Elastoplastic deformation processes in materials with cubic symmetry of properties

M N Krivosheina
Institute of Strength Physics and Material Science of the Siberian Branch of the Russian Academy of Sciences, Akademicheskii 2/4, Tomsk 634021, Russia
E-mail: marina_nkr@mail.ru

Abstract. Some results of studies of the processes of elastoplastic deformation in a material with a cubic symmetry of elastic and plastic properties are presented. Cases of shock loading of a cylinder from a single crystal alloy on a rigid target (Taylor test) along three different directions ([111], [001] and [011]) are considered. These directions are characterized by the fact that along them propagation of longitudinal and transverse waves with different speeds is possible. Using the example of solving the Taylor test problem, it is shown that the differences in elastic properties along the [011] directions in cubic crystals determine elastoplastic deformations.

1. Introduction
Elastoplastic deformation of materials characterized by cubic symmetry of properties depends on the direction of loading relative to the axes of symmetry of the material. For such materials, the index surfaces of the elastic characteristics have a geometry that differs significantly from spherical. Especially differences are great in the elastic properties along the [111], [001] and [011] directions. The investigation of elastic properties in these directions in natural experiments is traditionally since the propagation of longitudinal and transverse waves occurs in cubic crystals in these directions. As a rule materials characterized by cubic symmetry of properties have auxeticity (deformation of the same sign in the direction perpendicular to the direction of loading), noticeable anisotropy of Young’s modulus and yield strengths. It is known that 70% of single crystals with cubic symmetry of properties are auxetics; therefore the study of elastic and plastic properties and features of the processes of elastoplastic deformation in such single crystals is relevant [1–5].

This paper presents an analysis of the features of deformation of a single crystal alloy VZhM8, which has cubic symmetry of properties, under dynamic loading. Alloy VZhM8 contains Cr (3 vol %), Mo (3.5 vol %), W (4.2 vol %), Re (6.3 vol %), Ta (6 vol %), Al (5.7 vol %), Co (5.5 vol %), Ru (6 vol %). The directions of shock loading are considered to be the directions [001], [011] and [111]. The mathematical model takes into account the anisotropy of the elastic and plastic properties of VZhM8, as well as the dependence of the speeds of propagation of elastic and plastic waves on the direction. The maximum elastoplastic deformations differ by 4 times for different loading directions for a cylinder made of VZhM8 alloy with an initial shock loading rate of 50 m/s. The aim of the work is to study the regularities of the processes of elastoplastic deformation in a single crystal with cubic symmetry of properties using the example of a heat-resistant nickel alloy VZhM8.
The study was conducted by numerical simulation using original programs. The calculations are carried out by the finite element method. The results of this work can be applied in the simulation of fast processes [6, 7].

2. Mathematical model of elastic deformation of anisotropic material

To simulate the processes of deformation in anisotropic materials a system of equations is used, which describes non-stationary adiabatic motions of a compressible anisotropic medium [8]:

continuity equation
\[ \frac{d\rho}{dt} + \rho \text{div} \vec{v} = 0, \]  (1)

continuum motion equations
\[ \rho \frac{d\vec{v}^k}{dt} = \frac{\partial \sigma^{ki}}{\partial x_i} + F^k, \]  (2)

energy equation
\[ \frac{dE}{dt} = \frac{1}{\rho} \sigma^{ij} e_{ij}, \]  (3)

where \( \rho \) is the medium density; \( \vec{v} \) is speed vector; \( F^k \) are the mass vector components; \( \sigma^{ij} \) are the contravariant components of the symmetric stress tensor; \( E \) is the specific internal energy;

\[ e_{ij} = \frac{\nabla_i v_j + \nabla_j v_i}{2}, \]  (4)

where \( e_{ij} \) are the components of the symmetric strain rate tensor, \( v_i \) are the components of the velocity vector; \( i, j = 1, 2, 3 \). Depending on the orientation of the calculated coordinate system relative to the crystallographic axes of the single crystal, plastic deformation can develop under isotropic or anisotropic hydrostatic stress. For the cases of orientation of the calculated coordinate system relative to the crystallographic axes of a single crystal, in which the elastic properties can be described using 2 or 3 technical constants, isotropic hydrostatic stress occurs in the elastic and plastic deformations, otherwise anisotropic. For example, under shock loading of a single crystal along the [011] direction, the elastic deformation of a cubic single crystal is determined by the values of two Young modulus, two shear modulus, and three Poisson coefficients. All values of technical constants are uniquely determined by the values of three elastic constants and the values of Euler angles, which determine the rotation of the computational coordinate system relative to the crystallographic axes. The calculations were carried out using a mathematical model that includes the decomposition of the total stress tensor into the deviator part and the “anisotropic” hydrostatic stress [9]:

\[ \sigma_{ij} = S_{ij} - P_e \lambda_{ij}, \]  (5)

