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Young's modulus surface and Poisson's ratio curve for tetragonal crystals*

Zhang Jian-Min(张建民)[a)†], Zhang Yan(张 研)[a)],
Xu Ke-Wei(徐可为)[b)], and Ji Vincent[c)]

[a)] *College of Physics and Information Technology, Shaanxi Normal University, Xi'an 710062, China*
[b)] *State Key Laboratory for Mechanical Behavior of Materials, Xi'an Jiaotong University, Xi'an 710049, China*
[c)] *ICMMO/LEMHE UMR CNRS 8182, Université Paris-Sud 11, 91405 Orsay Cedex, France*

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This paper gives the general expressions for the compliance s'_{ijkl}, Young's modulus $E(hkl)$ and Poisson's ratio $\upsilon(hkl,\theta)$ along arbitrary loading direction $[hkl]$ for tetragonal crystals. The representation surface for which the length of the radius vector in the $[hkl]$ direction equals $E(hkl)$ and representation curve for which the length of the radius vector with angle θ deviated from the reference directions $[00\bar{1}]$, $[100]$, $[00\bar{1}]$, $[10\bar{1}]$ and $[11\bar{2}]$ equals $\upsilon(100,\theta)$, $\upsilon(001,\theta)$, $\upsilon(110,\theta)$, $\upsilon(101,\theta)$ and $\upsilon(111,\theta)$ respectively, are constructed for nine tetragonal crystals (ammonium dihydrogen arsenate, ammonium dihydrogen phosphate, barium titanate, indium, nickel sulfate, potassium dihydrogen arsenate, potassium dihydrogen phosphate, tin and zircon). The characteristics of them are analysed in detail.

Keywords: tetragonal crystals, elastic properties, representation surfaces, representation curves
PACC: 0340D, 0630M, 4630C, 6220D

1. Introduction

Thin films have been used extensively in decorative, protective, electronic, magnetic and optical devices and systems. These films usually have strong textures and so anisotropic elasticity.[1−8] The anisotropic elasticity can result in the directionally dependent stress and strain energy,[9−16] abnormal grain growth and texture transformation in thin films.[17−22] In x-ray diffraction method for determining residual stresses in a polycrystalline specimen, only those grains properly oriented to diffract at each tilt contribute to the diffraction profile. This selectivity makes the x-ray elastic constants (XREC) $s_1(hkl) = -\dfrac{\upsilon(hkl)}{E(hkl)}$ and $\dfrac{1}{2}s_2(hkl) = \dfrac{1+\upsilon(hkl)}{E(hkl)}$ connecting the relative change in inter-planar spacing (or lattice strain $\varepsilon = \dfrac{d(hkl)-d_0(hkl)}{d_0(hkl)}$) to the stresses vary with the particular set of planes (hkl) chosen for measurement.[23] In bulk materials, the resulting macroscopic properties are usually calculated by considering the directionally dependent values averaged over all orientations in space.[24]

The purpose of this paper is to obtain the general expressions for elastic compliance constant (in short, the compliance) s'_{ijkl}, Young's modulus $E(hkl)$ and Poisson's ratio $\upsilon(hkl,\theta)$ for arbitrary lattice plane (hkl) of tetragonal crystals. The calculations have been made for nine tetragonal crystals (ammonium dihydrogen arsenate, ammonium dihydrogen phosphate, barium titanate, indium, nickel sulfate, potassium dihydrogen arsenate, potassium dihydrogen phosphate, tin and zircon), and the representation surface for which the length of the radius vector in the $[hkl]$ direction equals $E(hkl)$ and representation curve for which the length of the radius vector with angle θ deviated from the reference directions $[00\bar{1}]$, $[100]$, $[00\bar{1}]$, $[10\bar{1}]$ and $[11\bar{2}]$ equals $\upsilon(100,\theta)$, $\upsilon(001,\theta)$, $\upsilon(110,\theta)$, $\upsilon(101,\theta)$ and $\upsilon(111,\theta)$ for examples are constructed as well.

2. General compliance transformation relation

Three orthogonal coordinate systems, cubic crystal axes (A_i), lattice plane systems (L_i) and measurement systems (M_i), used in the following analysis are shown in Fig.1.

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†E-mail: jianm_zhang@yahoo.com

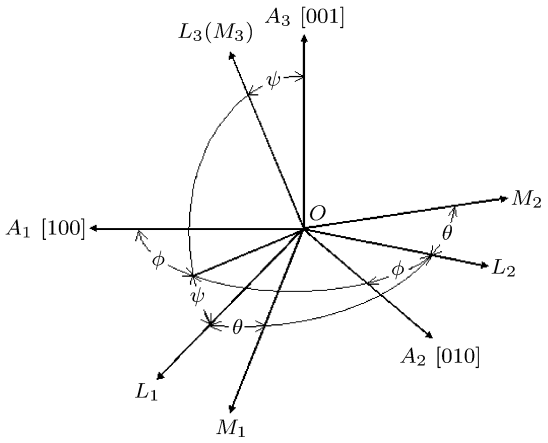


Fig.1. Three orthogonal coordinate systems of tetragonal crystal axes (A_i), lattice plane systems (L_i) and measurement systems (M_i).

The lattice plane systems (L_i) are defined such that L_1 and L_2 axes are in the lattice plane (hkl) so L_3 axis is along the normal direction of the lattice plane (hkl) (noted with Miller indices in crystal axes (A_i)).

