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Computer Simulation of Spall Crack Formation

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ABSTRACT: Molecular dynamics investigation of central impact of thin plate impactor to target from the same material is presented. Two types of impactor are considered: plate impactor and cup impactor. Cup impactor is usually used in nature experiments to avoid boundary effect from the impactor borders in order to obtain uniform deformation of the target. The presented computer experiments show that the walls of the cup give a strong boundary effect that leads to focusing of the shock waves in the centre part of the spall crack.

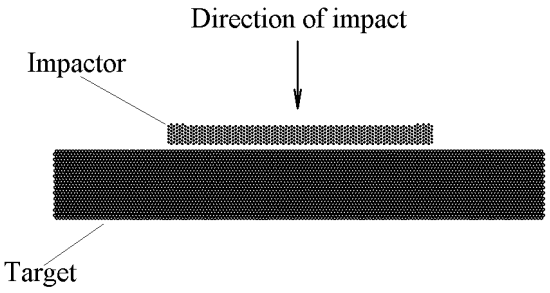

Figure 1. The initial state of the specimens.

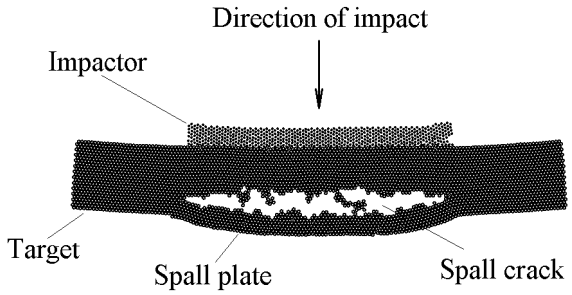

Figure 2. The specimens after impact.

1 INTRODUCTION

The method that is used in these investigations is close to a standard molecular dynamics method. The main distinction of our consideration is that the particles are interpreted not as atoms or molecules, but as elements of mesoscopic scale level, such as grains of material. In this case the considered model can describe many futures of the fracture process (Krivtsov & Zhilin 1997, Krivtsov 1999). The time dependencies of the quantities that can be measured in nature experiments (Mescheryakov & Divakov 1994, Mescheryakov et al. 1994), such as average velocity on the free surface of the target, mesoparticle velocity dispersion, are similar with the time dependencies obtained from the computer simulation.

One of the main advantages of the molecular dynamics approach is that it can be simply used with any shape of the specimens. After the model is tested in simple cases, the method can be used for complicated impact problems. In the presented investigation two shapes of impactor are considered: the simplest (the plate impactor) and the frequently used in practice (the cup impactor).

2 METHODS

To simplify the model, a monoatomic two-dimensional lattice with standard Lennard-Jones 6–12 potential (Eckstein 1991) was chosen for molecular dynamics simulation, as shown in (1)

$$U(r_{ij}) = \epsilon \left[\left(\frac{r_0}{r_{ij}} \right)^{12} - 2 \left(\frac{r_0}{r_{ij}} \right)^{6} \right] , \qquad (1)$$

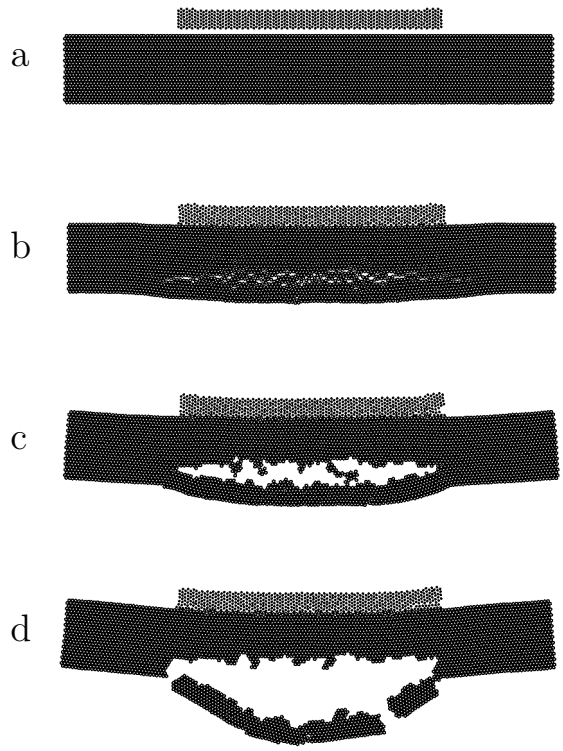

Figure 3. Sequential stages of impact, plane impactor.

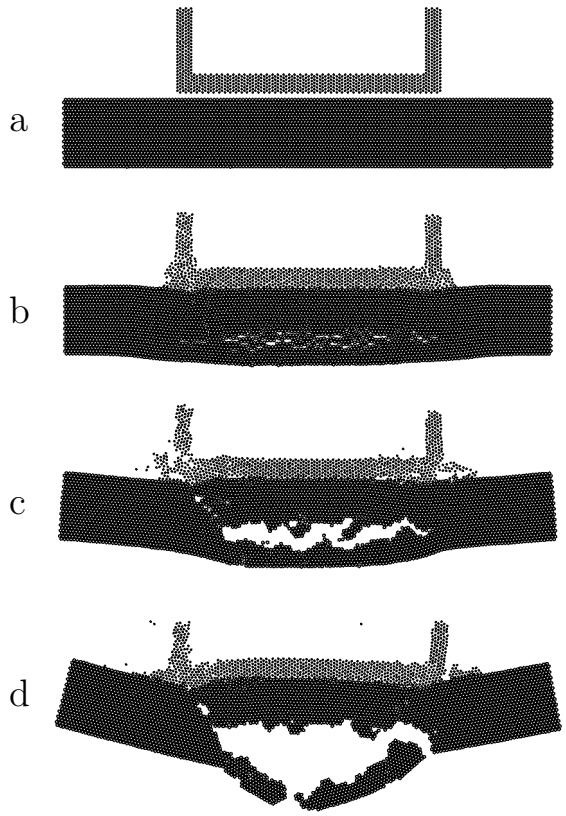

Figure 4. Sequential stages of impact, cup impactor.