where \( S_{ij} \) are the total stress deviator components, \( \lambda_{ij} \) is the generalized Kronecker symbol, \( P_e \) is the mean pressure. In the field of elastic deformations \( S_{ij} = C_{ijkl} \varepsilon_{kl} \), \( \lambda_{ij} = C_{ijkl} \delta_{kl}/(3K_a) \), \( K_a = C_{ijkl} \delta_{ij} \delta_{kl}/9 \), \( P_e = \varepsilon_V C_{ijkl} \delta_{ij} \delta_{kl}/3 \), where \( K_a \) is the generalized bulk strain modulus, \( \delta_{kl} \) is Kronecker symbol, \( \varepsilon_{kl} \) are the deformation deviator components, \( C_{ijkl} \) are the elastic constants defined in directions that coincide with the directions of the calculated coordinate system, \( \varepsilon_V \) is volumetric deformation of anisotropic medium. In the field of elastic deformations \( \varepsilon_V = \varepsilon_{11} + \varepsilon_{22} + \varepsilon_{33} \). In the field of plastic deformations \( \varepsilon_V = (V_0 - V)/V \). The volumetric deformation of the anisotropic medium does not change when the direction of the deformation changes, but due to different compressibility factors of the material in different directions, it causes anisotropic hydrostatic stress in cases when \( \lambda_{ij} \) is not equal to one. The use of numerical calculations in the field of elastic deformations of the decomposition of the total stress tensor in the form of (5) is equivalent to calculations in full stresses. The total stresses in the field of
plastic deformations were also calculated by formula (5). In the present work, this approach is extended to the region of plastic deformations and it was assumed that the pressure anisotropy coincided in the region of elastic and plastic deformations. When modeling plastic deformation of anisotropic material, the average pressure $P_e$ in the material was calculated using the Mie–Gruneisen equation as a function of specific internal energy $E$ and current density:

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

where $K_0, K_1, K_2, K_3$ are the material constants, $V, V_0$ are the current and initial volumes. In the field of plastic deformations, $P_e$ was also multiplied by the values of the coefficients $\lambda_{ij}$. The components of the total stress deviator were calculated using the flow theory. The associated law of flow is used to calculate the plastic deformation in the form

$$d\varepsilon^p_{ij} = d\lambda \frac{\partial F}{\partial \sigma_{ij}},$$

the parameter $d\lambda = 0$ at elastic deformation, at plastic is always positive, is defined by means of a condition of plasticity, $d\varepsilon^p_{ij}$ are the components of plastic deformation, $F$ is the plasticity function. The Mises-Hill plasticity condition, written through stress deviators for transtropic material with regard to isotropic hardening, has the form [10]

$$F(S_{ij}, R) = \frac{S_{22}^2}{r_1^2} + \frac{S_{22}^2}{r_2^2} + \frac{S_{33}^2}{r_3^2} + \frac{S_{12}^2}{r_4^2} + \frac{S_{23}^2}{r_5^2} + \frac{S_{31}^2}{r_6^2} - R^2 = 0,$$

where $r_i$ is determined through yield limits for tensile and shear transtropic material, $R$ is the isotropic hardening function. From the experimental studies presented in [10] it is known that the function $R$ characterizing isotropic hardening is invariant to the type of stress state, is determined from experiments on simple loading and depends linearly on the accumulated plastic deformation $\varepsilon^p$: $R(\varepsilon^p) = 1 + \xi \varepsilon^p$, where $\varepsilon^p = \int |d\varepsilon^p_{kl}|$, $k, l = 1, 2, 3.$

3. Statement of the problem

The impact of a cylinder of a single crystal alloy VZhM8 on a rigid wall with an initial velocity of 50 m/s is considered. The axis of symmetry of the cylinder in each problem coincides with one of the three axes in which the elastic, plastic, and strength properties in cubic crystals are traditionally investigated: [111], [001], and [011]. In the first case, the direction of the axis of symmetry of the cylinder coincide with the directions [111] and the other two axes coincides with the [211] and [011] direction. In the second case, the direction of the axis of symmetry of the cylinder and the other two coincides with the direction of the crystallographic axes [001], [010] and [100]. In the third case, the axis of symmetry of the cylinder coincides with the [011] direction, and the other axes coincides with the [100] direction. Those in the first and second cases, axisymmetric problems are solved, and in the third case, a three-dimensional stress state is realized in the cylinder. The differences in each case of the axes of symmetry of a single crystal alloy relative to the axis of symmetry of the cylinder leads to the fact that in all three problems the values of technical elastic constants and velocities of propagation of elastic waves in the direction of each coordinate axis have different values.

