Proceedings of XXX Summer School "Advanced Problems in Mechanics", St.-Petersburg, Russia. 2002. Accepted.

Spall crack parameters dependence on the velocity dispersion in 3D spall process simulation

I. B. Volkovets

Abstract

It is known from the plate impact experiments that a higher mesoparticle velocity dispersion corresponds to a higher spall strength of material [1]. Computer investigation of this fenomenon was considered in [2] for a two-dimensional computational model using molecular dynamics method. It was obtained in [2] that the spall strength dependence on the velocity deviation has a maximum approximately at 10% of the dissociation velocity.

Taking this result as a basis, this work reproduces the same computational experiment for a three-dimensional model with much greater number of particles.

1 Setup of the computer experiment

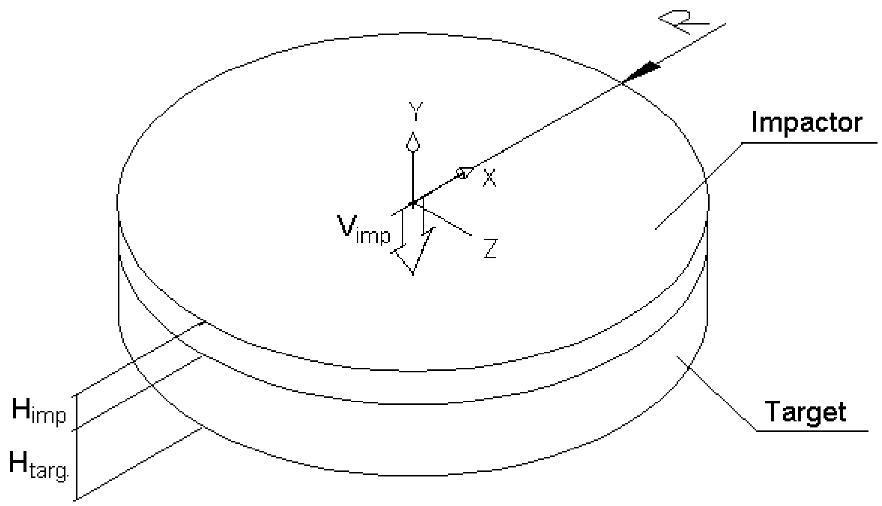

Fig. 1. Initial position of the impactor and the target.

A bulk cylindrical crystal with a monoatomic lattice is considered. The particles in the crystal are interpreted as mesoscopic level elements. As it is shown in Fig. 1, the upper part of the crystal is an impactor and the lower part is a target. The only difference between the target and the impactor is that the particles in the impactor have got an initial velocity in the downward direction. This method of the impactor placement allows to avoid any defects in the contiguous surface. To simulate a mesoparticle velocity dispersion [1] the random velocities are added to all particles in the crystal. To describe the intensity of the random velocities the term "velocity deviation" is used, which is the square root of the velocity dispersion.

The computer experiment is the time integration of the equations of motion for each particle using the method of central differences. The forces between the particles are calculated using the Lennard-Jones potential

$$\Pi(r) = D\left[\left(\frac{a}{r}\right)^{12} - 2\left(\frac{a}{r}\right)^{6}\right], \tag{1}$$

where D is the bond energy, a is the equilibrium distance between the particles. To decrease the calculation time the interaction between two particles is taken to be zero when the interparticle distance is greater than a cut-off distance, which is equal to $2.1a$. This approximation allows an interaction between three nearest atoms in a perfect atomic chain. Let us note that the bond energy between the first and the third atom is little bit more than 3% of the bond energy D between the nearest neighbors. The interaction energy between the first and the fourth atom is ten times smaller — 0.3% of D.

Proportion between H_{imp} and H_{targ} (see Fig. 1) is $H_{imp}/H_{targ} = 1/2$. Proportion between the height and the radius of the specimen is $(H_{imp} + H_{targ})/R = 9/26$, as in the real experiments by Yu. I. Mescheryakov [1].

