



## **Molecular Dynamics Simulation of Impact Fracture in Polycrystalline Materials**

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(Accepted: 10 July 2002)

**Abstract.** Technique for creation of polycrystalline computer materials is presented. The method considered allows for the obtaining of not only polycrystalline particle packings with various grains sizes but also the creating of materials with the preset value of porosity. Plate impact experiments were performed to compare strength properties of mono- and polycrystalline computer materials and also to investigate influence of the material porosity on the shock wave penetration and spallation processes. The experiments show significant differences in the impact fracture processes between mono- and polycrystalline materials. Smearing the shock waves due to heterogeneity of the granular structure of the polycrystals decreases localization effects, and the fracture occupies larger areas but with the smaller level of injury. Porosity adds significant resistance due to the strong plastic deformation during the pore collapsing. This effect can strongly decrease the penetration distance of the shock wave and even prevent the spallation.

**Key words:** Molecular dynamics, Impact fracture, Polycrystal.

### **1. Introduction**

One of the main challenges in using the molecular dynamics technique for simulating macroscopic behavior of materials is that all regular particle packings produce computer materials with anisotropic mechanical properties. Though generally it is possible to choose interparticle potentials to obtain isotropic conditions for elastic moduli, there is no way of satisfying isotropic conditions for inelastic and strength properties. This may be why molecular dynamics, which is widely used in modeling crystalline materials, still has limited applications in the case of homogeneous isotropic solids.

The approach, which allows for bypassing this problem, is to construct polycrystalline particle packings with random distribution of the monocrystal grain orientations. This method can produce isotropic computer materials which can satisfy a very wide range of mechanical, thermodynamic, and physical properties. Obviously this technique requires much more computer resources, because the elementary volume is now the monocrystal grain, containing hundreds of particles at least. Therefore the full-scale use of polycrystalline computer materials was started only recently, following the sharp increase in the power of the modern computers. Recent advances in nanotechnologies also stimulated molecular dynamics-aided research in the area of nanocrystal materials [1]. Polycrystalline computer materials can also be applied for simulating macroscopic mechanical properties of the rock materials [2], especially for simulating such processes as percussive drilling [3], where impact fracture is of primary importance.

In the present paper, methods for construction of polycrystalline computer materials with various porosity will be considered, and then mechanical properties of these materials will be studied using the plate impact experiments. The simulation technique is described in [4], where the conventional molecular dynamics method is used [5]. Material is simulated by 2D set of particles interacting via prescribed potential forces; simulation is made by integrating Newton's equations of motion for each particle. For the sake of simplicity, a standard Lennard-Jones 6–12 potential is used to describe interaction between the particles for the impact experiments. For polycrystal creation, more general Mie potentials are used, which can be described by the formula

$$U(r) = \varepsilon \left[ \left( \frac{\sigma}{r} \right)^n - \left( \frac{\sigma}{r} \right)^m \right], \quad n > m$$

where  $U(r)$  is the interaction energy between two atoms separated by distance  $r$ , the quantity  $\varepsilon$  characterizes the strength of the interaction, and  $\sigma$  is a characteristic length scale. The Lennard-Jones potential is a partial case of the Mie potential for  $m = 6$ ,  $n = 12$ .

## 2. Creation of Polycrystalline Computer Materials

Creation of computer polycrystals is a serious challenge, because it can be done in different ways, and the properties of the obtained computer materials depend generally on the procedure adopted. Still, there is very limited understanding of how the mechanical properties of the computer materials depend on the method of their construction. Let us refer to some methods of polycrystal creation. The first method is based purely on geometrical approaches. This method requires less computational time and resources, but usually it is difficult to obtain lattices with natural random distribution of the monocrystals; also, the particle equilibrium at the grain interfaces can be doubtful. Nevertheless, the geometrical method can produce nice polycrystalline packings, such as in [1], where the Voronoi construction method is applied for polycrystal creation. Another method is based on molecular dynamics simulation, where the desired packing can be obtained as a result of particles motion under certain conditions. These methods obviously require much more time for computation but can be easier from the algorithmical point of view. One of these methods is the melting of an ideal monocrystal lattice with sequential cooling [5, 6]. Another method [6] of this kind uses an unstable crystal lattice as initial condition. In the process of the molecular dynamics simulation, this lattice spontaneously changes itself to another stable lattice with a polycrystalline structure.