The transformation matrix ($b_{\rm rt}$) from tetragonal crystal axes (A_i) to lattice plane systems (L_i) can be obtained through the following two rotations, one by an angle ϕ about the A_3 axis, and another by ψ about L_2 axis

$$(b_{\rm rt}) = \begin{pmatrix} \cos\psi & 0 & -\sin\psi \\ 0 & 1 & 0 \\ \sin\psi & 0 & \cos\psi \end{pmatrix} \begin{pmatrix} \cos\phi & \sin\phi & 0 \\ -\sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} \cos\psi\cos\phi & \cos\psi\sin\phi & -\sin\psi \\ -\sin\phi & \cos\phi & 0 \\ \sin\psi\cos\phi & \sin\psi\sin\phi & \cos\psi \end{pmatrix}. \quad (1)$$

For tetragonal crystals, the transformation matrix ($b_{\rm rt}$) can be expressed explicitly in terms of the Miller indices of the (hkl) plane

$$(b_{\rm rt}) = \begin{pmatrix} \dfrac{hL}{\sqrt{h^2+k^2}\sqrt{h^2+k^2+L^2}} & \dfrac{kL}{\sqrt{h^2+k^2}\sqrt{h^2+k^2+L^2}} & -\dfrac{\sqrt{h^2+k^2}}{\sqrt{h^2+k^2+L^2}} \\ -\dfrac{k}{\sqrt{h^2+k^2}} & \dfrac{h}{\sqrt{h^2+k^2}} & 0 \\ \dfrac{h}{\sqrt{h^2+k^2+L^2}} & \dfrac{k}{\sqrt{h^2+k^2+L^2}} & \dfrac{L}{\sqrt{h^2+k^2+L^2}} \end{pmatrix}, \quad (2)$$

where $L = \dfrac{a}{c}l$, a and c are lattice constants of the tetragonal crystal.

The measurement systems (M_i), in which the stresses σ_{kl} are evaluated from measured strains ε_{ij}, are obtained by rotating further the lattice plane systems (L_i) about its own L_3 axis an angle θ. Thus, the transformation matrix ($a_{\rm rt}$) from tetragonal crystal axes (A_i) to measurement systems (M_i) can be represented as

$$(a_{\rm rt}) = \begin{pmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \cos\psi\cos\phi & \cos\psi\sin\phi & -\sin\psi \\ -\sin\phi & \cos\phi & 0 \\ \sin\psi\cos\phi & \sin\psi\sin\phi & \cos\psi \end{pmatrix} = \begin{pmatrix} \cos\theta\cos\psi\cos\phi - \sin\theta\sin\phi & \cos\theta\cos\psi\sin\phi + \sin\theta\cos\phi & -\cos\theta\sin\psi \\ -\sin\theta\cos\psi\cos\phi - \cos\theta\sin\phi & -\sin\theta\cos\psi\sin\phi + \cos\theta\cos\phi & \sin\theta\sin\psi \\ \sin\psi\cos\phi & \sin\psi\sin\phi & \cos\psi \end{pmatrix}. \quad (3)$$

With Eq.(2), the transformation matrix ($a_{\rm rt}$) can also be expressed explicitly in terms of the Miller indices of the (hkl) plane

$$(a_{\rm rt}) = \begin{pmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \dfrac{hL}{\sqrt{h^2+k^2}\sqrt{h^2+k^2+L^2}} & \dfrac{kL}{\sqrt{h^2+k^2}\sqrt{h^2+k^2+L^2}} & -\dfrac{\sqrt{h^2+k^2}}{\sqrt{h^2+k^2+L^2}} \\ -\dfrac{k}{\sqrt{h^2+k^2}} & \dfrac{h}{\sqrt{h^2+k^2}} & 0 \\ \dfrac{h}{\sqrt{h^2+k^2+L^2}} & \dfrac{k}{\sqrt{h^2+k^2+L^2}} & \dfrac{L}{\sqrt{h^2+k^2+L^2}} \end{pmatrix}$$

$$=\begin{pmatrix} \frac{hL}{\sqrt{h^2+k^2}\sqrt{h^2+k^2+L^2}}\cos\theta-\frac{k}{\sqrt{h^2+k^2}}\sin\theta & \frac{kL}{\sqrt{h^2+k^2}\sqrt{h^2+k^2+L^2}}\cos\theta+\frac{h}{\sqrt{h^2+k^2}}\sin\theta & -\frac{\sqrt{h^2+k^2}}{\sqrt{h^2+k^2+L^2}}\cos\theta \\ -\frac{hL}{\sqrt{h^2+k^2}\sqrt{h^2+k^2+L^2}}\sin\theta-\frac{k}{\sqrt{h^2+k^2}}\cos\theta & -\frac{kL}{\sqrt{h^2+k^2}\sqrt{h^2+k^2+L^2}}\sin\theta+\frac{h}{\sqrt{h^2+k^2}}\cos\theta & \frac{\sqrt{h^2+k^2}}{\sqrt{h^2+k^2+L^2}}\sin\theta \\ \frac{h}{\sqrt{h^2+k^2+L^2}} & \frac{k}{\sqrt{h^2+k^2+L^2}} & \frac{L}{\sqrt{h^2+k^2+L^2}} \end{pmatrix}. \tag{4}$$