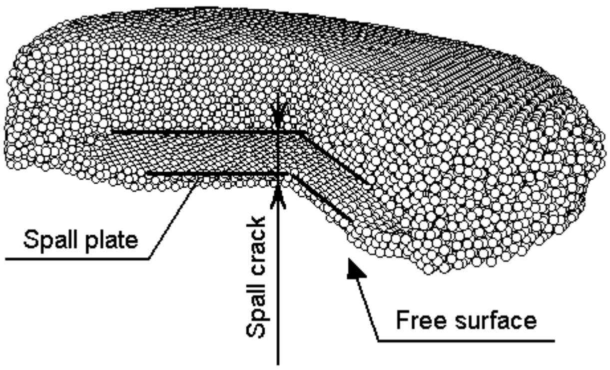

Fig. 2. Section of the model after impact.

The unit of distance is the equilibrium interparticle distance a; the unit of velocity is the dissociation velocity v_d (velocity needed to separate two particles from the equilibrium to the infinity). The time step used for integration is $0.01T_0$, where

$$T_0 = 2\pi\sqrt{m/C}, \qquad C = \Pi''(a) = 72D/a^2 \tag{2}$$

is the period of one-particle harmonic oscillator. An additional macroscopic time unit $t_s = (H_{imp} + H_{targ})/v_0$ is used. It is the time needed for the elastic wave to pass through the total height of the crystal. Velocity $v_0 = 6v_d$ is the elastic wave velocity in 1D chain. The number of particles used for calculation, N, is about 1.6 millions. This corresponds to the radius of impactor $R = 100a$. In the most comprehensive experiments N reaches 100 millions. The specimen is a crystal with FCC lattice. The impact is performed along the edge of the cubic cells of the lattice.

The values to be measured in the computer experiments are the free surface velocity and the width of the spall crack (see Fig. 2). To avoid boundary effects only the central part of the spall plate is used for measuring. The spall effect could be clearly detected using the free surface velocity graph and the spall crack width graph. Fig. 3 illustrates the free surface velocity graph obtained from two computer

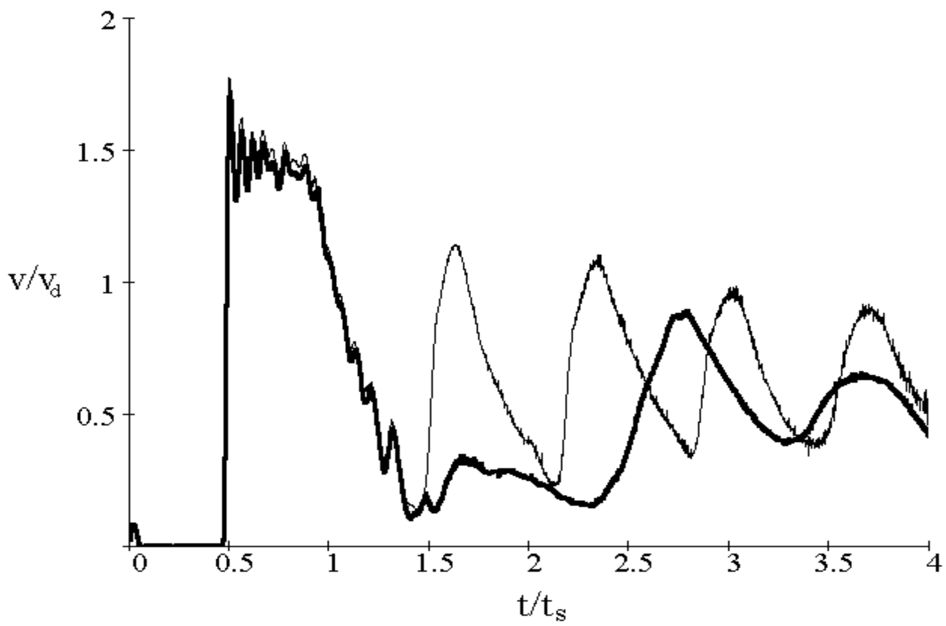

Fig. 3. Free surface velocity graph for two different impactor velocities, v_{imp}. Bold curve corresponds to $v_{imp} = 1.6v_d$. Thin curve corresponds to $v_{imp} = 1.65v_d$. Velocity deviation $\Delta V = 0.1v_d$.

experiments. The bold curve was obtained from an experiment without spall. Other curve shows the spall effect. Oscillations of this curve are the oscillations in the spall plate. Fig. 4 shows the spall crack width graph for the same pair of experiments. Let us note that 3% increase of the impactor velocity completely changes the form of the graphs.