In the present work the second method, based on the molecular dynamics technique, is used. But unlike in the papers cited above, here we are interested in obtaining polycrystalline materials with various porosity, which is important for simulating the plastic behavior of materials. Porosity is also essential for the rock materials modeling. The need to have a certain level of porosity makes it impossible to use directly the methods mentioned above. Though, for investigation purposes, it is useful to have a number of specimens with different porosity, it would be very costly to generate them separately. That is why the method suggested below is based on sequential preparation of the specimens with decreasing porosity from a single set of particles.

The first step is use of the condensation technique, which is as follows: The particles initially are randomly distributed in a rectangular area – Figure 1(a) (white is used for the particles and black for the background). Unfortunately, the initial density of the random distribution cannot be very high, because the particles cannot be placed initially much closer

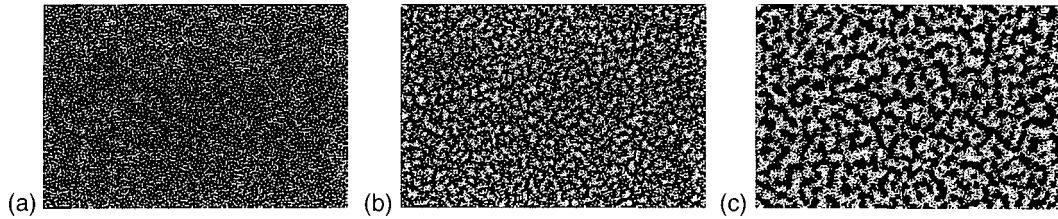


Figure 1. Agglomeration of particles: (a) initial configuration with the particles randomly distributed in a rectangular area, (b) agglomeration in progress, (c) final stage.

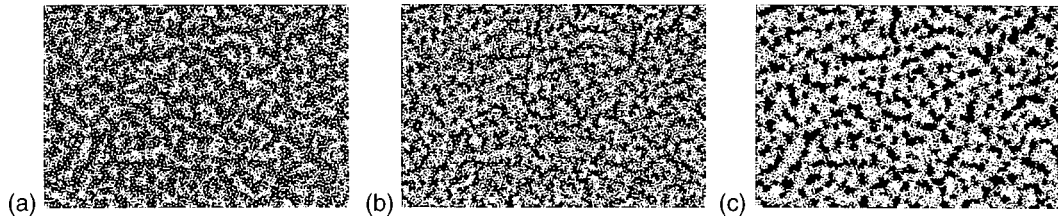


Figure 2. Additional particles are added to the configuration: (a) new particles are filling voids, (b) agglomeration in progress, (c) final stage.

to each other than the equilibrium distance (otherwise, huge repulsion forces between the particles will appear, which will produce high velocities of the particles motion and the computation instability). That is why the following method is used for creating the random initial distribution: each new particle obtains its random coordinates, then if in the vicinity of these coordinates no another particle exists, the particle is added to the configuration. Otherwise, the coordinates are recalculated to another random value until the necessary space for the new particle is found. The mentioned vicinity is chosen to be the circle with the radius equal to the particle equilibrium distance. This technique allows for the obtaining of approximately 60% density, relative to the density of the hexagonal crystal lattice. The initial configuration of this kind is shown in Figure 1(a). Then owing to the action of the attraction forces the particles coalesce, forming porous material – Figure 2(b, c). Small viscose friction proportional to the velocities of the particles is used to remove excess kinetic energy from the system.