In measurement systems (M_i), the basic equation relating stress σ_{kl} to strain ε_{ij} is the generalized form of Hooke's law[25]

$$\varepsilon_{ij}=s'_{ijkl}\sigma_{kl}\quad(i,j,k,l=1,2,3), \tag{5}$$

where s'_{ijkl} are the compliances in the measurement systems (M_i) and the summation is taken automatically from 1 to 3 for repeated suffix indices. Equation (5) stands for nine equations, each with nine terms on the right-hand side. The 81 compliances s'_{ijkl} form a fourth-rank tensor and can be transformed from the compliances of the crystal s_{mnop} in the tetragonal crystal axes (A_i)

$$s'_{ijkl}=a_{im}a_{jn}a_{ko}a_{lp}s_{mnop}. \tag{6}$$

The symmetry of s_{mnop} (or s'_{ijkl}) in the first two and the last two suffixes, that is $s_{mnop}=s_{nmop}$ and $s_{mnop}=s_{mnpo}$, makes only 36 of the 81 components s_{mnop} (or s'_{ijkl}) independent and possible to use a matrix notation. The first two suffixes are abbreviated into a single one running from 1 to 6, and the last two are abbreviated in the same way, according to following scheme:

Tensor notation: 11 22 33 23, 32 31, 13 12, 21

Matrix notation: 1 2 3 4 5 6

At the same time factors of 2 and 4 are introduced as follows:

$s_{mnop}=s_{ij}$ when i and j are $1,2$ or 3,

$2s_{mnop}=s_{ij}$ when either i or j are $4,5$ or 6,

$4s_{mnop}=s_{ij}$ when both i and j are $4,5$ or 6.

The components of the stress and the strain tensors are also written in a single suffix running from 1 to 6

$$\begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ & \sigma_{22} & \sigma_{23} \\ & & \sigma_{33} \end{bmatrix} \Rightarrow \begin{bmatrix} \sigma_1 & \sigma_6 & \sigma_5 \\ & \sigma_2 & \sigma_4 \\ & & \sigma_3 \end{bmatrix}, \tag{7}$$

$$\begin{bmatrix} \varepsilon_{11} & \varepsilon_{12} & \varepsilon_{13} \\ & \varepsilon_{22} & \varepsilon_{23} \\ & & \varepsilon_{33} \end{bmatrix} \Rightarrow \begin{bmatrix} \varepsilon_1 & \frac{1}{2}\varepsilon_6 & \frac{1}{2}\varepsilon_5 \\ & \varepsilon_2 & \frac{1}{2}\varepsilon_4 \\ & & \varepsilon_3 \end{bmatrix}. \tag{8}$$

We have omitted the lower left-hand half of the array, since the stress and the strain tensors are symmetrical about the leading diagonal.

The array of s_{ij} (or s'_{ij}) forms 6×6 squares and Eq.(5) takes a compact form

$$\varepsilon_i=s'_{ij}\sigma_j\qquad(i,j=1,2,\cdots,6). \tag{9}$$

For the materials with tetragonal structure, as is well known, only 6 (s_{11}, s_{12}, s_{13}, s_{33}, s_{44} and s_{66}) of the 36 components s_{ij} are independent. We have omitted the lower left-hand half of the array as well, since the matrix is symmetrical about the leading diagonal.

$$(s_{ij})=\begin{pmatrix} s_{11} & s_{12} & s_{13} & 0 & 0 & 0 \\ & s_{11} & s_{13} & 0 & 0 & 0 \\ & & s_{33} & 0 & 0 & 0 \\ & & & s_{44} & 0 & 0 \\ & & & & s_{44} & 0 \\ & & & & & s_{66} \end{pmatrix}. \tag{10}$$

Using Eqs.(6) and (10), and the rules for transforming between the 2 suffixes notation and the 4 suffixes notation mentioned above, we can obtain a general compliance transformation relation for tetragonal crystals from crystal axes (A_i) to measurement systems (M_i)

$$\begin{aligned} s'_{ijkl} =& s_{11}[a_{i1}a_{j1}a_{k1}a_{l1} + a_{i2}a_{j2}a_{k2}a_{l2}] + s_{12}[a_{i1}a_{j1}a_{k2}a_{l2} + a_{i2}a_{j2}a_{k1}a_{l1}] + s_{13}[a_{k3}a_{l3}\delta_{ij} + a_{i3}a_{j3}\delta_{kl}] \\ &+ \frac{1}{4}s_{44}[a_{j3}a_{l3}\delta_{ik} + a_{j3}a_{k3}\delta_{il} + a_{i3}a_{l3}\delta_{jk} + a_{i3}a_{k3}\delta_{jl}] \\ &+ \frac{1}{4}s_{66}[(a_{i1}a_{j2} + a_{i2}a_{j1})(a_{k1}a_{l2} + a_{k2}a_{l1})] + (s_{33} - 2s_{13} - s_{44})a_{i3}a_{j3}a_{k3}a_{l3}, \end{aligned} \tag{11}$$

where δ_{ij} is the Kronecker delta function defined by

$$\delta_{ij} = \begin{cases} 1 \ (i = j), \\ 0 \ (i \neq j). \end{cases} \tag{12}$$

