Simulation for elasto-plastic behavior of artificial 3D-structure under shock wave loading

V. Romanova, R. Balokhonov, E. Soppa¹, S. Schmauder¹ and P. Makarov

Institute of Strength Physics and Materials Science, SB RAS, Pr. Academicheskii 2/1, 634021 Tomsk, Russia
¹ Staatliche Materialprüfungsanstalt, Universität Stuttgart, Stuttgart, Germany

Abstract. From the mesomechanical point of view, the internal structure of a material considerably influences its plastic deformation pattern at the meso-scale level. Structural effects in real materials are three-dimensional. It is a challenge to perform 3D-modeling for material behavior under loading, taking into account an internal structure. In this paper, a special routine is applied to generate a 3D polycrystalline structure. A dynamic problem is solved to calculate 3D-polycrystal behavior under plane shock wave using a finite-difference approximation. The results of 3D simulations are analyzed and compared with those obtained in the framework of a 2D formulation.

1. INTRODUCTION

From the viewpoint of modern mechanics and physics of solids [1-3], the internal structure of a material under deformation exerts a predominating influence on the elasto-plastic behaviour at the meso-scale level. Experimental and theoretical investigations [1-6] indicate a key role of internal heterogeneity for the development of stress concentration and plastic strain localisation under loading.

The majority of the experimental methods of in situ investigations of plastically deformed materials are mostly reduced to surface observations [1-3, 6]. In this connection, a numerical simulation including the consideration of an internal structure in an explicit form shows promise for studying plastic deformation patterns in the bulk of heterogeneous media.

The main idea is to introduce an internal structure into the material region for which the calculation is performed by prescribing appropriate physical properties to computational cells corresponding to different structural elements.

Except for the simplest geometrical shape (e.g. spherical), the explicit calculations of an internal structure have been mainly performed in a 2D formulation. This fact has been attributed to both the extra complexity of the 3D mechanical problem and the requirements to power characteristics of computing facilities, more stringent in view of complex 3D models.

Note that the 2D-simulation of heterogeneous structures has given a considerable impetus to describing and understanding some elasto-plastic phenomena [1, 3-6] not addressed before, such as local stress concentration and relaxation, plastic strain localisation, etc., even though the 3D effects were beyond this study. Though intuition suggests that these results could be at least qualitatively extended to the 3D-case, providing similar patterns of elasto-plastic deformation in the bulk of material, additional calculations are required to prove or disprove this assumption and delineate the frames of its validity.

In this connection, the subject of this paper is to calculate a 3D polycrystalline test-piece subjected to deformation in a plane shock wave. A special procedure to design an artificial polycrystalline structure is given in Section 2. In Section 3, the elasto-plastic behaviour of the artificial polycrystalline structure under the shock wave loading is then calculated by the finite-difference method [7]. Finally, the 3D numerical results are analysed and compared with those calculated within 2D modelling.
2. COMPUTER DESIGN OF AN ARTIFICIAL 3D-STRUCTURE

The design of a 3D-structure filling a finite volume with irregularly shaped elements without gaps and overlapping is a topical problem of modern computational mechanics. In this section we design a polycrystalline 3D-structure whose mechanical behaviour will be further numerically calculated. The procedure of filling a finite 3D-volume with structural elements includes the following steps.

1. The volume to be filled with structural elements is discretized by the computational grid and three-dimensional coordinates are defined for each discrete point.

2. Each cell of the discretized volume is assigned a so-called structural index (SI), which reflects that this point belongs to a certain structural element. Initially all points possess the same SI equal to zero, which implies an initial homogeneity throughout the volume. At the next step, some cells are assigned specific structural indices different from zero. In such a way, they are treated as nucleating centres (NCs) of new structural elements.

In this work, NCs of different sorts were randomly distributed over the volume using the random number generator commonly used in programming. The appropriate nodes were assigned structural indices randomly varied from 1 to the number of NCs. For the sake of simplicity, it was assumed that the growth of all structural elements obeyed the same law, according to which each volume surrounding appropriate nucleating centre increments as spherically-shaped, and the growth rate was assumed to be uniform as well.