Then, if higher density is required, this procedure can be continued. Now additional particles can be easily added to the system, because a lot of voids appear during the condensation process. The particles are added until there is free space (Figure 2(a)). Again the condensation is performed (Figure 2(b, c)). This process can be repeated until the necessary density is obtained. The sequential stages of such process are shown in Figure 3, where the maximum number of the particles added to the system is around 10 000. The density varies from 60% at the beginning to 95% at the end. During this process, a set of specimens with sequentially increasing density are obtained, which is much faster than preparing them separately. To speed up the computation, the Mie 4–6 potential was used, instead of the Lennard-Jones 6–12 potential, because it produces a more dense agglomeration of the particles. Then, after the desired porosity is obtained, the potential can be changed to the Lennard-Jones or another one which is more appropriate for further simulation. In case of the Lennard-Jones potential, this change provides dilatation of the material, which results in decreasing the specimen's porosity – see Figure 4(a).

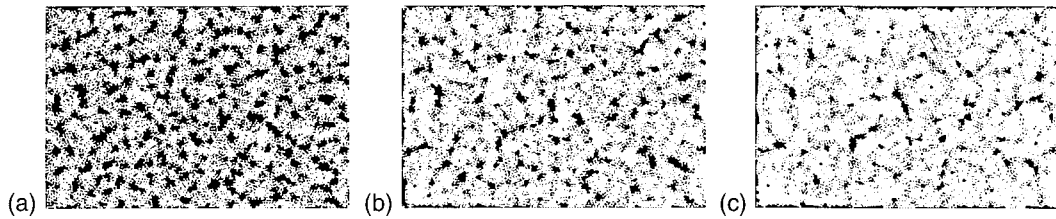


Figure 3. Continuation of the polycrystal creation process – final stages after sequential cycles of filling-agglomeration.

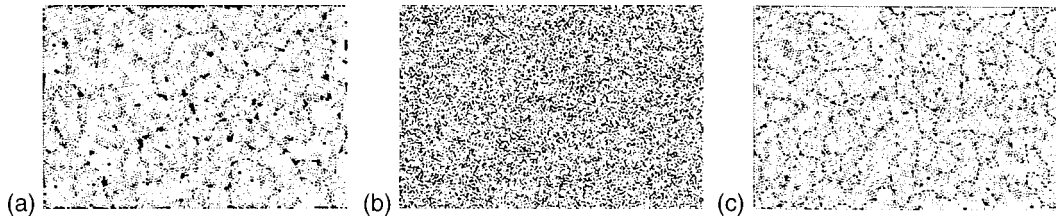


Figure 4. (a) The configuration after the potential has been changed to the Lennard-Jones one, (b) melted configuration, (c) the configuration after cooling.

After the specimens are obtained and their configurations are recorded, they require some additional processing. The simplest procedure is cooling of the specimen, which means that it is being held under the action of small viscous forces acting on each particle until they finally reach an equilibrium configuration. But usually more comprehensive processing is needed, especially if the properties of the polycrystalline packing should be alternated. In this case the specimens are subjected to additional melting with sequential cooling. This process is shown in Figure 4. The melting practically means that a random velocity is added to each particle, so that the kinetic energy of the particles will be far higher than the bond energy in the material. In several time steps this kinetic energy breaks the inner structure of the material and transmits the material to a uniform fluidized state. Then the cooling is applied by means of the distributed viscous forces. The melting allows for the obtaining of more uniform inner polycrystalline structure of the material. Additionally, the speed of the cooling allows for varying the grain size in the material. In Figure 5(a, b) two specimens are shown, which were obtained with different magnitude of the friction forces during the cooling process. Figures show that the sizes of the monocrystalline grains are much smaller for the faster cooling.