3. Young's modulus

Young's modulus $E(hkl)$ along the normal direction of the lattice plane (hkl) or $L_3(M_3)$ axis as shown in Fig.1 is defined as the ratio of the stress σ_3 to the strain ε_3 along M_3 axis. From Eq.(9), we know that $\dfrac{1}{E(hkl)} = s'_{33}$. Using Eqs.(11) and (12) and then Eqs.(3) and (4), we can obtain

$$\begin{aligned} \frac{1}{E(hkl)} = s'_{33} =& s_{11}[a_{31}^4 + a_{32}^4] + (2s_{12} + s_{66})a_{31}^2a_{32}^2 + (2s_{13} + s_{44})a_{33}^2 + (s_{33} - 2s_{13} - s_{44})a_{33}^4 \\ =& s_{11}(\cos^4\phi + \sin^4\phi)\sin^4\psi + (2s_{12} + s_{66})\sin^4\psi\cos^2\phi\sin^2\phi \\ &+ (2s_{13} + s_{44})\cos^2\psi + (s_{33} - 2s_{13} - s_{44})\cos^4\psi \\ =& \frac{s_{11}(h^4 + k^4) + (2s_{12} + s_{66})h^2k^2 + (2s_{13} + s_{44})(h^2 + k^2)L^2 + s_{33}L^4}{(h^2 + k^2 + L^2)^2}. \end{aligned} \tag{13}$$

Substituting the handbook values of the compliances s_{11}, s_{12}, s_{13}, s_{33}, s_{44} and s_{66} of the nine tetragonal crystals (ammonium dihydrogen arsenate, ammonium dihydrogen phosphate, barium titanate, indium, nickel sulfate, potassium dihydrogen arsenate, potassium dihydrogen phosphate, tin and zircon)[26] into Eq.(13), we can obtain Young's modulus $E(hkl)$ along arbitrary direction $[hkl]$. The representation surfaces, for which the length of the radius vector in the direction $[hkl]$ equals to $E(hkl)$, are shown in Fig.2 for ammonium dihydrogen arsenate, barium titanate and nickel sulfate as examples.

From representation surfaces of Young's modulus for all nine tetragonal crystals considered, following characters can be drawn. Firstly, for all nine tetragonal crystals considered, the representation surface of Young's modulus has the same symmetry as the crystal. Second, according to the detail shape of the representation surface, the tetragonal materials can be grouped into three classes. For ammonium dihydrogen arsenate, ammonium dihydrogen phosphate, potassium dihydrogen arsenate, potassium dihydrogen phosphate and zircon, Young's modulus surface has two round protuberances along [001] and [00$\bar{1}$] directions and four non-round protuberances along [100], [010], [$\bar{1}$00] and [0$\bar{1}$0] directions. In the second group (barium titanate and indium), Young's modulus surface has eight non-round protuberance corners and six depressions at the centres of the faces (two round depressions along [001] and [00$\bar{1}$] directions and four non-round depressions along [100], [010], [$\bar{1}$00], and [0$\bar{1}$0] directions). In the third group (nickel sulfate and tin), Young's modulus surface has two round protuberances along [001] and [00$\bar{1}$] directions and four depressed grooves along [100], [010], [$\bar{1}$00] and [0$\bar{1}$0] directions, The values of Young's modulus along [100], [001], [110], [101] and [111] specific directions are listed in Table 1.

