temperature, which flows like a liquid. The development of Richtmeyer–Meshkov instability leads to the formation of jets and the subsequent separation of droplets (see figure 9). These results are qualitatively consistent with data obtained in MD modeling [21–23] at high shock wave intensity.

7. Conclusions

The MD study of high-velocity impact, carried out for aluminum and copper samples, shows that the deposited nanoparticles make the free surface more resistant to spall fracture initiated by a reflecting compression pulse. There is severe plastic deformation at the lateral surface of the nanoparticles due to unloading when the shock wave reaches the rear surface with the deposited nanoparticles. The amplitude of the tension pulse is limited due to the use of a part of the energy of the compression pulse on the plastic deformation; as a result, the destruction of the substance in tensile stresses is limited and suppressed. The size of the first layer of nanoparticles, closest to the surface, affects the increase in the spallation threshold. The greatest effect of strengthening is observed when the diameter of nanoparticles is equal to the cross section of the MD system that is, taking into account the periodic boundary conditions, when adjacent columns of particles are in contact. In this case, the violation of the integrity of the rear surface of the target is mainly due to the development of the Richtmeyer–Meshkov instability accompanied by the ejection of jets of matter [21–23].
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