The boundary conditions are very important during the cooling process. For the above experiments the boundary conditions were not periodic, as it is usually done for such experiments. The reason is that for further experiments the specimens with free surfaces are needed,

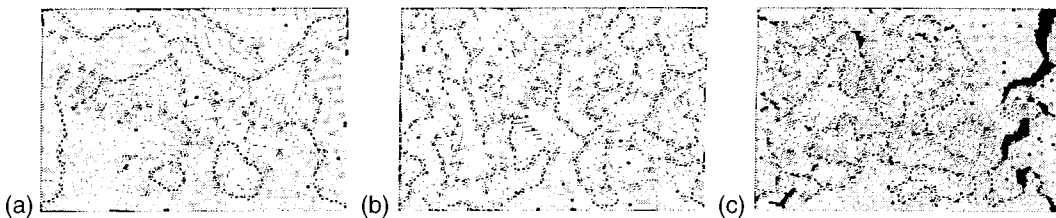


Figure 5. Influence of the speed of cooling on the material structure: (a) slow cooling, (b) fast cooling – ten times faster than (a), (c) fracture due to the thermal stresses in the material.

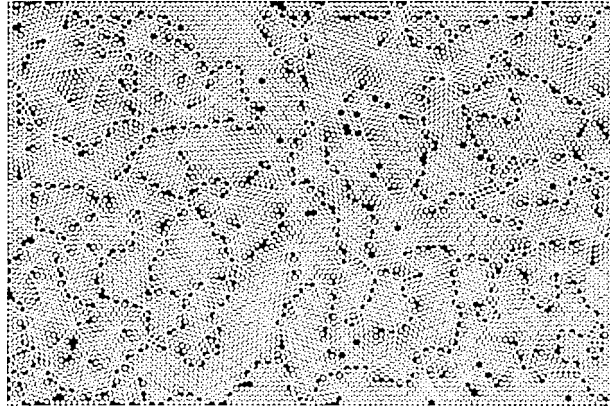


Figure 6. Polycrystalline material with 5% porosity, obtained by the described technique.

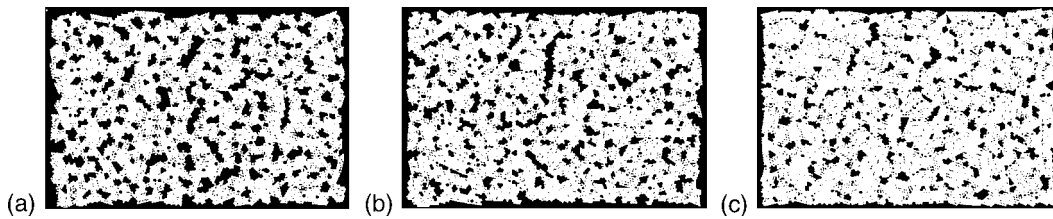


Figure 7. Polycrystalline materials with higher porosity after cooling: (a) 12%, (b) 17%, (c) 21%.

so it is more convenient to have already formed surfaces after the specimen's creation. During the simulation, the interaction between the particles and the area boundaries was simulated using the potential, which is proportional to the one acting between the particles. The magnitude of the boundary potential is usually a bit higher than the interparticle interactions so as to prevent void formation at the boundaries. But during the cooling process, especially if the porosity is significant, the boundary conditions should be released to zero. Otherwise, the material can be broken by the thermal stresses, which appear due to the material contraction while cooling, as is shown in Figure 5(c). In the figure the crack produced by the thermal tension is clearly visible.

The final result of the polycrystal creation with 5% porosity is shown in Figure 6. The specimen is magnified to visualize the inner structure of the material. Different types of imperfections of the crystal structure such as voids, dislocations, and grain boundaries can be observed in the figure. The final polycrystalline specimens with higher porosity are shown in Figure 7. After the material with the required porosity is prepared, it can be used in various computer tests to determine its mechanical properties. Quasistatic tests for elastic and strength property determination are described in [2]. In the current paper, we will focus on the dynamic fracture tests.

### 3. Computer Experiments on Impact Fracture

In the presented work the plate spallation experiments were chosen to compare properties of the mono- and polycrystalline computer materials. The plate impact experiments produce a simple deformation at very high strain rates, which makes these experiments an essential tool for calibrating and validating material models that aspire to general applicability [7].