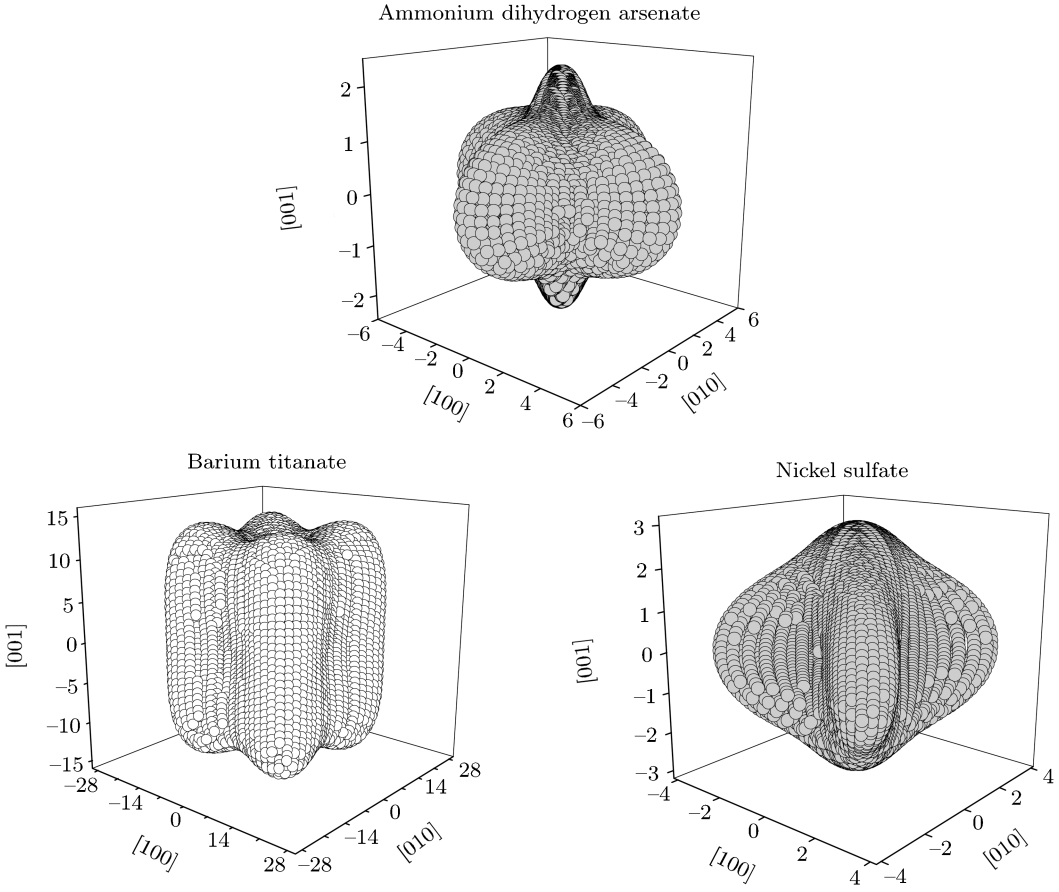


Fig.2. Representation surfaces of Young's modulus for tetragonal crystals ammonium dihydrogen arsenate, barium titanate and nickel sulfate. The length of the radius vector in the $[hkl]$ direction equals to $E(hkl)$ (in units of $10^{10}\mathrm{N/m^2}$).

Table 1. The values of Young's modulus (in units of $10^{10}\mathrm{N/m^2}$) along [100], [001], [110], [101] and [111] specific directions for tetragonal crystals.

crystals	$E(100)$	$E(001)$	$E(110)$	$E(101)$	$E(111)$
Ammonium dihydrogen arsenate	5.9172	2.2472	3.2468	2.0822	2.4096
Ammonium dihydrogen phosphate	5.0000	2.1882	1.8832	2.5494	2.9211
Barium titanate	13.7930	9.2593	23.474	16.715	17.455
Indium	0.6693	0.5348	1.4306	1.2958	1.2342
Nickel sulfate	1.5385	2.9070	4.3197	2.1822	1.9472
Potassium dihydrogen arsenate	5.2632	3.7037	2.0833	2.9851	3.2258
Potassium dihydrogen phosphate	6.7568	5.1282	2.0812	3.7943	4.0735
Tin	6.8493	11.7650	10.6380	10.1110	9.0162
Zircon	7.1942	4.5249	4.6189	3.8023	4.1647

4. Poisson's ratio

As is well known that, a simple tension stress produces, in general, not only longitudinal strain but also lateral strains. The ratio of the negative values of lateral (or transverse) strain to the longitudinal strain is known as Poisson's ratio. Suppose that the crystal is acted on by a uniaxial stress σ_3 along normal direction of the lattice plane (hkl) or M_3 axis as shown in Fig.1. From Eq.(9), the transverse strains ε_1 along M_1 axis and longitudinal strain ε_3 along M_3 axis can be written in terms of the compliance as follows:

$$\varepsilon_1 = s'_{13}\sigma_3, \tag{14}$$

$$\varepsilon_3 = s'_{33}\sigma_3. \tag{15}$$

Therefore, Poisson's ratio $\upsilon(hkl)$ for an arbitrary plane (hkl) can be expressed as

$$\upsilon(hkl) = -\frac{\varepsilon_1}{\varepsilon_3} = -\frac{s'_{13}}{s'_{33}}. \tag{16}$$

The expression of s'_{33} is already given by Eq.(13), the expression of s'_{13} can be obtained by using Eqs.(11) and (12) and then Eqs.(3) and (4),

$$\begin{aligned}
s'_{13} =& s_{11}(a_{11}^2a_{31}^2 + a_{12}^2a_{32}^2) + s_{12}(a_{11}^2a_{32}^2 + a_{12}^2a_{31}^2) + s_{13}(a_{13}^2 + a_{33}^2) + s_{66}a_{11}a_{12}a_{31}a_{32} + (s_{33} - 2s_{13} - s_{44})a_{13}^2a_{33}^2 \\
=& s_{11}\left[(\cos\theta\cos\psi\cos\phi - \sin\theta\sin\phi)^2\cos^2\phi + (\cos\theta\cos\psi\sin\phi + \sin\theta\cos\phi)^2\sin^2\phi\right]\sin^2\psi \\
&+ s_{12}\left[(\cos\theta\cos\psi\cos\phi - \sin\theta\sin\phi)^2\sin^2\phi + (\cos\theta\cos\psi\sin\phi + \sin\theta\cos\phi)^2\cos^2\phi\right]\sin^2\psi \\
&+ s_{13}(\cos^2\theta\sin^2\psi + \cos^2\psi) \\
&+ s_{66}(\cos\theta\cos\psi\cos\phi - \sin\theta\sin\phi)(\cos\theta\cos\psi\sin\phi + \sin\theta\cos\phi)\cos\phi\sin\phi\sin^2\psi \\
&+ (s_{33} - 2s_{13} - s_{44})\cos^2\theta\sin^2\psi\cos^2\psi \\
=& \left\{\frac{s_{11}}{h^2+k^2}\left[\left(\frac{h^2L}{\sqrt{h^2+k^2+L^2}}\cos\theta - hk\sin\theta\right)^2 + \left(\frac{k^2L}{\sqrt{h^2+k^2+L^2}}\cos\theta + hk\sin\theta\right)^2\right]\right. \\
&+ \frac{s_{12}}{h^2+k^2}\left[\left(\frac{hkL}{\sqrt{h^2+k^2+L^2}}\cos\theta - k^2\sin\theta\right)^2 + \left(\frac{hkL}{\sqrt{h^2+k^2+L^2}}\cos\theta + h^2\sin\theta\right)^2\right] \\
&+ s_{13}\left[(h^2+k^2)\cos^2\theta + L^2\right] \\
&+ \frac{s_{66}}{h^2+k^2}\left(\frac{hkL}{\sqrt{h^2+k^2+L^2}}\cos\theta - k^2\sin\theta\right)\left(\frac{hkL}{\sqrt{h^2+k^2+L^2}}\cos\theta + h^2\sin\theta\right) \\
&\left.+(s_{33} - 2s_{13} - s_{44})\frac{(h^2+k^2)L^2}{h^2+k^2+L^2}\cos^2\theta\right\}\frac{1}{h^2+k^2+L^2}.
\end{aligned} \tag{17}$$