3. Finally, the volume under consideration is filled with the grain structure in a step-by-step fashion controlled by the following algorithm. At each step in the processing time, the volumes surrounding the nucleating centres are incremented by preset values in accordance with the law of growth. After the volumes of structural elements have been incremented, for each computational cell with a zero SI so far belonging to none of the structural elements it is checked whether its coordinates fall within any of the volumes. If so, the cell is considered to belong to this structural element and its SI is assigned an appropriate value different from zero. Otherwise it retains the zero SI and is checked again at the next step of the processing time. Such a procedure is repeated until the growing grains has filled 100% of the volume, that means there are no cells with a zero SI.

Presented in Figure 1 is the artificial structure with the following parameters: grid size is $100 \times 100 \times 100$, the number of NCs and their sorts are 100 and 42, respectively.

It should be noted that the resulting structural elements deviate widely from a spherical shape despite the fact that all of them were grown in the same manner and at the same rate. Such an irregularity mainly resulted from the non-uniform distribution of the nucleating centres over the initial volume.

![Figure 1. Schematic illustration of the flyer-plate test and polycrystalline test-piece under calculation.](image-url)
3. MATHEMATICAL FORMULATION OF THE THREE-DIMENSIONAL PROBLEM OF DYNAMIC LOADING

Assuming that a medium under plastic deformation retains its continuity at the meso and macro scale levels, we apply mathematical tools and a numerical method of continuum mechanics [7]. A system of differential equations in terms of a barotropic medium includes

1. The equation of continuity
   \[ \frac{\partial \rho}{\partial t} - \nabla \cdot \rho \mathbf{U} = 0 \]

2. The equation of motion
   \[ \rho \ddot{\mathbf{U}} = \sigma_{ij,j} \]

3. The expression for stress tensor components
   \[ \sigma_{ij} = -\rho \delta_{ij} + \mathbf{S}_{ij} \]

where \( i, j = 1, 3 \); \( \mathbf{U}_i = \dot{x}_i \) and \( x_i \) are the velocity vector components and Cartesian coordinates, respectively; \( V = \frac{\rho_0}{\rho} \) is the relative volume, and \( \rho_0 \) and \( \rho \) are the reference and current densities. The upper dot denotes a time derivative.

The pressure was defined from the barotropic equation

\[ P = A \frac{\rho}{\rho_0} - 1 + B \left( \frac{\rho}{\rho_0} \right)^2 - C \left( \frac{\rho}{\rho_0} \right)^3 \]

The deviatoric stresses are given by the Prandtl-Reuss model for the elasto-plastic medium

\[ \dot{\mathbf{S}}_{ij} = \mu \dot{\mathbf{E}}_{ij} - \frac{1}{3} \dot{\varepsilon}_{kk} \delta_{ij} \]

where \( \mu \) is the shear modulus. The strain rate tensor is

\[ \dot{\mathbf{E}}_{ij} = \frac{1}{2} (\dot{\mathbf{U}}_{ij} + \dot{\mathbf{U}}_{ji}) \]

To eliminate an increase in stress due to rigid rotations of medium elements, we define deviatoric stresses through the Jaumann derivative

\[ \dot{\mathbf{S}}_{ij} = \mathbf{S}_{ij} - \mathbf{S}_{ik} \mathbf{w}_{jk} - \mathbf{S}_{jk} \mathbf{w}_{ik} \]

where \( \mathbf{w}_{ij} = \frac{1}{2} (\dot{\mathbf{U}}_{ij} - \dot{\mathbf{U}}_{ji}) \) is the material spin tensor.

The plastic behaviour is controlled by the von Mises yield criterion, according to which

\[ \sqrt{\mathbf{S}_{ij} \mathbf{S}_{ij}} = Y_0 \]

where \( Y_0 \) is the material yield point. Under plastic yielding, the deviatoric stresses are corrected by multiplying by the term \( \frac{Y_0}{\sqrt{3} \mathbf{S}_{ij} \mathbf{S}_{ij}} \).