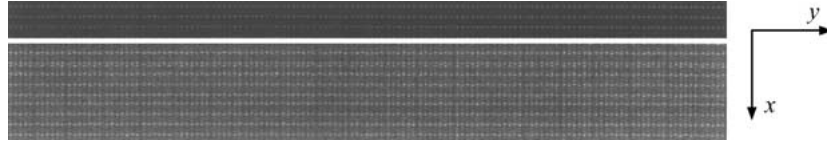


Figure 8. Initial configuration for the spallation experiment. Black – impactor, gray – target.

The history of molecular dynamics computer simulations of shock waves covers several decades; the references can be found in the review paper [8]. Here let us mention paper [5] where the noticeable differences were obtained in spallation scenario between mono- and polycrystalline particle arrangements. In papers [4, 9] the influence of the heterogeneity caused by the thermal motion in the monocrystalline materials on the spallation processes was studied. In [4] it was shown that this kind of heterogeneity could lead to drastic changes in the shape of the spall crack, increasing finally the spall strength of the material.

The computational model for the impact experiment on spallation is presented in Figure 8, where the initial particle's configuration is shown. The computational technique is the same as in [4]. The particles are filling two rectangles, representing the impactor (black) and the target (gray). The impactor is placed with a small gap from the target. In Figure 8 the particles are arranged in the perfect triangular (hexagonal) lattice. The orientation of the lattice is the same for the impactor and the target, where one of the sides of the lattice triangles is extended along  $y$ -axis. The Lennard-Jones 6–12 potential is used to describe interaction between the particles. There is no difference between the impactor and target particles. The total number of particles is about 30 000. Initially the target has zero velocity; the impactor has a constant velocity directed towards the target, where the value of the impactor velocity is about 25% of the wave speed in the perfect crystal. Free boundary conditions on all boundaries are applied. This is different from [5], where periodical boundary conditions were used for the  $y$  direction. Free boundary conditions allow for observing boundary effects, which vary significantly for the different particle arrangements. The thermal energy of the particles motion (that is proportional to the kinetic energy of the stochastic component of the particles velocities) is taken to be negligible with respect to the kinetic energy of the impactor.

The configuration after the spallation is shown in Figure 9. From the figure it follows that the spall crack boundaries in the central part of the target are absolutely straight. This is the result of the low thermal energy and coincidence between the impactor and target lattices. Multiple spallation is seen in Figure 9, which can occur for the sufficiently high impact velocities. Specific fracture localization is well seen in the vicinity of the side boundaries. This is the result of wave reflection from the free boundaries of the specimen.

Now let us consider the results of the second impact experiment (Figure 10), where impactor is the same as before, but the target is made from the polycrystalline material, which

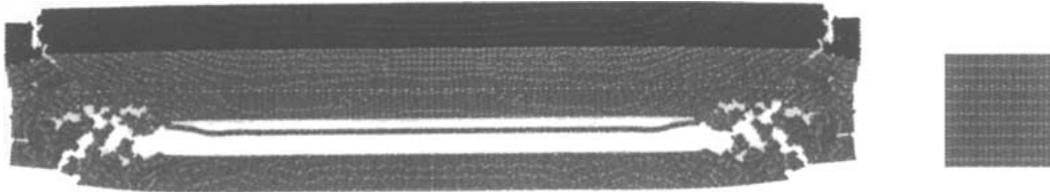


Figure 9. Spallation in monocrystal target. The rectangle shows an element of the original target material (before impact).



Figure 10. Spallation in polycrystal target. The rectangle shows an element of the original target material (1% porosity).