Fig. 5 shows results of two computer experiments with different velocity deviations: $\Delta V = 0.05v_d$ and $\Delta V = 0.15v_d$. The character of the spall fracture is different. The left picture corresponds to the less deviation and the spall fracture is quite smooth. In the right one the contiguity exists and there are some randomly located atoms between the crack edges.

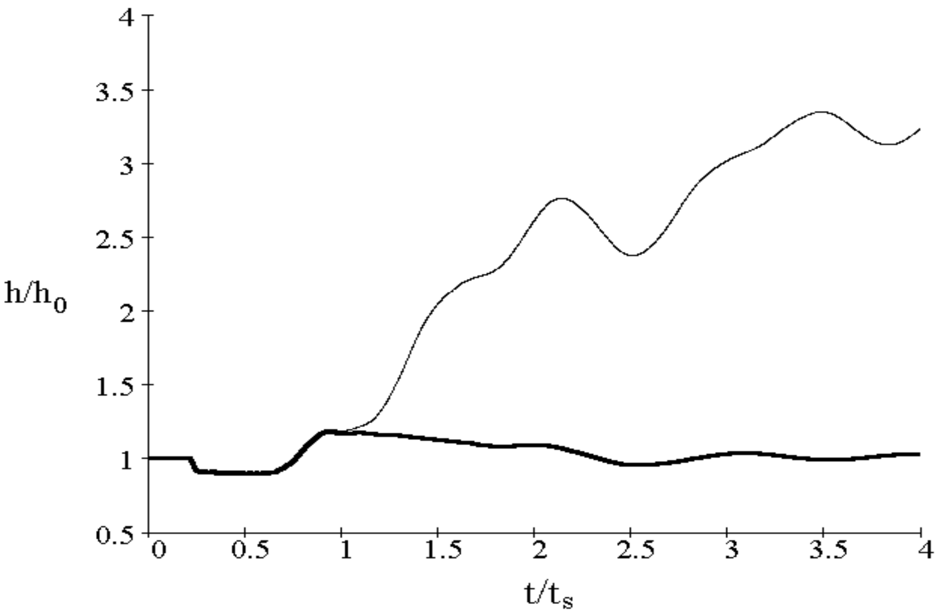

Fig. 4. Spall crack width graph for two different impactor velocities. Parameters of experiments are the same as in Fig. 3.

2 Results

To study the spall crack width dependence on the velocity deviation the series of the computer experiments was performed. Fig. 6 shows the relation between the velocity deviation and the maximal spall crack width. The increase of deviation from 0 to $0.15v_d$ causes the decrease of the maximal crack width value, as it shown in Fig. 6. Further increase of the deviation leads to growth of the crack width. Thus the spall strength characteristics has a maximum at the values of deviation about $0.15v_d$.

Fig. 7 corresponds to the spall velocity dependence on the velocity deviation. The spall velocity is the difference between the first maximum and the first minimum on the time dependence of the free surface velocity (see Fig. 3). Graph in Fig. 7 demon-