The parameter \( \lambda \) in (5) has the meaning of the power of plastic deformation energy: \( \lambda < 0 \) under elastic deformation, and \( \lambda > 0 \), provided that Eq. (8) is fulfilled.

The system of Eqs. (1) - (8) was numerically solved by the finite difference method [7] for a cubic grid. The partial differential equations are discretized in space and time, so that coordinates \( x_i \) and velocities \( \mathbf{U}_i \) are calculated in the nodes, while the stress and strain tensor components, volume and density are related to the cells. The node velocities and strain rate tensor components are calculated at an intermediate time with the n+1/2 index, and the remaining values are defined at the n, n+1, ... time steps.

The 3D calculation has been performed for a polycrystalline test-piece under a plane shock wave as schematically presented in fig. 1. Differently-coloured grains were distinguished by their yield stresses:

\[ Y_0 = (Y_0) + (Y_0) \left( \frac{N_{ph} - 2i}{N_{ph}} \right) \]
where \( \langle Y_0 \rangle \) is the average dynamic yield point, \( N_{ph} \) is the number of NCs sorts, and index \( i \) varies from 1 to \( N_{ph} \). Referring to the structure image in fig.1, the darker the grain colour, the lower its yield stress.

The material constants are presented in Table 1. The spatial step of the computational grid was \( 5 \times 10^{-4} \) cm along all three dimensions.

**Table 1. Material constants**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>( \rho_0 ), g/cm(^3)</th>
<th>( \mu_0 ), GPa</th>
<th>( \langle Y_0 \rangle ), GPa</th>
<th>( A ), GPa</th>
<th>( B ), GPa</th>
<th>( C ), GPa</th>
</tr>
</thead>
<tbody>
<tr>
<td>Value</td>
<td>2.7</td>
<td>27.7</td>
<td>0.34</td>
<td>76.5</td>
<td>165.9</td>
<td>42.8</td>
</tr>
</tbody>
</table>

Considering the triaxial compression, we disregarded the unloading waves from consideration to be able to arrive from the side surfaces. Referring to fig. 1, the boundary conditions were given in the form

\[
\sigma_{ij}(h_1, x_2, x_3, t) = 0, \quad i = 1..3, \quad j = 1..3 \\
U_i(x_1, x_2, x_3, 0, t) = U_i(x_1, x_2, h_3, t) = U_i(x_1, h_2, x_3, t) = U_i(0, x_2, x_3, t) = 0, \quad i = 2,3 \quad (10)
\]

Here \( h_1 \), \( h_2 \) and \( h_3 \) are the test-piece lengths along the \( x_1 \), \( x_2 \) and \( x_3 \) directions, respectively.

At \( t = 0 \), a shock wave front was specified at the surface \( x_1 = 0 \) as a jump in the normal component of the velocity vector, whereas other values were equal to 0. Under further calculation, the amplitude of \( U_1 \) at the surface nodes was kept constant to avoid the unloading effects

\[
U_1(0, x_1, x_2, x_3, t) = V_0, \quad \text{where} \quad V_0 = 500 \text{ m/sec}.
\]

**4. CALCULATION RESULTS**

In the 3D case, along with the complexity of the computational procedure, visualisation and analysis of the calculation results also become more difficult. Due to its heterogeneity, every layer of the test-piece exhibits an individual stress-strain pattern that, in addition, evolves in time. In this section we, therefore, give only some representative illustrations of deformation patterns, velocity vector fields and stress profiles on cutting-planes oriented parallel (figs. 2, 3 and 4(a)) and perpendicular (fig. 5) to the shock wave front, with the conclusions drawn for the general case.

*Figure 2*. Deviations of velocity vectors from those obtained for a homogeneous medium: 3D (left) and 2D (right) simulations.

