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**POISSON'S RATIO FOR TETRAGONAL CRYSTALS**

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General expressions for Poisson's ratio are derived for tetragonal crystals; simplified forms are given for cases involving symmetry directions.

**Isotropic media; tetragonal symmetry**
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POISSON'S RATIO FOR TETRAGONAL CRYSTALS

Abstract

General expressions for Poisson's ratio are derived for tetragonal crystals; simplified forms are given for cases involving symmetry directions.

Introduction

Poisson's ratio, ν, is defined for isotropic media as the quotient of lateral contraction to longitudinal extension arising from application of a simple tensile stress; in most materials, this dimensionless number is positive. In crystals, ν takes on different values, depending on the directions of stress and strain chosen. The ratio finds application in a variety of areas of applied elasticity and solid mechanics, for example, as indication of the mechanical coupling between various vibrational modes of motion.

The maximum value of $\nu = +1/2$ is obtained in the incompressible medium limit, where volume is preserved; for ordinary materials, values of +1/4 to +1/3 are typical, but in crystals $\nu$ may vanish, or take on negative values. Analytical formulas for Poisson's ratio are expressed in terms of elastic constants. For the case of crystals of general anisotropy, these expressions are quite unwieldy, but for tetragonal crystals the symmetry elements reduce the complexity considerably.

Crystals of tetragonal symmetry include a number of ferroelectrics as well as lithium tetraborate, a nonferroelectric with substantial piezoelectric coupling and temperature-compensated properties. These materials are potentially important for high technology applications such as cellular radio and microwave collision avoidance radar. Each of the seven tetragonal point groups is characterized by one of two elastic matrix schemes, so it is necessary to distinguish among the point groups. The distinction relates to symmetry; those groups that appear as holohedral under classical x-ray analysis (classes 4-bar 2m, 422, 4mm, and 4/m mm) have an elastic matrix in which $c_{16}$ and $s_{16}$ constants do not appear; the remainder (classes 4-bar, 4, and 4/m) retain the $c_{16}$ and $s_{16}$ entries. The presence of piezoelectricity is neglected.
Expressions Relating Tetragonal Stiffnesses and Compliances

Relations for Poisson’s ratio are most simply expressed in terms of the elastic compliances \([s_{\nu\mu}]\). It is often the case, however, that the most accurate determinations of the elastic constants (resonator and transit-time methods) yield values for the stiffnesses \([c_{\nu\mu}]\) directly; the conversion relations are given below. For the tetragonal system, the elastic stiffness and compliance matrices have identical form. Referred to the \(x_k\) axes as defined in the IEEE Standard, the matrices are, including the \(c_{16}\) and \(s_{16}\) entries:

\[
\begin{array}{ccccccc}
C_{11} & C_{12} & C_{13} & 0 & 0 & C_{16} & S_{11} & S_{12} & S_{13} & 0 & 0 & S_{16} \\
C_{12} & C_{11} & C_{13} & 0 & 0 & -C_{16} & S_{12} & S_{11} & S_{13} & 0 & 0 & -S_{16} \\
C_{13} & C_{13} & C_{33} & 0 & 0 & 0 & S_{13} & S_{13} & S_{33} & 0 & 0 & 0 \\
0 & 0 & 0 & C_{44} & 0 & 0 & 0 & 0 & 0 & S_{44} & 0 & 0 \\
0 & 0 & 0 & 0 & C_{44} & 0 & 0 & 0 & 0 & 0 & S_{44} & 0 \\
C_{16} & -C_{16} & 0 & 0 & 0 & C_{66} & S_{16} & -S_{16} & 0 & 0 & 0 & S_{66} \\
\end{array}
\]

