Computer simulation of 2D dynamic fracture: anisotropic effects in spall crack formation

Pavel V. Tkachev Anton M. Krivtsov

pavel_tkachev@mail.ru

Abstract

2D problem of a plate impact fracture interaction is analysed using the particle dynamics method. An ideal single-crystal particle packing with Lennard-Jones pair potential is used. Dependence of the spall velocity on the system geometry is analysed. Influence of the crystal lattice orientation on the fracture scenario is investigated.

1 Introduction

The plate impact experiments produce a simple deformation at very high strain rates, which makes these experiments to be convenient tool for studying dynamics fracture processes [1, 2]. The particle dynamics method allows to analyze kinetic processes in the fracture zone, where it is very difficult to perform such analysis using continuum mechanics methods [3, 4]. Following the particle dynamics technique in the current work the material is represented as a set of particles. Interaction between particles is defined by an interaction potential. General property of the potential is repulsion at a short range and attraction at a long range. The material structure and the initial velocities of the particles are set before the computer simulation.

The equations of motion have the form

$$m\ddot{\underline{r}}_{k} = \sum_{n=1}^{N} \frac{f\left(|\underline{r}_{k} - \underline{r}_{n}|\right)}{|\underline{r}_{k} - \underline{r}_{n}|} \left(\underline{r}_{k} - \underline{r}_{n}\right), \tag{1}$$

where \underline{r}_k is the radius-vector of the particle with number k, N is the total number of particles, m is the particle mass, $f(r) = -\Pi'(r)$ is the interaction force between particles. In this paper the Lennard-Jones potential is used

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

where a is the equilibrium distance between particles, D is the bond energy. The simulation consists of Cauchy problem solving for equations (1) with the interaction potential (2). Initial conditions are the initial coordinates and initial velocities of the particles.

Further we will use the dissociation velocity v_d , which is the minimum velocity required for the particle of mass m to go from the equilibrium to the infinity in the potential field with bond energy D:

$$v_d = \sqrt{\frac{2D}{m}}.$$
(3)

2 Statement of the problem



Figure 1: Initial conditions

The initial setup at the macrolevel is shown in Figure 1. The bottom plate is target, initially it has zero velocity. The upper plate is impactor, its initial velocity is directed towards the target. The height of the impactor is h, the height of the target is H.



Figure 2: Orientation of the crystal lattice: a) horizontal b) vertical.

At the microlevel the material is represented by the ideal triangular crystal lattice, same for the impactor and target. Horizontal (Figure 2a) and vertical (Figure 2b) orientation of the crystal lattice will be considered. Each impactor particle has the same initial velocity directed towards the target. In the horizontal direction periodic boundary conditions or free boundary conditions are used, in the vertical direction only free boundary conditions are used.

3 Simulation results

The computer experiments show that with increasing the number of particles and the height of the impactor the spall velocity converges to the dissociation velocity. For the vertical orientation of the crystal lattice the spall velocity converges to the dissociation velocity faster then for the horizontal orientation.



Figure 3: Fracture in case of a) horizontal b) vertical orientation of the crystal lattice.

The spall strength depends on the crystal orientation. Character of the fracture is also different for the different crystal orientations. Let us show it on the results of two computer experiments with different orientations of the lattice – see Figures 3. Initially the impactor height is equal to the target height; total height of the specimen is twice greater then the total width. Free boundary conditions in all directions are used. The total number of particles in the impactor and target is 100 000. The initial impactor velocity is equal to the velocity of dissociation.

According to the figures, for the horizontal orientation of the crystal lattice the orientation of the spall crack is horizontal (Figure 3a); for the vertical crystal lattice the crack orientation is vertical (Figure 3b). Actually in the latter case the fracture scenario is different from spallation — the specimen breaks in two nearly equal vertical fragments. It is well known that for the small deformations crystal with triangular lattice is isotropic. However, for big deformations the mechanical properties of the lattice are substantially anisotropic, which results in the fracture scenario shown in Figure 3b.

Acknowledgements

This work was supported by Russian Foundation for Basic Research, grant No 02-01-00514.

References

[1] Mescheryakov Y. I., Divakov A. K., Zhigacheva N. I. Shock-induced phase transformation and vortex instabilities in shock loaded titanium alloys. *Shock waves*. 2000. **10**. 43–56.

- [2] Rajendran A. M., Dietenberger M. A., Grove D. J. A void growth-based failure model to describe spallation. *Journal of Applied Physics*. 1989. 65(4). 1521–1527.
- [3] Krivtsov A. M. Relation between Spall Strength and Mesoparticle Velocity Dispersion. International Journal of Impact Engineering. 1999. 23(1). 466– 476
- [4] Krivtsov A. M. Molecular Dynamics Simulation of Plastic Effects upon Spalling. *Physics of the Solid State*. 2004. **46**(6). 1055–1060.

Pavel V. Tkachev and Anton M. Krivtsov, Institute for Problems in Mechanical Engineering Russian Academy of Sciences, Bolshoy pr. V. O., 61, St. Petersburg, 199178, Russia.