Studies of the propagation of elastic and plastic waves in cubic single crystals

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Abstract. The study of the elastic and plastic properties of a single crystal with cubic symmetry of mechanical properties under dynamic loading was carried out. In the work, the method of numerical simulation shows the effect on the output of an elastic precursor and a plastic compression wave of the orientation of the calculated coordinate system relative to the direction of loading. It is shown that the rotation of the calculated coordinate system by 45° around the axis of loading of the projectile and the target in the framework of numerical simulation of the process of shock loading affects the stress state of the target and the velocity profile of its rear surface. This is explained by the fact that in the plane of loading the elastic and plastic properties in a single crystal with cubic symmetry of properties change in accordance with the values of Euler angles.

1. Introduction

The main objectives of the study of shock wave processes arising in solids are the prediction of destruction, the implementation of physical and mechanical transformations, and the construction of equations of state for the studying materials. To do this, the shock loading of targets from the studying material simulate in natural experiments then determine the particle velocity on the rear surfaces of these targets. The compression and extension wave profiles obtained in the natural experiments which reflect the dynamics of wave interactions determine the presence of elastoplastic deformations and fracture in the material. Relations are used under the assumption that a one-dimensional deformation process is implemented in the targets for mathematical processing of the results of natural experiments. The processes of material deformation are accompanied by changes in compressibility, and this leads to features in the form of profiles of compression and extension waves. High strain rates are locally realized in various technological processes during the processing of metals during natural experiments. They allow one to investigate elementary acts of deformation and fracture under stress conditions close to comprehensive tension. In materials having anisotropy of mechanical properties, a uniform deformed state gives rise to an uneven stress state due to different volume compressibility of the material in different directions. This fact is confirmed by differences in the propagation velocities of elastic and plastic waves in anisotropic materials for different directions. Investigations of shock wave processes in anisotropic materials using computer modeling in a three-dimensional formulation provide additional information by taking into account the anisotropy of all mechanical properties including compressibility anisotropy. For example, in [1] using numerical simulation of shock loading...
of a zinc single crystal the difference between the profiles of shock waves reaching the rear surface of the target in cases of loading along the [0101] and [0001] axes is shown.

For shock loading along the [0001] axis in a zinc single crystal, there is no separation into an elastic precursor and a plastic compression wave on the shock wave velocity profile. This is explained by the proximity of the volume compressibility values in the region of elastic and plastic strains in the [0001] direction in the zinc single crystal. The consequence of this is the proximity of the values of the propagation velocities of elastic longitudinal and volumetric waves in this direction in a zinc single crystal. In single crystals with cubic symmetry of properties in some planes, a continuous change in mechanical properties is observed and a nontrivial problem arises of choosing the directions of the axes of the coordinate system in this plane. The use of methods for numerical simulation of shock loading of targets made of anisotropic materials in order to study their mechanical characteristics allows us to identify some features of their deformation processes.

On the example of studying the processes of elastoplastic deformation of a single-crystal target with cubic symmetry of properties, the influence of applying a three-dimensional statement of the problem on the exit velocity of an elastic precursor is shown in the paper. To do this, we simulated the shock loading of the target along the [001] direction for two cases of orientation of the coordinate axes. In the first case, the two other calculated coordinate axes coincide with the directions [010] and [100], in the second case - with the directions [011] and [011]. All these axes lie in the same (001) plane of the single crystal, but in this plane there are differences in properties in different directions. In natural experiments, such a separation of the calculated axes within the same loading plane is impossible.

When processing the results of natural experiments, equations are used that are obtained under the assumption of the realization of one-dimensional motion of a continuous compressible medium [2]. The aim of the work is to find differences in the results of calculations of the stress state of the target from the single crystal obtained only by rotating the calculated coordinate system by 45° around the axis of shock loading.

2. Mathematical model of elastoplastic deformation of anisotropic target material

System of equations described the unsteady adiabatic motions of a compressible anisotropic medium is used that for modeling the processes of deformation in anisotropic materials [3]

- continuity equation:

$$\frac{d\rho}{dt} + \rho \text{div} \vec{v} = 0, \quad (1)$$

- equations of motion of a continuous medium:

$$\rho \frac{d\vec{v}^k}{dt} = \frac{\partial \sigma^{ki}}{\partial x_i} + F^k, \quad (2)$$