Stiffness and compliance are matrix reciprocals; the seven independent components of each are related by:

\[
s_{11} = \frac{[(c_{33} / C_1) + (c_{66} / C_2)]}{2}; s_{12} = \frac{[(c_{33} / C_1) - (c_{66} / C_2)]}{2}
\]

\[(s_{11} + s_{12}) = [c_{33} / C_1]; (s_{11} - s_{12}) = [c_{66} / C_2]\]

\[s_{13} = -[c_{13} / C_1]; s_{16} = -[c_{16} / C_1]\]

\[s_{33} = [(c_{11} + c_{12}) / C_1]; s_{66} = [(c_{11} - c_{12}) / C_2]; s_{44} = 1 / C_{44}\]

\[C_1 = [c_{33}(c_{11} + c_{12}) - 2c_{13}^2]; C_2 = [c_{66}(c_{11} - c_{12}) - 2c_{16}^2]\]

These are inverted simply by an interchange of symbols \(c_{\nu\mu}\) and \(s_{\nu\mu}\). When \(c_{16}\) is set equal to zero in the above equations, the six relations for classes 4-bar, 4, and 4/m are recovered as:

\[
s_{11} = \frac{[c_{11}c_{33} - c_{13}^2]}{[(c_{11} - c_{12}) C_1]}
\]

\[
s_{12} = -\frac{[c_{12}c_{33} - c_{13}^2]}{[(c_{11} - c_{12}) C_1]}
\]

\[
s_{13} = -\frac{[c_{13} / C_1]; s_{33} = [(c_{11} + c_{12}) / C_1]}{s_{44} = 1 / C_{44} ; s_{66} = 1 / C_{66}}
\]
Definition of Poisson's Ratio for Crystals

Poisson's ratio for crystals is defined in general as \( v_{ij} = \frac{s_{ij}'}{s_{ii}'} \), where \( x_i \) is the direction of the longitudinal extension, \( x_i \) is the direction of the accompanying lateral contraction, and the \( s_{ij}' \) and \( s_{ii}' \) are the appropriate elastic compliances referred to this right-handed axial set. It suffices to take \( x_1 \) as the direction of the longitudinal extension; then two Poisson's ratios are defined by the orientations of the lateral axes \( x_2 \) and \( x_3 \): \( v_{21} = \frac{s_{12}'}{s_{11}'} \) and \( v_{31} = \frac{s_{13}'}{s_{11}'} \). Application of the definition requires specification of the orientation of the lateral coordinate set with respect to the crystallographic directions, and transformation of the compliances accordingly.

Relations for Rotated Tetragonal Compliances - General

The unprimed compliances are referred to a set of right-handed orthogonal axes related to the crystallographic axes in the manner defined by the IEEE standard. Direction cosines \( a_{mn} \) relate the transformation from these axes to the set specifying the directions of the longitudinal extension (\( x_1 \)), and the lateral contractions (\( x_2 \) and \( x_3 \)). General expressions for the transformed compliances that enter the formulas for \( v_{21} \) and \( v_{31} \), including the \( s_{12} \) terms, are:

\[
\begin{align*}
    s_{11}' &= s_{11} [a_{11}^4 + a_{12}^4] + s_{33} [a_{13}^4] + (s_{44} + 2 s_{13})[a_{13}^2][a_{13}^2 + a_{12}^2] + \\
             &\quad (s_{66} + 2 s_{12})[a_{12}^2] + 2 s_{16} [a_{11}a_{12}][a_{11}^2 - a_{12}^2] \\
    s_{12}' &= s_{11} [a_{11}^2a_{21}^2 + a_{12}^2a_{22}^2] + s_{33} [a_{13}^2a_{23}^2] + s_{44} [a_{13}a_{23}][a_{12}a_{22} + a_{11}a_{21}] + \\
             &\quad s_{66} [a_{11}a_{12}a_{21}a_{22}] + s_{12} [a_{11}^2a_{22}^2 + a_{12}^2a_{21}^2] + \\
             &\quad s_{13} [a_{23}^2(a_{11}^2 + a_{12}^2) + a_{13}^2(a_{21}^2 + a_{22}^2)] + \\
             &\quad s_{16} [a_{21}a_{22}(a_{11}^2 - a_{12}^2) + a_{11}a_{12}(a_{21}^2 - a_{22}^2)] \\
    s_{13}' &= s_{11} [a_{11}^2a_{31}^2 + a_{12}^2a_{32}^2] + s_{33} [a_{13}^2a_{33}^2] + s_{44} [a_{13}a_{33}][a_{12}a_{32} + a_{11}a_{31}] + \\
             &\quad s_{66} [a_{11}a_{12}a_{31}a_{32}] + s_{12} [a_{11}^2a_{32}^2 + a_{12}^2a_{31}^2] + \\
             &\quad s_{13} [a_{33}^2(a_{11}^2 + a_{12}^2) + a_{13}^2(a_{31}^2 + a_{32}^2)] + \\
             &\quad s_{16} [a_{31}a_{32}(a_{11}^2 - a_{12}^2) + a_{11}a_{12}(a_{31}^2 - a_{32}^2)]
\end{align*}
\]