Inserting Eqs.(13) and (17) into Eq.(16), we can obtain

$$\begin{aligned}
\upsilon(hkl,\theta) =& -\left\{s_{11}\left[(\cos\theta\cos\psi\cos\phi - \sin\theta\sin\phi)^2\cos^2\phi + (\cos\theta\cos\psi\sin\phi + \sin\theta\cos\phi)^2\sin^2\phi\right]\sin^2\psi\right. \\
&+ s_{12}\left[(\cos\theta\cos\psi\cos\phi - \sin\theta\sin\phi)^2\sin^2\phi + (\cos\theta\cos\psi\sin\phi + \sin\theta\cos\phi)^2\cos^2\phi\right]\sin^2\psi \\
&+ s_{13}(\cos^2\theta\sin^2\psi + \cos^2\psi) \\
&+ s_{66}(\cos\theta\cos\psi\cos\phi - \sin\theta\sin\phi)(\cos\theta\cos\psi\sin\phi + \sin\theta\cos\phi)\cos\phi\sin\phi\sin^2\psi \\
&\left.+(s_{33} - 2s_{13} - s_{44})\cos^2\theta\sin^2\psi\cos^2\psi\right\}\Big/\left[s_{11}(\cos^4\phi + \sin^4\phi)\sin^4\psi\right. \\
&\left.+ (2s_{12} + s_{66})\sin^4\psi\cos^2\phi\sin^2\phi + (2s_{13} + s_{44})\cos^2\psi + (s_{33} - 2s_{13} - s_{44})\cos^4\psi\right] \\
=& -\left\{\frac{s_{11}}{h^2+k^2}\left[\left(\frac{h^2L}{\sqrt{h^2+k^2+L^2}}\cos\theta - hk\sin\theta\right)^2 + \left(\frac{k^2L}{\sqrt{h^2+k^2+L^2}}\cos\theta + hk\sin\theta\right)^2\right]\right. \\
&+ \frac{s_{12}}{h^2+k^2}\left[\left(\frac{hkL}{\sqrt{h^2+k^2+L^2}}\cos\theta - k^2\sin\theta\right)^2 + \left(\frac{hkL}{\sqrt{h^2+k^2+L^2}}\cos\theta + h^2\sin\theta\right)^2\right] \\
&+ s_{13}\left[(h^2+k^2)\cos^2\theta + L^2\right] \\
&+ \frac{s_{66}}{h^2+k^2}\left(\frac{hkL}{\sqrt{h^2+k^2+L^2}}\cos\theta - k^2\sin\theta\right)\left(\frac{hkL}{\sqrt{h^2+k^2+L^2}}\cos\theta + h^2\sin\theta\right) \\
&\left.+(s_{33} - 2s_{13} - s_{44})\frac{(h^2+k^2)L^2}{h^2+k^2+L^2}\cos^2\theta\right\} \\
&\times \frac{h^2+k^2+L^2}{s_{11}(h^4+k^4) + (2s_{12}+s_{66})h^2k^2 + (2s_{13}+s_{44})(h^2+k^2)L^2 + s_{33}L^4}.
\end{aligned} \tag{18}$$

It is noted that, different from Eq.(13) for the expression of Young's modulus, Poisson's ratio depends not only on the lattice plane (hkl) but also on the angle θ deviated from reference direction $[hL\ kL\ -(h^2+k^2)]$ (L_1 axis) as shown in Fig.1. Substituting the handbook values of the compliances s_{11}, s_{12}, s_{13},