- energy equation:

$$\frac{dE}{dt} = \frac{1}{\rho} \sigma^{ij} e_{ij}. \quad (3)$$

Here $\rho$ — medium density; $\vec{v}$ — velocity vector; $F_k$ — components of the body force vector; $\sigma_{ij}$ — components of symmetric stress tensor; $E$ — specific internal energy.

$$e_{ij} = \frac{1}{2} (\nabla_i \nu_j + \nabla_j \nu_i), \quad (4)$$

where $e_{ij}$ — components of symmetric strain velocity tensor; $\nu_i$ — components of velocity vector; $i, j = 1, 2, 3$. 
Total strain tensor in the elastic and plastic strain region decomposes in the general case into spherical and deviator parts like for isotropic materials. Uniform volumetric deformation due to anisotropy of the compressibility of the material corresponds to anisotropic pressure in anisotropic materials. Therefore, the total stress tensor in the general case of elastic and plastic strains is decomposed into parts corresponding to the spherical and deviator parts of the total strain tensor, i.e. on the deviator part and anisotropic pressure [4]

$$\sigma_{ij} = S_{ij} - P\lambda_{ij},$$

where $S_{ij}$ are the components of the total stress deviator; $\lambda_{ij}$ is the generalized Kronecker delta; $P_e$ is the spherical part of the total stress tensor. In the elastic range

$$S_{ij} = C_{ijkl}e_{kl}, \quad \lambda_{ij} = \frac{C_{ijkl}\delta_{kl}}{3K_\alpha}, \quad K_\alpha = \frac{C_{ijkl}\delta_{kl}}{9}, \quad P_e = \frac{e_{ij}C_{ijkl}\delta_{ij}\delta_{ml}}{3},$$

where $K_\alpha$ is the generalized bulk modulus; $\delta_{kl}$ is the Kronecker delta; $e_{kl}$ are the strain deviator components; $C_{ijkl}$ are elastic constants, $e_V$ is the volume strain for an anisotropic medium. In the elastic range $e_V = \left(\varepsilon_{11} + \varepsilon_{22} + \varepsilon_{33}\right)$. The use of decomposition of the full stress tensor in the form (5) in the calculations of elastic stresses in the field of elastic strains is equivalent to the full stress calculations. In the plastic range $e_V = (V_0/V - 1)$, where $V$ and $V_0$ are the current and initial volumes. In the plastic range, the pressure $P_e$ for an anisotropic material is estimated by the Mie-Grüneisen equation

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

where $K_0$, $K_1$, $K_2$, $K_3$ — material constants.

The components of the total stress deviator were calculated by flow theory. Associated flow law is used to calculate the plastic strain in the form

$$d\varepsilon_{ij}^p = d\lambda \frac{\partial F}{\partial \sigma_{ij}},$$

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

As a plasticity condition, the Mises-Hill condition written for anisotropic materials through stress deviators taking into account isotropic hardening has the form [5]

$$F\left(S_{ij}, R\right) = \frac{S_{11}^2}{r_1} + \frac{S_{22}^2}{r_2} + \frac{S_{33}^2}{r_3} + \frac{S_{44}^2}{r_4} + \frac{S_{55}^2}{r_5} + \frac{S_{66}^2}{r_6} - R^2 = 0,$$

where $r_i$ is determined in terms of tensile and shear yield strengths for a transversally isotropic material, $R$ is the isotropic hardening function.

From experimental studies [6], it is known that the function $R$ characterizing isotropic hardening is invariant to the form of the stress state, is determined from experiments on simple loading and linearly depends on the accumulated plastic deformation $e^p$. 
where $R(e^p) = 1 + \xi e^p$, $k, l = 1, \ldots, 3$.

When simulating the plastic deformation of an anisotropic material, the average pressure $P_e$ in the material obtained using the equation of state was also multiplied by the coefficient $\lambda_{ij}$. Therefore, the condition of the same values of pressure anisotropy in the region of elastic and plastic deformations is realized. The used mathematical model allow to take into account the dependence on the direction of the coordinate axes of the volume compressibility values, as well as the propagation velocities of elastic longitudinal and body waves.

The elastoplastic deformation of the isotropic material of the projectile was carried out using the Prandtl-Reuss model. Stresses defined in the element of the projectile or target rigidly rotated in space are recalculated using the derivative of Yaumann [7].