Single-Axis Rotations

The general rotation relations given above for \( s_{11}' \), \( s_{12}' \), and \( s_{13}' \) simplify considerably for single-axis rotations. Longitudinal extension is along the \( x_1 \) axis; abbreviations \( c(\phi) \) and \( s(\phi) \) stand for \( \cos(\phi) \) and \( \sin(\phi) \), etc.
(A)  Rotation about $x_1$: $s_{11}' = s_{11}$
\[
s_{12}' = s_{12} [c^2(\theta)] + s_{13} [s^2(\theta)] = s_{12} + (s_{13} - s_{12})[s^2(\theta)]
\]
\[
s_{13}' = s_{13} [c^2(\theta)] + s_{12} [s^2(\theta)] = s_{13} + (s_{12} - s_{13})[s^2(\theta)]
\]
\[
v_{21} = \frac{(s_{12} + (s_{13} - s_{12})[s^2(\theta)])}{s_{11}} ; \quad v_{31} = \frac{(s_{13} + (s_{12} - s_{13})[s^2(\theta)])}{s_{11}}
\]

These expressions are independent of $s_{16}$, and have two-fold symmetry. When $\theta = \pi/4$, $v_{21} = v_{31} = (s_{12} + s_{13}) / 2 s_{11}$

(B)  Rotation about $x_2$: 
\[
s_{11}' = s_{11} [c^2(\psi)] + s_{33} [s^2(\psi)] + (s_{44} + 2 s_{13})[c^2(\psi)s^2(\psi)]
\]
\[
s_{12}' = s_{12} [c^2(\psi)] + s_{13} [s^2(\psi)] = s_{12} + (s_{13} - s_{12})[c^2(\psi)]
\]
\[
s_{13}' = s_{13} + s_{2} [c^2(\psi) s^2(\psi)] ; \quad s_{2} = (s_{11} + s_{33} - (s_{44} + 2 s_{13}))
\]
\[
v_{21} = \frac{s_{12}'}{s_{11}'} ; \quad v_{31} = \frac{s_{13}'}{s_{11}'}
\]

These expressions are independent of $s_{16}$, and have two-fold symmetry. When $\psi = \pi/4$, $v_{21} = 2 (s_{12} + s_{13}) / (s_{0} + s_{44})$
\[
v_{31} = (s_{0} - s_{44}) / (s_{0} + s_{44}) ; \quad s_{0} = (s_{11} + s_{33} + 2 s_{13})
\]

When $\psi = \pi/2$, $v_{21} = v_{31} = s_{13} / s_{33}$; Poisson’s ratio is isotropic when the longitudinal extension is along the four-fold symmetry axis.