Figure 2 shows the results of a 3D-calculation compared with those obtained in a 2D approximation. The velocity vectors deviated from those calculated for a homogeneous medium show that the 2D and 3D vector fields are comparable if not identical in a certain extent. In the 2D case, the ability of the material fragments to “rotate” is more clearly pronounced since the mode of plastic accommodation is confined within the only plane. The “vortices” mainly develop near the triple point zones of grains markedly differing in their yield characteristics. In the bulk of the material, greater degrees of freedom can result in a development of structural-accommodation modes other than those evolving in conditions of plane strain.
Fig. 3 indicates that plastic deformation patterns in 2- and 3D cases are quite similar qualitatively and quantitatively. The plastic strain localises mainly along the grain boundaries oriented in the direction of maximum tangential stresses. The plastic strain gradients are more pronounced near the boundaries between the grains exhibiting a high difference in their yield characteristics. It is worth noting that all the bands of localised deformation displayed in the images as darker lines border lighter zones indicating lower strain. This conclusion qualitatively agrees with the experimental data obtained by M.P. Bondar in [8] on microstructure of specimens compacted by explosion (see fig. 4(b)). The development of plastic deformation along the boundaries with higher ability to yielding results in unloading and stress relaxation in the adjacent sub-boundary zones of neighbouring grains.

A 3D simulation proved to be a useful tool for investigating the deformation modes developing in a cross-section parallel to the shock wave front, which was impossible in the framework of 2D formulation of the problem. Plotted in figure 4(a) as projections on $x_1x_2$-plane are the profiles of effective stresses $\sigma_{eff}(x_1, x_2, 0)$, corresponding to different moments of time. The average value of the stresses behind the front is equal to $\langle Y_0 \rangle$ and deviation from this value to about 15% corresponds to the yield points preset by Eq. (9).

Presented in fig. 5 are the velocity vector fields and plastic deformation pattern in the cross section $x_1 = 0.02$ cm parallel to the shock wave front. Considering figures 4(a) and 5 together we can make the following conclusions. At the beginning of the plastic front (see figs. 4(a) and 5(a), $t_1$) the deviation of velocity vectors from the direction of wave propagation manifests itself at first near the grain boundaries. As plastic front passes through the cross-section (figs. 4(a) and 5(b), $t_2$) the velocity field indicates the higher the grain deformability, the stronger the non-uniform motion it is involved into.

A correlation between the stress-profile and velocity field corresponding to $t_3$ shows that the non-uniform motion is mainly exhibited in the area of stress gradients that becomes practically uniform in the region of stress plateau behind the front. This fact agrees with the earlier assumption.
[4, 5] that the stress-strain gradients under triaxial compression are a primary reason for origination of bands of localized plastic deformation.

As in the case of a cutting-plane parallel to the wave direction, the plastic deformation pattern presented in fig. 5(c) demonstrates higher strain gradients in the vicinity of interfaces between grains with different ability for yielding.

![Figure 5](image_url)

**Figure 5.** Deviations of velocity vectors from those obtained for a homogeneous medium (a, b) and plastic deformation (c) in the cross-section \(x_1 = 0.02 \text{cm}\) (marked by dashed line in Fig. 4); \(t_1, t_2\) and \(t_3\) are the same as those in Fig. 4.

5. CONCLUSIONS

In this paper, 3D-simulations of elasto-plastic behaviour of a polycrystalline material under a plane shock wave have been performed. The results of the 3D-calculation have been analysed and compared with those obtained in the framework of a 2D-approximation. It has been shown that the 2D and 3D deformation patterns are comparable within a certain degree.

It should be marked, however, that the outlined conclusions hold for the specific case of deformation under a plane shock wave of a certain amplitude without unloading effects. It could hardly be extended to the case of other loading conditions without certain proofs calling for special calculations.

Acknowledgments

Support of the Russian Foundation for Basic Research through the grant №00-15-96174 «Scientific school of academician V.E.Panin on physical mesomechanics and computer-aided design of new materials» and the Deutscher Akademischer Austauschdienst (DAAD) through the project A0206390/REF.325 is gratefully acknowledged.

References