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Equations of state in materials beyond the assumption of isotropy of volume compressibility

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Abstract. The process of elastoplastic deformation is considered for materials whose symmetry of elastic properties is modeled by means of five or more independent elastic constants. In the simulation of shock loading of a zinc single crystal characterized by a transversal isotropy of elastic and plastic properties, it was assumed that there is no volume isotropy of compressibility. Different equations of state are applied in a three-dimensional arrangement in the condition of plastic deformation in the direction of each axis. They reflect the relationship of hydrostatic stress to the degree of compression of the material. It is shown that the application of various equations of state changes the propagation velocity of volume waves and introduces a change in the wave pattern of deformation in anisotropic materials.

1. Introduction

Uniform volumetric strain generates hydrostatic stress only in the case of isotropy of elastic properties in modeling elastic and plastic deformations in solids. The components of the stress tensor are divided into the spherical (hydrostatic stress) and deviator parts, as the components of the total deformation tensor in this case in the region of elastic and plastic deformations. For materials with 5 or more independent elastic constants\cite{1}, the question of separating of tensors of total stresses and total deformations into spherical and deviatorial parts remains unresolved. Traditionally, in the modeling of the deformation of anisotropic materials, it is assumed that uniform volumetric strain causes hydrostatic stress, i.e. the assumption of the isotropy of the volume compressibility of an anisotropic material is introduced\cite{2,3,4,5}. In the modeling of elastoplastic deformation of materials with a high degree of anisotropy, such an assumption may introduce errors. Therefore, in modeling the deformation of such materials, an anisotropic pressure is introduced, reflecting the degree of anisotropy of the compressibility of the material. This is relevant for materials whose elastic properties are described by five, six, seven and nine independent elastic constants. Such materials include: HCP - single crystals, plastically deformable composite materials, biomaterials and so on. The anisotropic pressure reflects the change in the shape of the spherical body under the action of external hydrostatic stress. In the region of elastic deformations, the introduction of anisotropic pressure is determined by
the expansion of the elastic deformation energy by the energy of the change in volume and the energy of the change in shape [6]. In the region of small plastic deformations, it is necessary to maintain the degree of pressure anisotropy for the correctness of the mathematical model, i.e. introduce two or three equations of state. In the region of developed plastic deformations, a gradual transition to a single equation of state is possible in the case when the anisotropy of the elastic properties changes with increasing pressure.

Within the framework of continuous medium mechanics, the results of numerical modeling of shock-loading a zinc single crystal target in the direction of [0001] and [1010], using anisotropic pressure in the region of elastic and plastic deformations, are presented in a three-dimensional statement. A good correspondence between the profiles of the forbidden velocities obtained numerically and in full-scale experiments is shown [7].

2. Model of mathematical modeling of elastoplastic deformation of anisotropic materials

The deformation in anisotropic materials is described by the system of equations for nonstationary adiabatic motion in a compressible anisotropic medium: continuity equation, motion equations of a continuous medium and energy equation.

A model, used in the calculations, included decomposition of the total stress tensor into a deviator part and an "anisotropic" hydrostatic stress [6]

\[
\sigma_{ij} = S_{ij} - P_e \cdot \lambda_{ij},
\]

here \( S_{ij} \) - the components of the total stress deviator, \( \lambda_{ij} \) - the generalized Kronecker delta and \( P_e \) - the spherical part of the total stress tensor. In the elastic range

\[
S_{ij} = C_{ijkl} \varepsilon_{kl} \text{, } \lambda_{ij} = \frac{C_{ijkl} \delta_{kl}}{3K_a} \text{, } K_a = \frac{1}{9}C_{ijkl} \delta_{ij} \delta_{kl} \text{, } P_e = \varepsilon_v C_{ijkl} \delta_{ij} \delta_{kl} / 3,
\]

where \( K_a \) - the generalized bulk modulus, \( \delta_{kl} \) - the Kronecker delta, \( \varepsilon_{vij} \) - the strain deviator components, \( C_{ijkl} \) - elastic constants and \( \varepsilon_v \) - the volume strain for the anisotropic medium.

The application of the expansion of the total stress tensor in the form (1) in numerical calculations in the region of elastic deformations is equivalent to calculations in total stresses. That is, in the region of elastic deformations, several relationships are realized between the volume deformation and the anisotropic pressure.

When passing from elastic deformations to plastic deformations, it is necessary to ensure the smoothness of the function of the anisotropic pressure, dependent on the volume deformations. Therefore, in the area of plastic deformations, the \( \lambda_{ij} \) coefficients obtained using the elastic constants are used.

Thus, having in the direction of each of the material's symmetry axes the relationship between volume deformations and anisotropic pressure coinciding with that in the region of elastic deformations, we ensure the smoothness of the functions of the equations of state in the transition from elastic strains to plastic deformations.