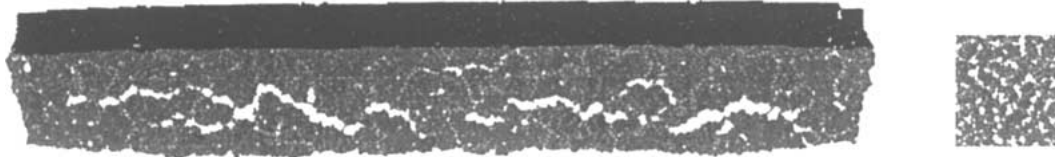


Figure 11. Spallation in polycrystal target. The rectangle shows an element of the original target material (15% porosity).

was prepared following the technique described above. The sample of the original material (as it was before the impact) is shown on the right of the figure. The original porosity is 1%. Comparing Figures 9 and 10, one can conclude that the fracture scenario is absolutely different for these two experiments. Instead of a single turnpike crack with straight boundaries, a lot of smaller cracks appeared in the polycrystalline material. These cracks are mainly following the monocrystal grain boundaries. The width of the cracks is smaller in the case of the polycrystalline material, but their orientation and location vary, so that the fracture covers a much wider region. This is in good agreement with the conclusion from [5] that the defects due to the grain boundaries could diffuse the sharpness of the tensile shocks in the material. A similar result was obtained in [4], where the diffusion of the shock wave sharpness was due to the thermal motion of the particles. The thermal effect also explains why in [5] the difference between the spallation of mono- and polycrystals was much lower than in the current experiments, since in [5] the considered initial thermal motion is much higher. Another reason why the effect of the polycrystalline packing is more significant in our case is that the sizes of the monocrystals are greater than the width of the target. Another result of the polycrystalline packing is that in Figure 10 the damage of the impactor plate is much higher than in Figure 9, which is due to the heterogeneity of the shock wave front, produced by the granular structure of the target.

The same experiment with the target made from material with much higher porosity (15%) is shown in Figure 11. Though the strength of this material is much weaker than the denser one, the spall fracture cracks are much smaller. Even more significant is this effect in Figure 12, where the same experiment was performed with 30% porous target. Actually, there is no spallation present in Figure 12. This can lead to the paradoxical conclusion that the porous Lennard-Jones material is stronger for the case of the spallation fracture. The reason

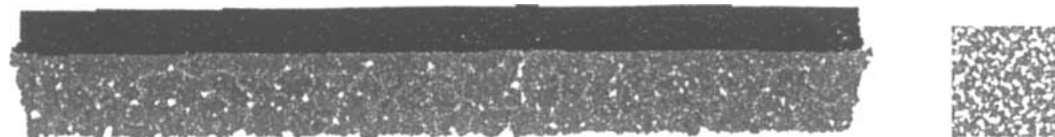


Figure 12. Result of the plate impact with polycrystal target. The original target porosity is 30%.

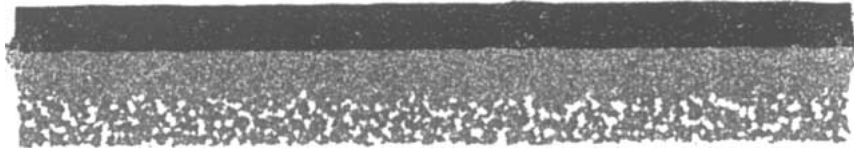


Figure 13. Penetration of plastic shock wave in the polycrystal target with 30% initial porosity.

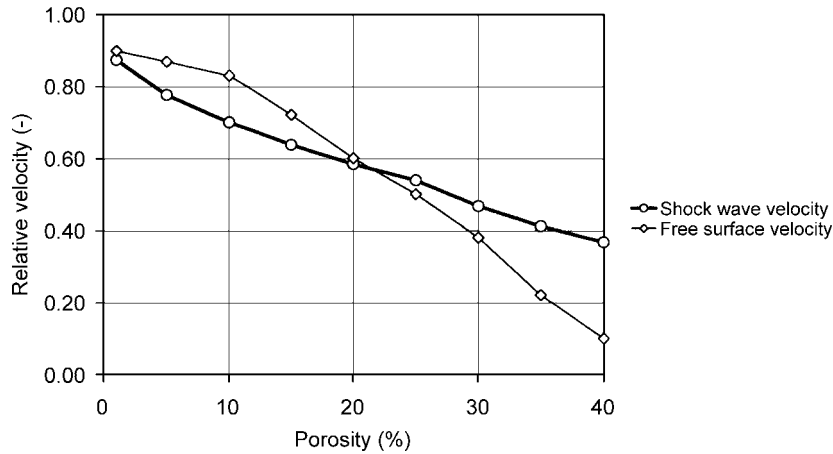


Figure 14. Shock wave velocity and free surface velocity as functions of the polycrystalline material porosity.