s_{33}, s_{44} and s_{66} into Eq.(18), we can readily obtain the Poisson's ratio $\upsilon(hkl,\theta)$ along an arbitrary direction in (hkl) lattice plane for each tetragonal crystal. As examples, variations of Poisson's ratio $\upsilon(hkl,\theta)$ with direction in five lower-index planes (100), (001), (110), (101) and (111) are shown in Fig.3 for tetragonal crystals ammonium dihydrogen arsenate (1), ammonium dihydrogen phosphate (2), barium titanate (3), indium (4), nickel sulfate (5), potassium dihydrogen arsenate (6), potassium dihydrogen phosphate (7), tin (8) and zircon (9). In these figures the length of the radius vector with angle θ deviated anticlockwise from the reference directions $[00\bar{1}]$, [100], $[00\bar{1}]$, $[10\bar{1}]$ and $[11\bar{2}]$ equals to $\upsilon(100,\theta)$, $\upsilon(001,\theta)$, $\upsilon(110,\theta)$, $\upsilon(101,\theta)$ and $\upsilon(111,\theta)$ respectively. It is noted that, for all nine tetragonal crystals considered, only in (001) plane Poisson's ratio is not direction dependent. This is because the [001] axis is a higher four-fold rotation axis in tetragonal crystals. In (100), (110), (101) and (111) planes, Poisson's ratio depends strongly on the direction. But as listed in Table 2 together with the values in (001) plane for comparison, the maximum (underlined) and the minimum values of Poisson's ratio are found along two orthogonal symmetry directions in each plane. Generally, the values of Poisson's ratio are positive, this implies that if a crystal is elongated in uniaxial tension direction, it will contract (as expected intuitively) in the plane perpendicular to the tension direction. This is always true in (111) plane. However, in the range of the angle θ listed in Table 3, the negative values of Poisson's ratio are found in four lower-index planes (100), (001), (110) and (101) of tetragonal crystals ammonium dihydrogen phosphate, indium, nickel sulfate, potassium dihydrogen arsenate and potassium dihydrogen phosphate. The negative values of Poisson's ratio were also found by Milstein *et al* for cubic crystals.[27−31]

Table 2. The maximum (underlined) and the minimum values of Poisson's ratio along two orthogonal symmetry directions in (100), (110), (101) and (111) planes of tetragonal crystals, the values in (001) plane are also listed for comparison.

plane	(100)		(001)		(110)		(101)		(111)	
direction	$[00\bar{1}]$	[010]	[100]	[010]	$[00\bar{1}]$	$[\bar{1}10]$	$[10\bar{1}]$	[010]	$[11\bar{2}]$	$[\bar{1}10]$
Ammonium dihydrogen arsenate	0.6568	<u>1.0237</u>	0.2494	0.2494	0.3604	<u>1.0130</u>	<u>0.5919</u>	0.2957	0.4910	<u>0.5139</u>
Ammonium dihydrogen phosphate	<u>0.6450</u>	–0.0850	0.2823	0.2823	0.2429	<u>0.5913</u>	<u>0.4914</u>	0.1428	0.2291	<u>0.5156</u>
Barium titanate	<u>0.4497</u>	0.4345	0.3019	0.3019	<u>0.7653</u>	0.0376	0.0364	<u>0.5357</u>	<u>0.2773</u>	0.2712
Indium	<u>0.6038</u>	0.3387	0.4824	0.4824	<u>1.2904</u>	–0.4135	–0.0107	<u>0.9122</u>	<u>0.5900</u>	0.2364
Nickel sulfate	0.0200	<u>0.7200</u>	0.0378	0.0378	0.0562	<u>0.2138</u>	–0.0562	<u>0.5248</u>	<u>0.2185</u>	0.1140
Potassium dihydrogen arsenate	–0.0526	<u>–0.1053</u>	–0.0370	–0.0370	–0.0208	<u>0.5625</u>	<u>0.2836</u>	–0.0448	0.0430	<u>0.4025</u>
Potassium dihydrogen phosphate	<u>0.2561</u>	–0.1149	0.1944	0.1944	0.0789	<u>0.6566</u>	<u>0.4931</u>	0.0397	0.1166	<u>0.5670</u>
Tin	0.1418	<u>0.3630</u>	0.2435	0.2435	<u>0.2202</u>	0.0106	0.0415	<u>0.3726</u>	<u>0.1993</u>	0.0862
Zircon	0.1007	<u>0.1151</u>	0.0633	0.0633	0.0647	<u>0.4319</u>	<u>0.3688</u>	0.0570	<u>0.2570</u>	0.2440

Table 3. The ranges of the angle θ corresponding to the negative values of Poisson's ratio in five lower-index planes (100), (001), (110), (101) and (111) for some tetragonal crystals.

crystals	$\upsilon(100)$	$\upsilon(001)$	$\upsilon(110)$	$\upsilon(101)$
Ammonium dihydrogen phosphate	75°–105°			
	255°–285°			
Indium			65°–115°	0°–5°
			245°–295°	175°–185°
				355°–360°
Nickel sulfate				0°–15°
				165°–195°
				345°–360°
Potassium dihydrogen arsenate	0°–360°	0°–360°	0°–10°	70°–110°
			170°–190°	250°–290°
			350°–360°	
Potassium dihydrogen phosphate	60°–120°			
	240°–300°			