3. Anisotropy of the elastic and plastic properties of the target’s material

The anisotropy of the elastic constants of a single crystal alloy is shown in figure 1 using the Pascal stress scale. Figure 1a shows the index surface of the Young’s modulus for a single crystal. The minimum and maximum values of Young’s modulus are in the range from 102.2 to 250.6 MPa. In figure 1, the green curve shows the anisotropy of the Young’s modulus in the 0XY plane, points 1 and 1’ correspond to the values of Young’s modulus in the 0X and 0Y directions equal to 102.2 MPa. Points 3 and 3’ correspond to the values of Young’s modulus in the directions 0X’ and 0Y’ equal to 193.2 MPa realized in the case of rotation of the directions of the axes 0X and 0Y by an angle of 45° in the plane 0XY. At other points (for example, 2 and 2’) on the curve in the 0XY plane, the Young’s modulus is greater than 102.2 MPa, but less than 193.2 MPa. It is clear that under shock loading of the single crystal in the direction perpendicular to the 0XY plane the reaction of the target from the single crystal will depend on the values of Young’s modulus taking values from 102.2 MPa to 193.2 MPa. But in numerical calculations, it is necessary to make a choice of two directions for the calculation coordinate system in the 0XY plane.

Rectangular Cartesian coordinate system is used in the numerical simulation of the process of deformation of a target from a single crystal. Two options for the directions of the coordinate axes were chosen to assess the influence of the choice of directions of the calculated coordinate system in the 0XY plane on the results of calculating the stress state of the target: either along [010] and [100], or with a rotation at an angle of 45° to the axes 0X and 0Y, i.e. [011] and [011].

The selected directions of the coordinate axes correspond to the minimum or maximum values of the Young’s modulus in the 0XY plane.

In the field of elastic deformations, the magnitude of the longitudinal compression modulus is either in all three directions 277.96 GPa, or in the direction 0Z also 277.96 GPa, and in the directions 0X and 0Y 360.8 GPa.

The Table 1 shows the values of technical elastic constants and propagation velocities of elastic (longitudinal and volumetric) waves for both cases of calculations. The propagation velocities of elastic longitudinal waves in the [011] direction are determined based on the relations for materials with cubic symmetry of properties [8,9]

$$\nu_{[011]} = \left( \frac{C_{11} + C_{12} + 2C_{44}}{2\rho} \right)^{\frac{1}{2}}$$

where $C_{ij}$ — components of the matrix of elastic constants of a material with cubic symmetry of properties. The elastic wave propagation velocities obtained on the basis of these relations are determined using the formulas relating the total stresses and total strains, i.e. taking into account the anisotropy of bulk compressibility.
**Figure 1.** Indication surface of the Young's modulus (a), section of the index surface of the Young's modulus in the 0XY plane (b) for the VZhM8 single crystal alloy.

**Table 1.** Properties of the materials of the projectile and target in three directions of the Cartesian coordinate system for two cases of calculations

| Material     | Young's modules | Poisson's ratios | Shear modules | Longitudinal wave velocity | The velocity of body waves in the directions |
|--------------|-----------------|-----------------|---------------|-----------------------------|---------------------------------------------|
| Steel        | $E = 204$ GPa   | $\nu = 0.3$     | $G = 79$ GPa  | $V_{l[001]} = 5539$ m/s     | $V_{ob[001]} = 5040$ m/s                   |
| VZhM8 [001], [010] and [100] | $E_x = E_y = E_z = 102.2$ GPa | $\nu_{xy} = \nu_{yz} = \nu_{zx} = 0.426$ | $G_{xy} = G_{yz} = G_{zx} = 118.7$ GPa | $V_{l[001]} = 5539$ m/s | $V_{ob[001]} = 5040$ m/s |
| VZhM8 [001], [011] and [011] | $E_x = 102.2$ GPa | $\nu_{yx} = 0.788$ | $G_{yx} = G_{zx} = 118.7$ GPa | $V_{l[011]} = 6311$ m/s | $V_{ob[011]} = 4867.5$ m/s |
|              | $E_y = 193.2$ GPa | $\nu_{yz} = -0.14$ | $G_{y} = 35.8$ GPa | $V_{l[011]} = 6311$ m/s | $V_{ob[011]} = 5372$ m/s |

The propagation velocity of volumetric waves in the case of propagation in the directions [001], [010] and [100] is 5040.3 m/s. The values of the plastic constants in the Cartesian coordinate system in three mutually perpendicular directions are as follows: either in all three directions the same $\sigma_T = 1050.8$MPa, or $\sigma_{TX} = 1050.8$MPa, $\sigma_{TY} = \sigma_{TZ} = 934$MPa [10]. Here $\sigma_T$ is the yield strengths of the target material along the directions $0X$, $0Y$, and $0Z$.