In the plastic range, the pressure \( P_e \) for an anisotropic material is estimated by the Mie-Grüneisen equation as a function of specific internal energy \( E \) and current density

\[
P_e = \sum_{n=1}^{3} K_n \left( \frac{V}{V_0} - 1 \right)^{n} \left[ 1 - K_0 \left( \frac{V}{V_0} - 1 \right) \right]^{2} + K_0 \rho E,
\]

where \( K_0, K_1, K_2, K_3 \) - material constants and \( V, V_0 \) - the current and initial volumes.

The total stress in the plastic range is also estimated by formula (1). The components of the total stress deviator are calculated according to the flow theory. The plastic strain is estimated using the non-associated flow rule:
\[ d\varepsilon_{ij}^p = d\lambda \frac{\partial F}{\partial \sigma_{ij}}, \]  

(3)

with \( d\lambda \) being zero in the elastic range and always positive in the plastic range (yield criterion), \( \varepsilon_{ij}^p \) - the plastic strain components and \( F \) - the yield function.

The von Mises–Hill criterion in terms of stress deviators for transversally isotropic materials with regard to isotropic hardening has the form [10]. The elastoplastic deformation of an isotropic material (projectile) is described using the Prandtl–Reuss model.

3. Problem statements for shock-loaded target of zinc single crystal

![Figure 1. Initial configuration of impactor and target](image)

The problem statement for our 3D finite element simulation of impacted Zn single crystals was the same as in experiments [7]. The elastic constants of the transversally isotropic Zn target were following [7]: \( C_{11} = 61041.7 \) MPa, \( C_{33} = 161018.1 \) MPa, \( C_{12} = 49987.7 \) MPa, \( C_{23} = 45126.2 \) MPa, and \( C_{44} = 63445.9 \) MPa. The simulation was performed using original software.

Figure 1 shows the initial configuration of the impactor (25 920 tetrahedrons) and target (227 430 tetrahedrons). The target was a Zn plate of thickness 1.7 mm, and the impactor was an Al plate with its initial velocity - \( v = 650 \) m/s.

4. Results of numerical simulation

The simulation results for impact loading demonstrate differences in the velocities of waves propagating in the Zn single crystal where it is assumed to have transversally isotropic bulk compressibility.

In this case the velocities of bulk waves estimated by (1) are 2741.7483 m/s along the axis \([0001]\) and 3382.909 m/s along \([10\bar{1}0]\). The velocities of longitudinal waves, which are unambiguously determined from elastic constants, are 2923 m/s along the axis \([0001]\) and 4749 m/s along \([10\bar{1}0]\). In the direction of \([0001]\), the propagation velocities of the longitudinal and volume waves are close, so in this direction is no splitting of the shock wave into an elastic precursor and a plastic shock. Figure 2 shows experimental free surface velocity profiles for Zn single crystal targets loaded along \([0001]\) and \([10\bar{1}0]\) [7]. The velocity profiles of free surfaces show the dependences in meters per second [m/s] over time in nanoseconds [ns].

In Fig. 3 shows analogous velocity profiles of free surfaces obtained by numerical modeling in a three-dimensional formulation using the mathematical model (1). In the simulation, the onset of the process is the instant of contact between the impactor and the target. The comparison is made only on the amplitudes of the initial sections of the velocities of the compression waves emerging on the free surface of the target, until the moment of spall fracture. In the case of shock loading target from a zinc...
single crystal along the direction [10\bar{1}0] in real and numerical experiments center point on the rear surface have the same velocities of elastic precursors - 140 m/s and the maximal velocity amplitudes are also close (450-400 m/s). Along the direction [0001] in real and numerical experiments no splitting of the shock wave into an elastic precursor and a plastic shock and the amplitudes of the maximum velocities of the rear surface are the same - to 550 m/s.

The flatness of the profiles of propagation velocities of elastic and plastic waves in numerical simulation is obtained because of the explicit difference schemes of dynamic numerical methods has own specifics. The dynamic yield strength of the Zn single crystal in the direction [10\bar{1}0] is 1800 MPa, and in the direction [0001], it is 3500 MPa.

![Figure 2](image1.png)  
**Figure 2.** Experimental free surface velocity profiles for Zn single crystal

![Figure 3](image2.png)  
**Figure 3.** Free surface velocity profiles for Zn single crystal obtained by numerical modeling

The role of the spherical part of the stress tensor in the total stress tensor increases during the deformation, accompanied by the processes of uniform compression: shock loading with concentration of stress waves, all-round pressing, angular pressing, etc.

The role of the spherical part of the stress tensor in the stress tensor is demonstrated on the example of the model problem. This is relevant for materials whose symmetry of elastic properties leads to the number of five or more independent elastic constants.