In the first case, the technical elastic constants are $E = 250.6$ GPa, $v = 0.28$, $G = 46.7$ GPa, $\sigma_T = 1219$ MPa, $\tau_T = 620$ MPa, longitudinal wave speeds $v_L = 6548$ m/s, shear wave speeds $v_S = 2646$ m/s, all $\lambda_{ij} = 1$. In the second case, the technical elastic constants are $E = 102.2$ GPa, $v = 0.426$, $G = 118.7$ GPa, $\sigma_T = 1160$ MPa, $\tau_T = 580$ MPa, longitudinal wave speeds $v_L = 5539$ m/s, shear wave speeds $v_S = 3619$ m/s, all $\lambda_{ij} = 1$. In the third case, the values of technical elastic constants differ in three mutually perpendicular directions: $E_x = 102.2$ GPa,
Figure 1. Increasing the cylinder radius along the OY axis: curve 1—the axis of symmetry of the cylinder is directed along the [111] axis; curve 2—along the [001] axis; curve 3—along the [011] axis.

\[ E_y = E_z = 193.2 \text{ GPa}, \ G_{xy} = G_{zx} = 118.7 \text{ GPa}, \ G_{yz} = 38.8 \text{ GPa}, \ \nu_{xy} = 0.788, \ \nu_{yz} = -0.140, \ \nu_{zx} = 1.489, \ \sigma_{TX} = 1050.8 \text{ MPa}, \ \sigma_{TY} = \sigma_{TZ} = 934 \text{ MPa}, \ \tau_T = 480 \text{ MPa}, \ \text{longitudinal wave speeds } v_L = 6311 \text{ m/s, shear wave speeds } v_{S1} = 3619 \text{ m/s and } v_{S2} = 1989 \text{ m/s, } \lambda_{11} = 0.932, \ \lambda_{22} = \lambda_{33} = 1.136 \] [11]. In this case, the cylinder material is characterized by auxeticity, the other two Poisson ratios exceed the value of 0.5. The density of the material is 9060 kg/m³.

4. Discussion

Figure 1 shows the increase in the cylinder radius along the OY axis at a height of 1 mm from the contact surface of the cylinder and the target. Curve 1 corresponds to the case when the axis of symmetry of the cylinder coincides with the direction [111], curve 2—[001], and curve 3—[011].

The change in the radius of the cylinder, shown by curve 3 along the axis OY until the moment of separation of the cylinder from the target (26.51 µs) is significantly less than on curve 1 and curve 2. This is explained by the presence of a negative Poisson coefficient in the ZOY plane, and as a result, during shock loading along the OZ axis until the cylinder is separated from the target, the elastic deformation in the direction of the OY axis is also compressive. The total elastoplastic deformation along the OY direction is approximately 3.5 times less under shock loading along the [011] direction than in the cases of [111] and [001]. Changes in the radius of the cylinder in the perpendicular direction—along the axis OX at a distance of 1 mm from the contact surface, demonstrate a different picture. If the axis of symmetry of the cylinder coincides with the [011] direction, the increase in the cylinder radius is more than 2 times greater than the increase in the cylinder radius for cases where the direction of the axis of symmetry of the cylinder coincides with the [111] or [001] axis.

From the analysis of the geometry of the curves in figure 1 and 2 it can be seen that already at a height of 1 mm from the contact surface of the cylinder and higher, the section of the cylinder acquires the geometry of an ellipse if the shock loading is modeled along the [011] axis. The cross sections of the cylinders remain round if the axes of symmetry of the cylinders coincide with the directions [111] or [001].
Figure 2. Increasing the cylinder radius along the $OX$ axis: curve 1—the axis of symmetry of the cylinder is directed along the [111] axis; curve 2—along the [001] axis; curve 3—along the [011] axis.

Figure 3. The change in the height of the cylinder: curve 1—the axis of symmetry of the cylinder is directed along the [111] axis; curve 2—along the [001] axis; curve 3—along the [011] axis.

The change in the length of the cylinder in time due to the arrival of an elastic wave from the contact surface of the cylinder and a rigid target to its free end is shown in figure 3. The velocity of propagation of a longitudinal wave along the axis of symmetry in a cylinder is maximum if it coincides with the [111] direction. Elastic and plastic properties along the [111] direction are also maximal from all the considered directions, therefore the minimum decrease in the cylinder height (by 1%) in this case is predictable (curve 1 in figure 3). If the direction of the crystallographic axis coincides with the axis of symmetry of the cylinder, the minimum elastic
properties along the [001] direction result in the maximum shortening of the cylinder (1.5%) along the axis of symmetry (curve 2 in figure 3). A shock loading of a cylinder, the axis of symmetry of which coincides with the direction [011], is accompanied by a shortening of the cylinder by 1.3%. The resulting cylinder lengths are determined by the plastic properties along the shock loading directions after the cylinders are separated from the target and they are maximum in the VZhM8 single crystal alloy along the [111] direction (curve 1 in figure 3).

The biggest differences for the three types of cylinders are shown by the final speed of the cylinder rebound from a rigid target. The change in the velocities of the centers of mass of the cylinders in time is shown in figure 4 for the three considered cases. The maximum constant speed is observed at the cylinder with the [001] direction—28.6 m/s, the minimum constant speed at the cylinder with the [111] direction—8.3 m/s. Differences in the final velocities of the cylinders after their impact on a rigid target show the influence of the orientation of the loading direction with respect to the axes of symmetry of the material on all parameters of their stress-strain states.

5. Conclusion
In the case of shock loading of the cylinder from a single crystal alloy VZhM8 along the [011] direction, the processes of elastoplastic deformation demonstrate a significant difference, which is determined by the auxeticity of the alloy. Under shock loading along the [011] direction with low velocities, the elastoplastic deformation is largely determined by the elastic properties.

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