Influence of auxeticity on the processes of elastic deformation in a single crystal VZhM8 in the direction [011]

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Abstract. The study of deformation processes in a cylinder made of monocrystalline heat-resistant nickel alloy VZHM8. Different variants of the orientation of the crystallographic axes of a single crystal of a VZhm8 nickel alloy relative to the axis of symmetry of the cylinder when it is shocks an rigid wall (Taylor test) are considered. It is shown that if the [011] direction coincides with the direction of shock loading of the cylinder, the initially circular sections of the cylinder turn into ellipses until the moment of rebound, which is explained by the influence of the negative Poisson’s coefficient.

1. Introduction
In connection with the intensive development of the aerospace industry, there is a need to use new materials in the nodes of structures operating in extreme conditions. Recently, much attention has been paid to the study of single crystal materials. Single crystals of metals and their alloys have enhanced strength properties and are used in aircraft and engine building [1–5]. Because of their structure, single crystals are characterized by a significant anisotropy of elastic properties, which affects the deformation processes in a single crystal product. Another feature of single crystals is that most of them have anomalous elastic characteristics, in particular, a negative Poisson’s ratio (auxetics). The presence of negative Poisson’s coefficients in some directions is typical of 70% of cubic symmetry single crystals and, in particular, of single crystals of heat-resistant nickel alloys.

The aim of the work is to study the laws of deformation processes in single-crystal heat-proof nickel alloy VZHM8. Alloy VZhM8 is the heat resistant Nickel aluminum alloy, rhenium and ruthenium doped. The research was conducted by numerical simulation using original programs. This set of programs allows taking into account in the mathematical model various types of symmetry of materials and extreme elastic characteristics of materials, including auxiticity.

2. Mathematical model of elastic deformation of anisotropic material
Dynamic loading of an anisotropic solid is modeled in the framework of continuum mechanics using the continuity equation and the equations of motion [6] in a three-dimensional formulation. The components of the symmetric strain rate tensor \( e_{ij} \) were calculated as follows \( e_{ij} = (\nabla_i v_j + \nabla_j v_i)/2 \), \( v_j \) are the velocity vector components; \( i, j = x, y, z \).
To determine the elastic deformation of an anisotropic material, the ratio of the total elastic deformations and stresses can be written in the form of a generalized Hooke’s law with a symmetric matrix of elastic compliances [7]:

\[
\begin{bmatrix}
\varepsilon_{xx} \\
\varepsilon_{yy} \\
\varepsilon_{zz} \\
\varepsilon_{xy} \\
\varepsilon_{xz} \\
\varepsilon_{yz}
\end{bmatrix} = \begin{bmatrix}
1/E_x & -\nu_{xy}/E_y & -\nu_{xz}/E_z & 0 & 0 & 0 \\
-\nu_{xy}/E_x & 1/E_y & -\nu_{yz}/E_z & 0 & 0 & 0 \\
-\nu_{xz}/E_x & -\nu_{yz}/E_y & 1/E_z & 0 & 0 & 0 \\
0 & 0 & 0 & 1/(2G_{xy}) & 0 & 0 \\
0 & 0 & 0 & 0 & 1/(2G_{xz}) & 0 \\
0 & 0 & 0 & 0 & 0 & 1/(2G_{yz})
\end{bmatrix}
\begin{bmatrix}
\sigma_{xx} \\
\sigma_{yy} \\
\sigma_{zz} \\
\sigma_{xy} \\
\sigma_{xz} \\
\sigma_{yz}
\end{bmatrix},
\]

(1)

where in \(v_{ij}/E_i = v_{ji}/E_j, i \neq j; i, j = x, y, z\).

The paper considers two variants for the location of the axes of coordinates relative to the crystallographic axes of the single crystal: in the first case, the loading direction coincides with the [001] axis of the single crystal, the other two axes of coordinates—with the [010] and [100] directions; in the second case the loading is applied along the [011] direction and other axis—with the [100] axis. The Cartesian coordinate system was used in the calculations. The direction of loading coincided with the axis \(OZ\).

Based on certain values of technical constants experimentally determined for the VZhM8 [5] alloy when loading direction along the single crystal [001], 7 values of the technical constants required for the calculations were calculated: 2 Young moduli values in 2 directions, 2 shear moduli and 3 Poisson’s ratios. Their magnitudes are \(E_x = 102.2\) GPa, \(E_y = E_z = 193.3\) GPa, \(G_{xy} = G_{xx} = 118.7\) GPa, \(G_{yz} = 35.8\) GPa, \(\nu_{xy} = 0.79\), \(\nu_{yz} = -0.14\), \(\nu_{xx} = 1.49\).