(C)  Rotation about $x_3$: $s_{11}' = [s_{11} + F(\varphi)] ; \quad s_{12}' = [s_{12} - F(\varphi)]$
\[
F(\varphi) = [c(\varphi)s(\varphi)][s_{1}[c(\varphi)s(\varphi)] + 2 s_{14}[c^2(\varphi) - s^2(\varphi)]]
\]
\[
s_{1} = (s_{46} + 2 s_{12} - 2 s_{11}) ; \quad s_{13}' = s_{13}
\]
\[
v_{21} = [s_{12} - F(\varphi)] / [s_{11} + F(\varphi)] ; \quad v_{31} = s_{13} / [s_{11} + F(\varphi)]
\]

When $\varphi = \pi/4$, $s_{16}$ does not appear:
\[
v_{21} = [4 s_{12} - s_{1}] / [4 s_{11} + s_{1}] ; \quad v_{31} = 4 s_{13} / [4 s_{11} + s_{1}]
Transformation Matrix for General Rotations

In order to derive the Poisson's ratio for the most general case, we consider the transformation matrix for a combination of three coordinate rotations: a first rotation about \( x_3 \) by angle \( \varphi \), a second rotation about the new \( x_1 \) by angle \( \theta \), and a third rotation about the resulting \( x_2 \) by angle \( \psi \). When these angles are set to zero, the \( x_1, x_2, x_3 \) axes coincide respectively with the reference crystallographic directions. For nonzero angles, the direction cosines \( a_{mn} \) are as follows:

\[
\begin{bmatrix}
    c(\varphi)c(\psi) - s(\varphi)s(\theta)s(\psi) \\
    - s(\varphi)c(\theta) \\
    s(\varphi)s(\psi) + s(\varphi)s(\theta)c(\psi)
\end{bmatrix}
\begin{bmatrix}
    s(\varphi)c(\psi) + c(\varphi)s(\theta)s(\psi) \\
    c(\varphi)c(\theta) \\
    s(\varphi)s(\psi) - c(\varphi)s(\theta)c(\psi)
\end{bmatrix}
\begin{bmatrix}
    - s(\theta)s(\psi) \\
    s(\theta) \\
    c(\theta)c(\psi)
\end{bmatrix}
\]

Substitution of these \( a_{mn} \) into the expressions for \( s_{11}', s_{12}', \) and \( s_{13}' \), and thence into the formulas \( v_{21} = s_{12}' / s_{11}' \) and \( v_{31} = s_{13}' / s_{11}' \) formally solves the problem for specified values of \( \varphi, \theta, \) and \( \psi \).

Poisson's Ratios for Specific Orientations

1) Longitudinal extension along an axis normal to the four-fold symmetry axis: \( \psi = 0 \); \( \varphi \) and \( \theta \) arbitrary. Direction cosines are:

\[
\begin{bmatrix}
    c(\varphi) \\
    - s(\varphi)c(\theta) \\
    s(\varphi)s(\theta)
\end{bmatrix}
\begin{bmatrix}
    s(\varphi) \\
    c(\varphi)c(\theta) \\
    - c(\varphi)s(\theta)
\end{bmatrix}
\begin{bmatrix}
    0 \\
    s(\theta) \\
    c(\theta)
\end{bmatrix}
\]

Rotated compliances are:

\[
s_{11}' = s_{11} + F(\varphi)
\]

\[
s_{12}' = s_{12} + (s_{13} - s_{12})s^2(\theta) - F(\varphi)c^2(\theta)
\]

\[
s_{13}' = s_{13} + (s_{12} - s_{13})s^2(\theta) - F(\varphi)s^2(\theta)
\]

\[
v_{21} = [s_{12} + (s_{13} - s_{12})s^2(\theta) - F(\varphi)c^2(\theta)] / [s_{11} + F(\varphi)]
\]

\[
v_{31} = [s_{13} + (s_{12} - s_{13})s^2(\theta) - F(\varphi)s^2(\theta)] / [s_{11} + F(\varphi)]
\]
When ϕ = 0 or π/2, F(ϕ) = 0; case (A). When ϕ = π/4, F(ϕ) = s₁/4, and

\[ \nu_{21} = \frac{[4 \ s_{12} + 4 \ (s_{13} - s_{12})[s^2(\theta)] - s_{1} \ [c^2(\theta)]]}{4 \ s_{11} + s_{1}} \]

\[ \nu_{31} = \frac{[4 \ s_{13} + 4 \ (s_{12} - s_{13})[s^2(\theta)] - s_{1} \ [s^2(\theta)]]}{4 \ s_{11} + s_{1}} \]