**4. Formulation of the problem**

The processes of elastoplastic deformation under shock loading by a steel projectile of a target made of VZhM8 single crystal alloy are considered [10]. In figure 2 shown the initial configuration of the projectile (D1) and target (D2) at the initial time. Boundary conditions: on the free surfaces of the projectile ($\Sigma$1) and the target ($\Sigma$2), the conditions of the absence of acting forces are satisfied, on the contact surfaces of the projectile and the target ($\Sigma$3) sliding conditions without friction are realized. The axis of symmetry of the target coincides with the direction [001] of the material and the axis (0Z) of the calculated coordinate system. The other two coordinate axes $0X$ and $0Y$ coincide with the directions [010] and [100] or [011] and [011] of the target material, respectively. Therefore, in both cases, an axisymmetric stress state is realized in the projectile and target. The initial velocity of the projectile is 600 m/s.
The density of the single crystal alloy VZhM8 $\rho = 9060$ kg/m$^3$. For a steel projectile, $\rho = 7850$ kg/m$^3$, $E = 204$ GPa, $\sigma_T = 640$ MPa. The finite element method modified for shock loading problems is used as a calculation method [10].

5. Results

Figure 3 shows the velocity profiles of the central part of the rear surface of the target for two calculations: when the axes 0$X$ and 0$Y$ are directed along the directions [011] (solid line) and when the axes 0$X$ and 0$Y$ are directed along the directions [010] and [100] (dashed line).

Figure 3$a$ shows the complete velocity profiles including the outputs of elastic precursors, the outputs of plastic compression waves, and also the outputs of spall pulses, reflecting the processes of occurrence of spall cracks in the material of the target. For a detailed discussion of the yield processes of elastic precursors in figure 3$c$ shows the propagation of fronts from 0.325 to 0.45 $\mu$s. It can be seen that the differences are observed in the exit velocities of elastic precursors and plastic compression waves. This is a consequence of the influence of the mechanical properties of the target in the directions perpendicular to the direction of shock. The back surface velocity profile shown by curve 1 corresponds to the case when in the directions perpendicular to the direction of shock the Young's modulus were almost 2 times larger and the yield strengths were 11% less. Since in both calculations the mechanical properties were set identical in the direction of shock, and the velocity profiles of the rear surfaces of the targets are different, these differences illustrate the non-uniformity of the deformation process realized in the target when it is loaded by a flat projectile.

Figure 3. The velocity profiles of the rear surfaces of the targets for calculating the shock loading of the targets along the [001] direction: 1 — the axes 0$X$ and 0$Y$ are directed along the [011] directions; 2 — the axes 0$X$ and 0$Y$ are directed along the [010] and [100] directions.
6. Conclusion
Non-uniformity of the elastoplastic deformation of the targets during the implementation of shock wave processes in them is shown for materials characterized by significant anisotropy of mechanical properties.

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References
[1] Krivosheina M N, Kobenko S V, Tuch E V, Kashin O A, Lotkov A I and Khon Yu A 2019 Mater. Sci. Technol. 5(7) 823
[2] Garkushin G V, Razorenov S V and Kanel G I 2008 Solid State Physics 50(5) 805
[3] Sedov L I 2004 Mekhanika Sploshnoy Sredy (Continuum mechanics) (Moscow: Nauka Publ) (In Russ)
[4] Solovyov A E, Golynets S A and Khvatsky K K 2017 Proc. 9 All-Russian Conference on Testing and Research of the Properties of Materials “Testmat” (Moscow) part 2 pp 1-10 (In Russ)
[5] Tsai S W and Wu E M 1971 J. Compos. Mater. 5 58
[6] Kosarchuk V V, Kovalchuk B I and Lebedev A A 1986 Strength of Materials 18(4) 473
[7] Anderson Ch E, Cox P A, Johnson G R and Maudlin P J 1994 Comput. Mechanics 15 201
[8] Solovyov A E, Golynets S A and Khvatsky K K 2017 Trudy VIAM (Proc. All-Russ. Inst. Aviation Materials) (10) 112 (In Russ)
[9] Goldstein R V, Gorodtsov V A, Lisovenko D S and Volkov M A 2016 Physical Mesomechanics 17(2) 97
[10] Petrushin N V, Svetlov I L and Ospennikova O G 2012 Vse Materialy Entsiklopedichesky spravochnik (All Materials Encyclopedic Reference) (5) 15 (In Russ)