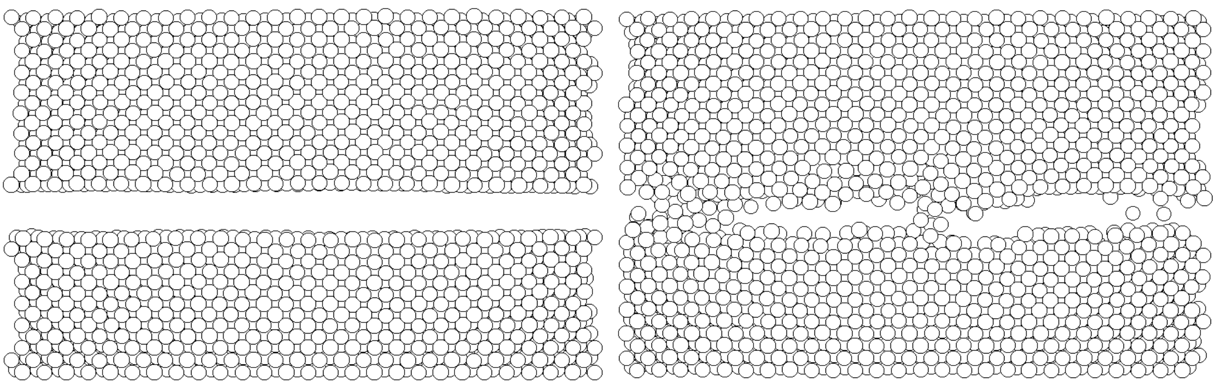

Fig. 5. Parts of the cross-sections of two crystals after an impact. The deviation for the left picture is $\Delta V = 0.05v_d$, for the right picture $\Delta V = 0.15v_d$. Impactor velocity $v_{imp} = 1.65v_d$ and the time passed from the moment of impact is $t = 1.4t_s$.

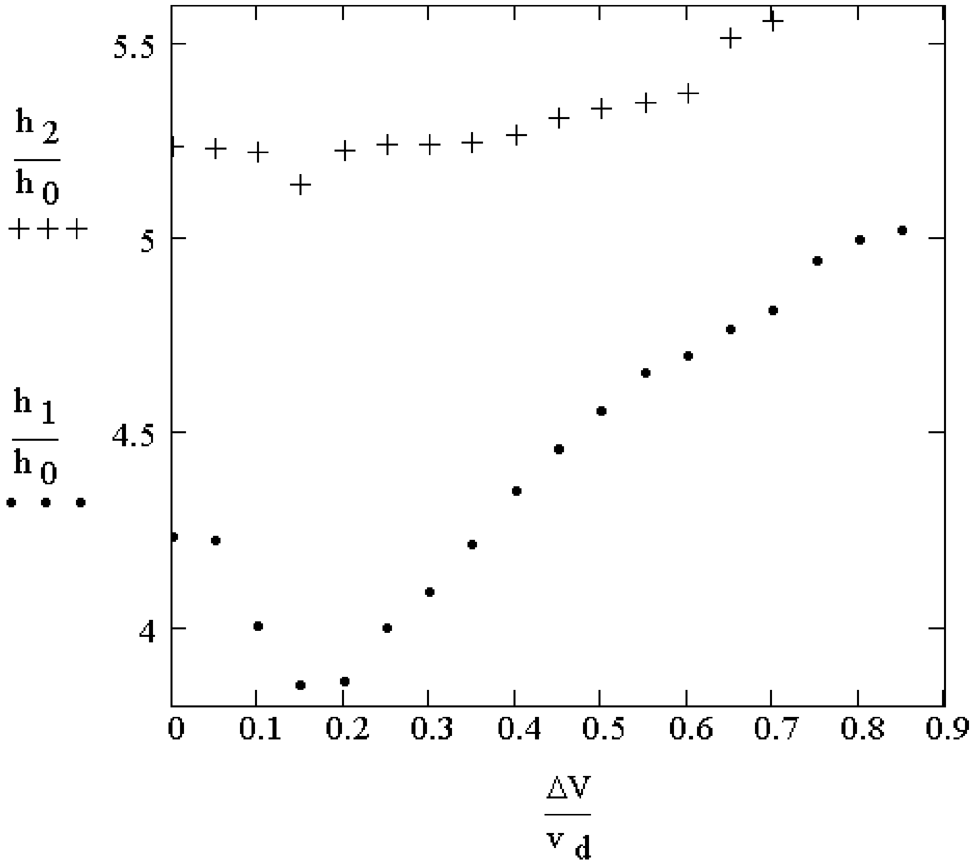

Fig. 6. The spall crack width dependence on the velocity deviation. h_1 is an average crack width for $v_{imp} = 1.68 v_d$, h_2 performs the same characteristics for $v_{imp} = 1.8 v_d$. h_0 is the initial distance between the atomic layers in the impact direction. Both curves were measured at the time $t = 1.5 t_s$.

strates that the spall velocity characteristics have the maximum approximately at the same value of deviation, which corresponds to the minimum of the spall crack width curve.