The values of the elastic constants correspond to the temperature of the gas turbine engine blades 800°C [6]. The differences in the values of the Young’s modulus obtained in natural experiments [5] in the \(OXY\) and \(OXZ\) planes demonstrate that in sections of the pointing surfaces the value of the Young’s modulus varies approximately by 2 times. The same is demonstrated by changes in the shear moduli and Poisson’s coefficients in the corresponding sections of the index surfaces.

The total stress tensor is generally decomposed into a stress deviator part and anisotropic pressure [8]:

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

(2)

where \(S_{ij}\) are the stress deviator tensor components; \(\lambda_{ij}\) is the generalized Kronecker symbol; \(P_e\) is the spherical part of the stress tensor. 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 bulk modulus; \(\delta_{kl}\) is the Kronecker symbol; \(\varepsilon_{kl}\) are the components of deviators of deformations; \(C_{ijkl}\) are the elastic constants, \(\varepsilon V\) is the volume strain for anisotropic medium. Coefficients \(\lambda_{ij}\) are equal to unity if the value of elastic compliance along each coordinate axis is constant: \(\lambda_{xx} = 1.136\), \(\lambda_{yy} = \lambda_{zz} = 0.932\).

The pressure anisotropy due to different compressibility in the [001] direction and the [011] directions is \(\lambda_{xx}/\lambda_{yy} = \lambda_{xx}/\lambda_{zz} = 1.22\). Accurate consideration of the anisotropy of the compressibility of the material is especially important at the calculation of the elastoplastic deformation and “viscous” destruction of anisotropic materials. The stresses defined in the element, rigidly rotated in space, are recalculated using the Jaumann derivative [9].

3. Statement of the problem of shock a cylinder from a single crystal VZhM8 alloy to a rigid wall

A numerical simulation of the impact of a cylinder of a single crystal alloy VZhM8 on a rigid wall with an initial velocity of 50 m/s was carried out. The direction of loading coincided with the axis of symmetry of the cylinder. Plastic deformation was not considered because of the need
Figure 1. The change in the radius of the cylinder along the axis $OX$: curve 1 corresponds to the case of loading along the [001] single crystal direction, the other two axes of coordinates are [010] and [100]; curve 2 corresponds to the loading along the [011] direction and other axis coincides with the [100] direction.

to single out the regularities of the processes of elastic deformation in cubic crystals depending on the direction of loading. In the first case, the loading direction along the [001] single crystal direction is considered. In the second case, the loading is applied along the [011] direction. The cylinder radius is 5 mm. On the contact surface of the cylinder and the rigid wall, slip-free conditions are realized. All calculations were performed using the original programs, the finite element method [9].

4. Numerical simulation results
Changes in the radius of the cylinders at a distance of 1 mm from the contact surface of the cylinder and the rigid wall along the axis $OX$ are shown in figure 1, and along the axis $OY$—in figure 2. As can be seen in figures 1 and 2, when the cylinder was loaded along the [001] direction, along the axes $OX$ and $OY$, the radius increases to a point in time of 36.6 $\mu$s, which corresponds to the moment of the cylinder rebound from the rigid wall (curves 1). When cylinder loading was carried out along the [001] direction, the deformation of the cylinder along the axes $OX$ and $OY$ are the same, that is, the problem is axisymmetric.

In the second case (curves 2 in figures 1 and 2), when the loading direction coincides with the [011] direction of the single crystal, a noticeable increase in the cylinder radius relative to the original along the axis $OX$ and a decrease in the cylinder radius relative to the initial along the axis $OY$ occurs (curve 2 in figure 1) until the moment of time 23.8 $\mu$s (the moment of the cylinder rebound from the rigid wall). The narrowing of the cylinder radius in the direction perpendicular to the loading direction, up to the moment of rebound, is due to the influence of the negative Poisson's coefficient in this plane. Despite the identical elastic properties of the material of both cylinders, the change in loading directions relative to the crystallographic axes of the cubic crystal leads to a significant change in the time of the cylinder rebound from the target.
Figure 2. The change in the radius of the cylinder along the axis $OY$: curve 1 corresponds to the case of loading along the [001] single crystal direction, the other two axes of coordinates are [010] and [100]; curve 2 corresponds to the loading along the [011] direction and other axis coincides with the [100] direction.

5. Conclusion
Thus, the results of numerical simulation of the impact of a cylinder from a single crystal VZhM8 alloy clearly demonstrate the influence of the crystallographic axes orientation of a single crystal relative to the calculated coordinate system of the cylinder on its deformation.

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