2) Longitudinal extension along an axis not normal to the four-fold symmetry axis, but with x₂ normal to the four-fold symmetry axis: θ = 0; ϕ and ψ arbitrary. Direction cosines are:

\[
\begin{bmatrix}
    [c(\phi)c(\psi)] & [s(\phi)c(\psi)] & [-s(\psi)] \\
    [ - s(\phi)] & [c(\phi)] & [ 0 ] \\
    [c(\phi)s(\psi)] & [s(\phi)s(\psi)] & [ c(\psi)]
\end{bmatrix}
\]

Rotated compliances are:

\[ s_{11}' = \left( s_{11} + F(\phi) \right)[c^2(\psi)] + \left( s_{13} + s_{33}[s^2(\psi)] + (s_{44} + 2 \ s_{13})[c^2(\psi)] \right) \]

\[ s_{12}' = s_{12}[c^2(\psi)] + s_{13}[s^2(\psi)] - F(\phi)[c^2(\psi)] \]

\[ s_{13}' = s_{13} + (s_{44} + F(\phi))[c^2(\psi)][s^2(\psi)] \]

\[ \nu_{21} = s_{12}' / s_{11}'; \ \nu_{31} = s_{13}' / s_{11}' \]

When ψ = π/4, s₁₁' = \left( s_{0} + s_{44} + F(\phi) \right) / 4:

\[ s_{12}' = \left( s_{12} + s_{13} - F(\phi) \right) / 2; \ s_{13}' = \left( 4 \ s_{13} + s_{2} + F(\phi) \right) / 4 \]

\[ \nu_{21} = 2 \ [s_{12} + s_{13} - F(\phi)] / \left( s_{0} + s_{44} + F(\phi) \right) \]

\[ \nu_{31} = \left( 4 \ s_{13} + s_{2} + F(\phi) \right) / \left( s_{0} + s_{44} + F(\phi) \right) \]

When ψ = π/2, s₁₁' = s₃₃ ; s₁₂' = s₁₃ \ ; s₁₃' = s₁₃:

\[ \nu_{21} = \nu_{31} = s_{13} / s_{33} \]

Conclusions

Poisson's ratio, with respect to rotated coordinate axes for tetragonal materials, has been obtained. Four cases are of particular interest:
• For longitudinal extension along $x_1$ and $x_3$ along the four-fold symmetry axis:

$$v_{21} = \frac{s_{12}}{s_{11}}, \quad v_{31} = \frac{s_{13}}{s_{11}}$$

• For longitudinal extension along an axis bisecting the original $x_1$ and $x_3$ axes; $x_2$ normal to the four-fold symmetry axis:

$$v_{21} = \frac{2(s_{12} + s_{13})}{(s_0 + s_{44})}$$

$$v_{31} = \frac{(s_0 - s_{44})}{(s_0 + s_{44})}$$

• For longitudinal extension along the four-fold symmetry axis, the result is independent of the azimuthal angle $\varphi$:

$$v_{21} = v_{31} = \frac{s_{13}}{s_{33}}$$

• For longitudinal extension along an axis bisecting the original $x_1$ and $x_2$ axes, and $x_3$ along the four-fold symmetry axis:

$$v_{21} = \frac{[4 s_{12} - s_1]}{[4 s_{11} + s_1]}$$

$$v_{31} = \frac{4 s_{13}}{[4 s_{11} + s_1]}$$

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