3 Conclusions

The results of 3D simulation are in good correspondence with the results obtained from the two-dimensional model [2]. The spall strength characteristics have the similar dependence on the particle velocity deviation. However, the observed effect in 3D is not so well pronounced as in 2D. Also some other differences were noticed. For 2D model the velocity deviation about $0.5 v_d$ causes fragmentation of the crystal, in 3D case there is no such effect even for the higher deviations up to v_d. The borders of the spall crack in 3D simulation are not so irregular as in 2D model. The impactor velocity necessary for spallation in 3D is greater than in 2D, where this velocity was about v_d. For 3D simulation v_{imp} must be greater than $1.6 v_d$ to produce spallation.

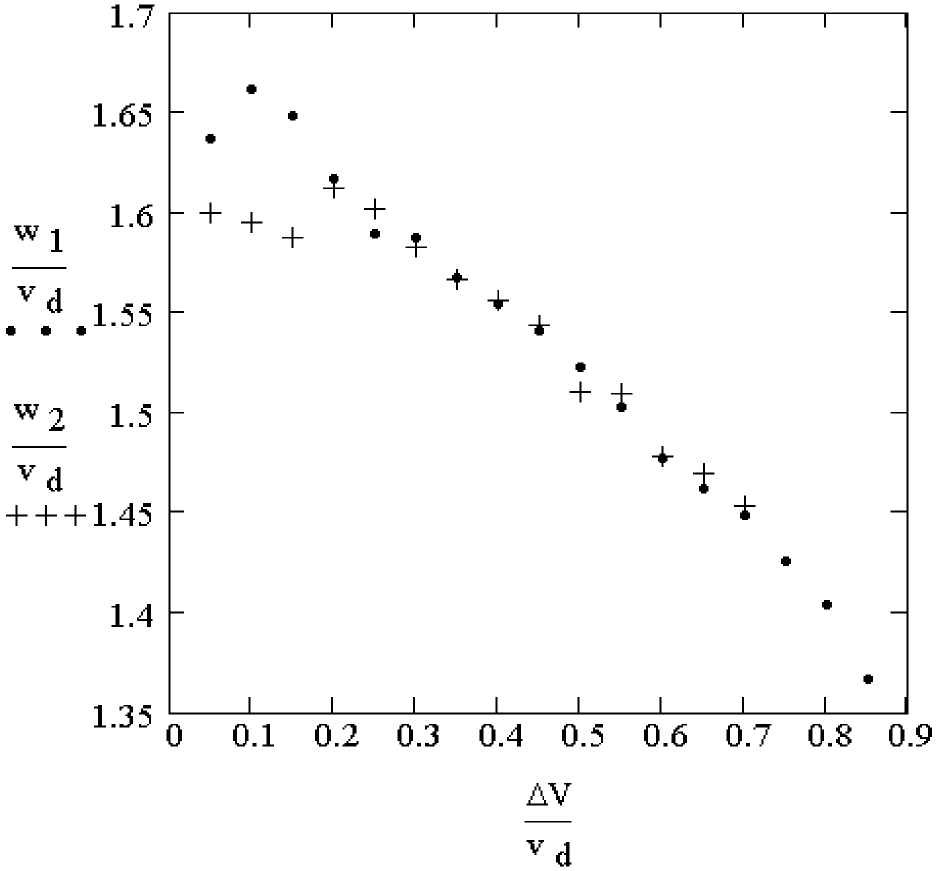

Fig. 7. The spall velocity dependence on the velocity deviation. w_1 is the spall velocity for $v_{imp} = 1.68 v_d$, w_2 corresponds to $v_{imp} = 1.8 v_d$.

Acknowledgements

The author is grateful to A. M. Krivtsov for the useful discussions. This work was supported by Russian Foundation for Basic Research, grant No 02-01-00514.

References

[1] Mescheryakov Y. I. and Divakov A. K. Multiscale kinetics of microstructure and strain-rate dependence of materials. *DYMAT Journal.* 1994. **4**. P. 271–287.

[2] Krivtsov A. M. Relation between Spall Strength and Mesoparticle Velocity Dispersion. *International Journal of Impact Engineering.* 1999. **23** (1). P. 466–476.

Ilya Volkovets, Molecular and Particle Dynamics Simulation Group, Institute for Problems in Mechanical Engineering RAS, Bolshoy pr. V. O. 61, St. Petersburg, 199178, Russia.