CUTS WITH NEGATIVE POISSON'S RATIO IN SOME CUBIC AND HEXAGONAL CRYSTALS

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ABSTRACT
In the paper a set of cubic, hexagonal and monoclinic crystals were investigated. Stereographic projections of Poisson's ratio were computed for each crystal. From these stereographic projections the Poisson's ratio for any directions of stretch and lateral strain in crystal were calculated and orientations of stretch and lateral strain with extremes values of Poisson's ratio were obtained. By analysis of the above results cuts with negative values of Poisson's ratio were revealed in zinc, molybdenum sulfide, polypropylene, graphite, carbon, natural minerals labradorite and augite, complex silicate and in a set of alloys. The angular dependences of stretched orientations corresponding to negative Poisson's ratio were determined. Elastic modules of crystals from the manual of Landolt-Bornstein were applied in calculations.

INTRODUCTION
Poisson's ratio is the ratio of lateral strain to the longitudinal strain during the stretching of a cylindrical rod along the rod axis. In almost all isotropic materials the Poisson's ratio is positive. Most ordinary materials have Poisson's ratio near 0.3. For many years negative Poisson's ratio materials were unknown and even thought to be impossible. Since then negative Poisson's ratio was discovered in several classes of materials: foams, polymers, chiral structures, laminated structures, crystals [3-9].

Anisotropic materials have properties that depend on direction. The Poisson's ratio of an anisotropic solid depends on directions of stretch and lateral strain. Stretching of anisotropic material can cause expansion in one direction and contraction in another direction. For example in crystals it is possible for Poisson's ratio to be negative in one direction and highly positive in another direction. Many crystals deformed in an oblique direction with respect to the cubic face diagonal [110] exhibit a negative Poisson's ratio for the resulting lateral deformation in the direction $[1\bar{1}0]$. The existence of negative Poisson's ratio for a stretch along a cube-face diagonal for some cubic metals were predicted by F. Milstein and K. Huang [7]. The auxetic behavior for some cubic metals and alloys with negative Poisson's ratio were investigated by R.H. Baughman, J. M. Shacklette, A. A. Zakhidov, S. Stafstrom [8]. The existence of negative Poisson's ratio in hexagonal monocrystalline of zinc in its basal plane were predicted by V.A. Lubarda and M.A. Meyers [9]. It was found by Y. Li [10] that in monocrystal of cadmium negative values of Poisson's ratio appear for some directions.

We calculated the stereographic projections of Poisson's ratio for a set of cubic, hexagonal and monoclinic crystals. This allows us to determine the Poisson's ratio for an arbitrary directions of stretch and lateral strain vectors in crystals. Then from these stereographic projections crystals with negative values of Poisson's ratio were revealed and the angular dependences of stretch directions with negative Poisson's ratio were obtained for the above crystals. The elastic modules of crystals from manuals of Landolt - Bornstein [1-2] were used in calculations.

A negative values of Poisson's ratio is not forbidden: the requirement that the strain energy for an elastic isotropic solid be non-negative leads to the restriction: $-1<\nu<0.5$ in three dimension and $-1<\nu<+1$ in two dimension. For anisotropic solids the allowed range is wider [13].

THEORY

Let us consider an anisotropic elastic body with the elastic compliances s_{ijkl}, related to an orthogonal coordinate system. The correspondence between compliances expressed in 2D suffix notation and 4D suffix notation is $s_{IJ} = 2^p s_{ijkl}$, where p is equal to the number of suffix greater than 3 in I and J, so $s_{1111} = s_{11}$, $s_{1123} = 2s_{14}$, $s_{2323} = 4s_{44}$.

If the body is stretched uniaxially by the stress σ_q in the direction defined by the unit vector q, characterized by an Euler's angles α and β, the stress components are: $\sigma_{ij} = \sigma_q q_i q_j$. If a stress tensor σ_{ij} and a strain tensor ε_{kl} are related by $\sigma_{ij} = c_{ijkl}\varepsilon_{kl}$, the corresponding strains are: $\varepsilon_{ij} = \sigma_q s_{ijkl} q_k q_l$. The longitudinal strain in the direction q is: $\varepsilon_q = q_i \varepsilon_{ij} q_j = \sigma_q q_i q_j s_{ijkl} q_k q_l$. Let the lateral strain in the direction m be characterized by an angle θ in the plane normal to q (or normal to the rod axis). Then the lateral strain in the direction m due to the stress σ_q in the ortogonal direction q is: $\varepsilon_m = m_i \varepsilon_{ij} m_j = \sigma_q m_i m_j s_{ijkl} q_k q_l$. So, the Poisson's ratio in the direction m due to the stress in the direction q is:

$$\nu_{mq} = -\frac{\varepsilon_m}{\varepsilon_q} = -\frac{m_i m_j s_{ijkl} q_k q_l}{q_\alpha q_\beta s_{\alpha\beta\gamma\delta} q_\gamma q_\delta} . \quad (1)$$

Thus the Poisson's ratio of anisotropic solid is a function of two Eulerian angles α and β, which identify the direction of the rod axis q, and an angle θ, which identifies the lateral strain direction in the cross-section plane of the rod.

METHOD OF CALCULATION

First we calculated the stereographic projections of Poisson's ratio by (1). Let us consider a set of rods with any directions of its axis. Then let us consider a set of angles θ_i for θ an angle of the lateral deformation in the cross-section plane of the rod. The stereographic projections of Poisson's ratio for these fixed angles θ_i were calculated from (1). From these stereographic projections orientations of stretched vectors q with negative values of ν were obtained for a set of cubic crystals.

Figure 2. The stereographic projection of Poisson's ratio in FeAl (25%Al) alloy for two angles $\theta_1 = 0°$ (left) and $\theta_2 = 45°$ (right) (x-axis is along $[100]$, y-axis is along $[010]$, z-axis is normal to this paper).

As an example the stereographic projections of Poisson's ratio in FeAl (25% Al) alloy for two angles $\theta_1 = 0°$, $\theta_2 = 45°$ and for any possible directions of rod axes are presented in Fig.2. On the stereographic projections the locations of stress directions with negative Poisson's ratio are clearly shows. The minimum and maximum Poisson's ratio for cubic crystals are usually for a stretch along a $[110]$ direction, which is a cube-face diagonal, and resulting lateral