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ON THE NEGATIVE POISSON RATIO IN MONOCRYSTALLINE ZINC

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1. Introduction

Consider an anisotropic body with the elastic compliance coefficients S_{ijkl}, relative to an orthogonal coordinate system. If the body is loaded uniaxially by stress σ_n in the direction defined by unit vector **n**, the stress components are $\sigma_{ij} = \sigma_n\, n_i n_j$, with the corresponding strains $\epsilon_{ij} = \sigma_n\, S_{ijkl}\, n_k n_l$. The longitudinal strain in the direction **n** is thus $\epsilon_n = n_i\, \epsilon_{ij}\, n_j = \sigma_n\, n_i n_j\, S_{ijkl}\, n_k n_l$. The lateral strain in the direction **m** due to stress σ_n in the orthogonal direction **n** is likewise $\epsilon_m = m_i\, \epsilon_{ij}\, m_j = \sigma_n\, m_i m_j\, S_{ijkl}\, n_k n_l$. The Poisson ratio in the direction **m** due to stress in the direction **n** is consequently

$$\nu_{mn} = -\frac{\epsilon_m}{\epsilon_n} = -\frac{m_i m_j S_{ijkl} n_k n_l}{n_\alpha n_\beta S_{\alpha\beta\gamma\delta} n_\gamma n_\delta}. \tag{1}$$

This is also equal to the transformed compliance ratio $-S'_{2211}/S'_{1111}$, provided that the coordinate axis $2'$ is in the direction **m**, and $1'$ in the direction **n** (Voigt [1], Nye [2]). The Young's modulus in the direction **n**, and the shear modulus between the orthogonal directions **m** and **n**, can be similarly written as:

$$\frac{1}{E_n} = n_i n_j S_{ijkl} n_k n_l, \frac{1}{G_{mn}} = 4 m_i n_j S_{ijkl} m_k n_l. \tag{2}$$

2. Negative Poisson Ratio in Single Crystals of Zinc

For a transversely isotropic material, whose axis of transverse isotropy is in the coordinate direction {0, 0, 1}, the Young's modulus is equal for any direction **n** on the cone around the axis of transverse isotropy. Thus, by taking $\mathbf{n} = \{0, \cos\theta, \sin\theta\}$ and $\mathbf{m} = \{0, -\sin\theta, \cos\theta\}$, where θ is the angle from the plane of isotropy, Eq. (1) gives

$$\nu_{mn} = -\frac{s_{13} + (s_{11} + s_{33} - s_{44} - 2s_{13})\sin^2\theta\cos^2\theta}{s_{11}\cos^4\theta + s_{33}\sin^4\theta + (s_{44} + 2s_{13})\sin^2\theta\cos^2\theta}. \tag{3}$$

The Voigt notation is used for the compliance coefficients, such that $S_{1111} = s_{11}$, $4S_{2323} = s_{44}$, etc.

If **m** is taken to be the direction {1, 0, 0}, the Poisson ratio ν_{1n} becomes

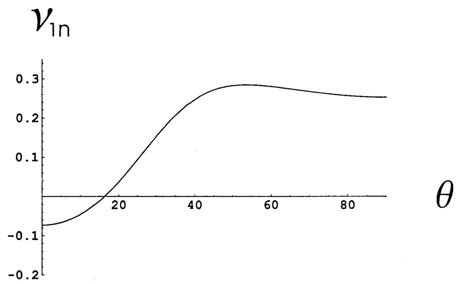

Figure 1. Variation of the Poisson ratio ν_{1n} in the direction 1 due to stress in the direction **n**, at an angle θ from the basal plane of a zinc crystal. The axis 1 is normal to the plane containing the axis of transverse isotropy and the direction **n**.

$$\nu_{1n} = -\frac{s_{12}\cos^2\theta + s_{13}\sin^2\theta}{s_{11}\cos^4\theta + s_{33}\sin^4\theta + (s_{44} + 2s_{13})\sin^2\theta\cos^2\theta}. \tag{4}$$

For common single hexagonal crystals, whose elastic constants are reported in the literature, the values of the compliance coefficients are such that the Poisson ratios ν_{mn} and ν_{1n} are positive for all θ. However, for single crystals of zinc: $s_{11} = 8.22$, $s_{33} = 27.7$, $s_{44} = 25.3$, $s_{12} = 0.60$, and $s_{13} = -7.0$, in units of $(TPa)^{-1}$ (Landolt-Börnstein [3]), so that the coefficients s_{11} and s_{12} are of the same sign. Consequently, for $\theta = 0$ we obtain from Eq. (4) that $\nu_{12} = -s_{12}/s_{11} \approx -0.073 < 0$. Thus, the Poisson ration of monocrystalline zinc in its basal plane is negative. Furthermore, the Poisson ratio ν_{1n} becomes equal to zero if $\theta = \theta_0$, defined by $\tan^2\theta_0 = -s_{12}/s_{13}$, which gives $\theta_0 \approx 16.3^0$, i.e., ν_{1n} is negative if the angle from the plane of isotropy is in the range $0 < \theta < \theta_0$. This is shown in Fig. 1.

The negative values of the Poisson ratio for transversely isotropic material are not precluded by stability requirements. The positive definiteness of the compliance matrix imposes the bounds on the Poisson ratio in the plane of isotropy, such that $-1 < \nu_{12} < 1$. The Poisson ratio ν_{mn} in the plane containing the axis of transverse isotropy is, on the other hand, always positive (Fig. 2). The two end values $\nu_{13} = -s_{13}/s_{33} \approx 0.253$ and $\nu_{31} = -s_{13}/s_{11} \approx 0.852$ clearly satisfy stability conditions $\nu_{13}\nu_{31} < 1$ and $1 - 2\nu_{13}\nu_{31} > \nu_{12}$, required in general for any transversely isotropic material.

In an early study of elastic constants in single crystals of zinc (Goens [4], Hanson [5]), negative values of the Poisson ratio in the basal or other crystallographic planes were not indicated. They were not mentioned in the later references either (e.g., Hearmon [6], Huntington [7]). The existence of the negative Poisson ratio for certain orientations in fcc crystals, however, is well-known and has been theoretically studied by using lattice elasticity models (i.e., Milstein [8]). A similar study may be worthwhile for hexagonal crystals of zinc.

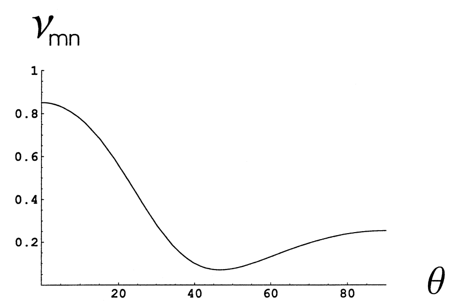

Figure 2. Variation of the Poisson ratio ν_{mn} in the direction **m** due to stress in the orthogonal direction **n**. Both directions are in the plane containing the axis of transverse isotropy of a zinc crystal.

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