Within the framework of continuous medium mechanics, a numerical simulation of the loading of spherical bodies from a single crystal of zinc in a three-dimensional setting is carried out. The calculations were carried out using a mathematical model that allows one to take into account the "anisotropic" hydrostatic stress in the material of a zinc single crystal according to the formula (1).

Calculations of the dynamic loading of bodies by a pulse of uniform compression were also performed by the finite element method [8] in a three-dimensional statement using original programs. The discretization of the volumetric configurations of the spherical body is performed with the 77000 tetrahedra (Fig. 4).

![Figure 4](image3.png)  
**Figure 4.** Uniform compression of a ball in 3D statement
The orientation [0001] of a zinc single crystal coincided with the axis OX and orientation \([10\overline{1}0]\) coincided with the axes OY and OZ. A numerical simulation of the deformation of a 10 mm diameter spherical body from a zinc single crystal by a 4GPa uniform compression pulse during 3 μs was carried out. This numerical problem illustrates the propagation of elastoplastic deformations in a spherical body. The magnitude of the 4GPa pulse ensures the occurrence of elastoplastic deformations in the direction of all three axes. After 3μs the load does not act on the spherical body and the propagation of elastoplastic waves continue.

In Fig. 5 shown the changes in the radius of a spherical body under the action of uniform compression pulse for two variants of the expansion of the total stress tensors onto the ball and deviation parts: curve 1 – for the case of assuming the bulk isotropy of a transversely isotropic material and curve 2 – for the case of assuming the bulk anisotropy of a transversely isotropic material according to model (1). Negative values correspond to a decrease in the radius of a spherical body over time with respect to the initial value and positive values – an increase in the radius.

The elastic properties along the axes OY and OZ are the same; therefore, in the OYZ plane, the stress state is axisymmetric. In Fig. 5a, curves 1 and 2 show changes in the radius of a spherical body under the action of a compression pulse along the OY and OZ axes for 2 types of mathematical models. In Fig. 5b curves 1 and 2 show changes in the radius of a spherical body under the action of a compression pulse along the OX axis. Zinc single crystal has the minimum values of the elastic properties along the OX axis.

Using curve 2 in Fig. 5 it is shown that at the initial stage the deformation of the compression of a spherical body along the [0001] axis is much larger than the compression deformation along the \([10\overline{1}0]\) axis and compression along the [0001] axis continues until the load is removed by 3 μs. At 3μs, the initially spherical body has the shape of an ellipsoid with a maximum elongation along the \([10\overline{1}0]\) axis.

After the load is stopped, the body expands elastically along the [0001] direction. During loading a spherical body from a zinc single crystal by an impulse of uniform compression of 4 GPa for 3 microseconds, elastoplastic deformations occur in all three mutually perpendicular directions, that is, along the axes [0001] and [10\overline{1}0]. The elastoplastic deformation changes not only the degree of compression of the spherical body, but also forms a stable the ellipsoid after one compression cycle. Further, over time, only elastic changes in the shape of the ellipsoid are observed in time, they are less than plastic and the maximum compression of the ellipsoid is preserved along the [0001] axis. Zinc single crystal is characterized by minimal elastic properties in the direction [0001], but maximal
plastic properties in the direction [0001], and the wave pattern of deformation leads to maximum final deformation in the direction [0001] (Fig. 6, curve 2). As a result, the maximum decrease in the radius of the spherical body in the direction [0001] is more than 7%, and in two perpendicular directions, corresponding to the direction [1010], it is 3% (Fig. 6). If the time of action of the compression pulse is greater than the propagation time of the compression wave to the center of the ball for all directions, than final picture of the elastoplastic deformation is similar to the final picture of elastoplastic deformation under static loading and the ellipsoid has compression along the OX [0001] axis and stretching along the OY and OZ axes [1010].

If the assumption of the isotropy of the volume compressibility of an anisotropic material is made in the mathematical model, at a time of 3 μs the spherical body restores the original shape (curves 1 in Figures 5a and 5b). In this case, the transversal isotropy of the elastic and plastic properties of a zinc single crystal determines only the initial degree of compression of a spherical body and does not affect its finite geometric form.

5. Conclusion

The application of the hypothesis of volume compressibility anisotropy in the numerical simulation of the elastoplastic deformation of an initially spherical body from a zinc single crystal with its dynamic loading by a pulse of uniform compression predicted a change in its shape to a biaxial ellipsoid. The application of the hypothesis of the isotropy of the volume compressibility of transversely isotropic zinc material in this case does not reflect the final change in its shape. Consequently, in the numerical modeling of elastoplastic deformation in materials characterized by anisotropy of elastic properties with five, six, seven, and nine independent elastic constants, it is important to apply the hypothesis of volume compressibility anisotropy in problems with a high level of developed volume deformations.

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