for this phenomenon can be found if we compare the inner structure of the material before and after the impact. The rectangular cuts of the original target material are shown in the right sides of Figures 10–12. It is clearly seen that the porosity of the material is much lower after the impact. This effect can be observed in Figure 13, where the middle stage of the impact experiment with 30% porous target is shown. The plastic shock wave moves through the target compressing the material and collapsing the pores, so that the shock wave front is clearly visible.

The results of the computer experiments with the different porous materials are summarized in Figure 14, where the shock wave velocity and the free surface velocity are plotted as functions of the porosity of the polycrystalline material. The shock wave velocity is measured using the time necessary for the plastic front to reach the free surface of the target. The free surface velocity is taken at the moment of time when it reaches its maximum value. Both velocities are plotted as relative quantities with respect to the values corresponding to the single crystal material. The graphs show that the both velocities decrease when the material porosity grows. The shock wave velocity shows more or less linear dependence on the porosity. The free surface velocity dependence is more nonlinear; it changes slowly for the low porosity, but for the higher porosity it decreases very fast practically tending to zero. The last fact shows that nearly all the energy of the shock wave is lost when it reaches the free surface. This explains why the spallation for the higher values of porosity is not observed. In the porous material a lot of energy is spent for the plastic deformation, which results in higher wave resistance. This proves the thesis that plastic strains associated with pore collapsing can be significant in spallation processes [10].

Let us note also one more distinct effect of the porous polycrystalline packing: the influence of the side boundaries, which is very high for the monocrystal target (Figure 9), is much lower for the polycrystalline targets (Figures 10–12), especially with the high porosity.



This is because the reflection of the shock waves from the grain boundaries and resistance due to the pore collapsing prevents focusing of the fracture in some localized area, as it happens in Figure 9.

#### 4. Conclusions

In the current work the technique for creation of the polycrystalline computer materials was described and comparison of the spallation computer experiments for mono- and polycrystalline particle packings is presented. The considered technique allows us to obtain not only the random polycrystalline packing but also materials with preset porosity. The presented computer experiments show that the polycrystalline computer materials can possess in the impact processes behavior which is strongly different from that for the monocrystals. The main feature of the polycrystals is smearing the shock waves due to heterogeneity of the granular structure of the polycrystals. This leads to decrease in the localization effects, which are usual for ideal monocrystals. This effect is similar (but of the higher magnitude) to the effect of smearing the shock waves in ideal crystals due to the thermal motion of the particles [4]. Material porosity introduces additional resistance for the shock wave penetration in the material. The speed of the shock wave penetration is smaller for the more porous material, and the relation between the shock wave speed and material porosity is close to linear. Free surface velocity decreases sharply for the higher porosity, which practically means that all the energy of the shock wave can be easily dissipated in the porous material due to the plastic deformations caused by the pore collapsing. This is also proved by the fact that no spallation was observed in the high-porous materials at the impact velocity, which easily breaks the monocrystal target. Thus at this point the porous material is much stronger than the ideal crystal, because the porous material can absorb energy due to the strong plastic deformations in its microstructure. But obviously this conclusion corresponds only to more or less plate impacts; for example in the case of sharp indenter, the strength of the porous material is far less than for the material with low porosity.

#### Acknowledgements

This work was partly completed during the author's stay at the Department of Engineering, Aberdeen University, U.K. The author thanks M. Wiercigroch for his support and useful discussions.

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