where $U(r_{ij})$ is the interaction energy between atoms i and j separated by distance r_{ij}, ϵ is the strength of the interaction, and r_0 is a characteristic length scale. In order to decrease calculation time, the potential is usually truncated at a finite distance, beyond which the interaction is taken to be zero. In the considered numeric experiments the cut-off distance was chosen to be $2.1\,r_0$. In this case, the interaction potential has contributions from the first, second, and third nearest particles in the perfect crystal. However, the contribution of the second and the third neighbours to the total energy are minimal. Hence, r_0 is approximately the equilibrium, nearest-neighbour atomic separation. In order to describe nonelastic losses of energy small dissipative forces proportional to the particles velocities were added. The simulation technique employed in this work is standard molecular dynamics method (Allen & Tildesley 1987, Eckstein 1991). In this method, the trajectories of each atom are followed through time by integrating Newton's classical equations of motion.

The computation model is presented in Figure 1. The impactor and the target are circular plates. In Figure 1 the particle two-dimensional model of the impactor and target cross-section is presented. The impactor is placed at an initial distance from the target greater than the cut-off distance of the interparticle potential. Initially the particles are arranged on a triangular lattice. Both impactor and target are made from the same particles. The total number of particles in Figure 1 is about 5000. Free boundary conditions on all boundaries is used.

Initially the target has zero velocity, the impactor has velocity directed along the vertical axis towards the target (see "direction of impact" in Figure 1). In addition to the initial velocity of each particle a random velocity is added which is chosen from a two-dimensional random uniform distribution (Krivtsov 1999). The impactor velocity is 260 m/s, strength characteristics of material are close to titanium. The sizes of the specimens in Figure 1 are proportional to the sizes of the specimens that were used in the nature experiments (Mescheryakov & Divakov 1994, Mescheryakov et al. 1994). Figure 1 shows the impactor and the target before impact, Figure 2 shows them after impact. It is well to see the spall crack in the target. The thickness of the spall plate is equal to the impactor thickness, how it should from theory. Form and width of the spall plate, the shape of the crack are far similar to results obtained

from the nature experiments (Mescheryakov & Divakov 1994, Mescheryakov et al. 1994, Chevrier & Klepaczko 1997).

3 RESULTS

In Figure 3 sequential stages of the impact are shown. Figure 3a corresponds to the moment of time just before the impact. In Figure 3b it is well to see appearance of microcracks. In Figure 3c all microcracks join in one turnpike crack, and in Figure 3d splinters formation takes place.

Figure 4 shows the same results for the other shape of impactor — the cup impactor. Figure 4a shows the initial state of the specimens, in Figure 4b the microcracks appears in the spall area, in Figure 3c the microcracks join in the turnpike crack, and in Figure 3d the spall plate is being broken in splinters.

Comparison of Figure 3 and Figure 4 shows that the cup shape of the impactor leads to localisation of the fracture in the central area of the target. The width (the horizontal size) of the spall crack for the plane impactor is grater then width of the target (Fig. 3c), but for the cup impactor the width of the spall crack is less then the width of the target (Fig. 4c). The fracture degree is grater for the case of the cup impactor.

4 DISCUSSION AND CONCLUSIONS

The results of the computation are in a good agreement with the main features of the real spall process: form and width of the spall plate, appearing of microcracs, formation and shape of the spall crack. There are also a good agreement in the quantities that can be calculated on the base of the continuum mechanics (such as longitudinal strain and mass velocity) and in the quantities that can be measured in both computer and real experiments, such as free surface velocity and mesoparticle velocity dispersion on the free surface (Krivtsov & Mescheryakov 1998). These conclusions give certainty that the quantities that can't be measured in reality (such as velocity dispersion inside the material) can be estimated from the presented computer experiments. After tests on simple specimens, the computer experiments can be used to investigate impacts with a complex shapes of impactor and target.

Cup impactor is often used in nature experiments to avoid boundary effect from the impactor borders in order to obtain uniform deformation of the target. The presented computer experiments give an unexpected result: the walls of the cup give a strong boundary effect that leads to focusing of the shock waves in the center part of the spall crack.

The computer model used to obtain the considered results is very simple: ideal monoatomic lattice with Lennard-Jones potential. If we consider the particles as elements of microscopic scale level (for example, atoms) then the results can be interpreted in the other way: we have investigated spall formation in an ideal monocrystal. Of course the considered model is very crude to describe kinetics and dynamic strength properties of real solids, but the general tendencies it should describe properly. For exact results more accurate models are desirable (other potentials of interaction, different types of particles, 3D simulation), but the main tendencies should be similar.

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