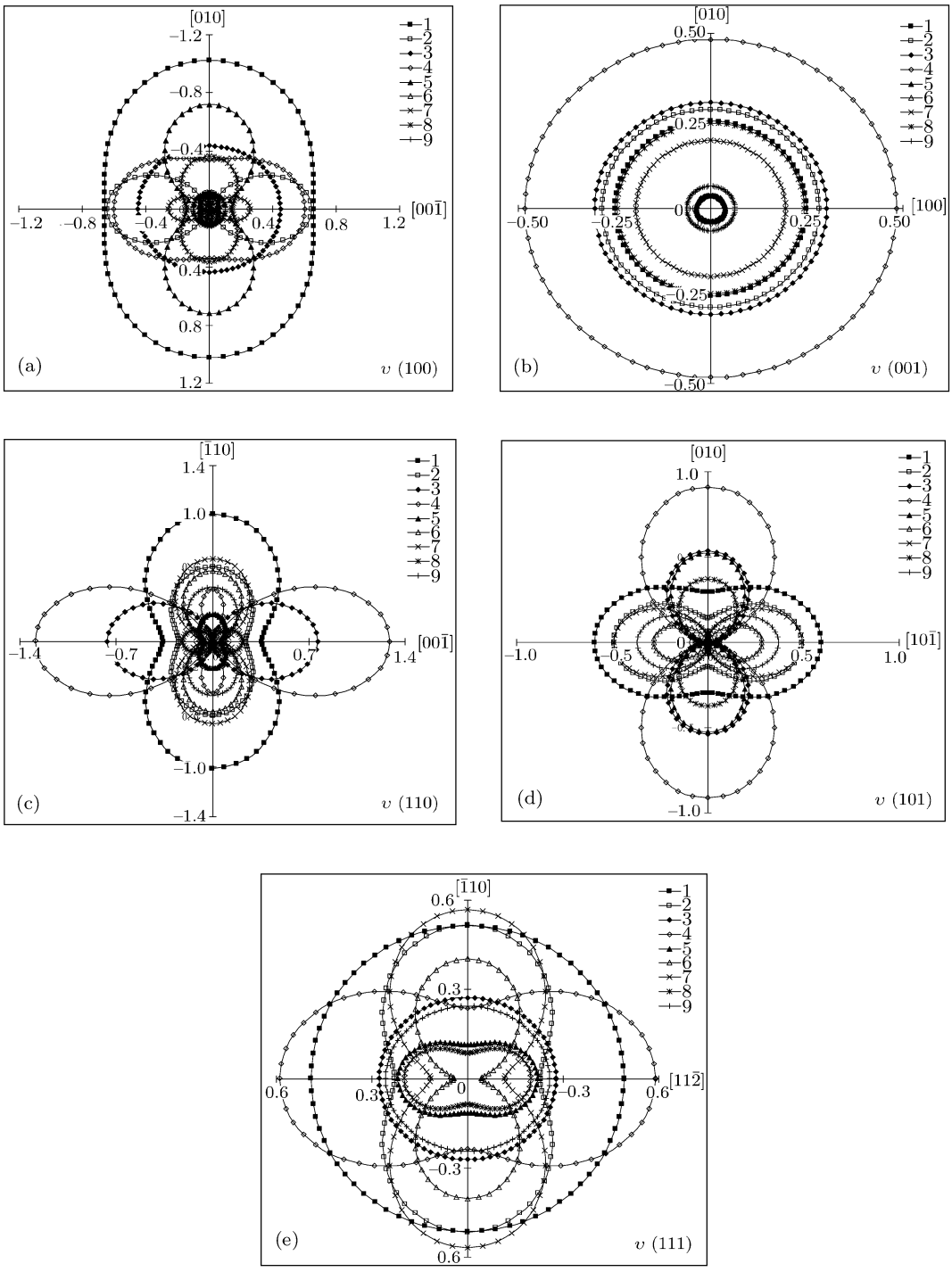


Fig.3. Representation curves of Poisson's ratio $\upsilon(hkl,\theta)$ for five lower-index planes (100), (001) (110) (101) and (111) of tetragonal crystals ammonium dihydrogen arsenate (1), ammonium dihydrogen phosphate (2), barium titanate (3), indium (4), nickel sulfate (5), potassium dihydrogen arsenate (6), potassium dihydrogen phosphate (7), tin (8) and zircon (9), in which the length of the radius vector with angle θ deviated anticlockwise from the reference directions [00$\bar{1}$], [100], [00$\bar{1}$], [10$\bar{1}$] and [11$\bar{2}$] equals $\upsilon(100,\theta)$, $\upsilon(001,\theta)$, $\upsilon(110,\theta)$, $\upsilon(101,\theta)$ and $\upsilon(111,\theta)$ respectively.

5. Conclusions

Young's modulus and Poisson's ratio are two important physical parameters of the materials and are not isotropic but depend on a specific direction in question. The general expressions for the compliance s'_{ijkl}, Young's modulus $E(hkl)$ and Poisson's ratio $\upsilon(hkl,\theta)$ along arbitrary loading direction $[hkl]$

are given for tetragonal crystals. The representation surface for which the length of the radius vector in the $[hkl]$ direction equals to $E(hkl)$ and representation curve for which the length of the radius vector with angle θ deviated from the reference directions $[00\bar{1}]$, $[100]$, $[00\bar{1}]$, $[10\bar{1}]$ and $[11\bar{2}]$ equals to $\upsilon(100,\theta)$, $\upsilon(001,\theta)$, $\upsilon(110,\theta)$, $\upsilon(101,\theta)$ and $\upsilon(111,\theta)$ for examples, are constructed for nine tetragonal crystals (ammonium dihydrogen arsenate, ammonium dihydrogen phosphate, barium titanate, indium, nickel sulfate, potassium dihydrogen arsenate, potassium dihydrogen phosphate, tin and zircon). Following conclusions are obtained.

(1) For ammonium dihydrogen arsenate, ammonium dihydrogen phosphate, potassium dihydrogen arsenate, potassium dihydrogen phosphate and zircon, Young's modulus surface has two round protuberances along [001] and $[00\bar{1}]$ directions and four non-round protuberances along [100], [010], $[\bar{1}00]$, and $[0\bar{1}0]$ directions.

(2) For barium titanate and indium, on the contrary, Young's modulus surface has two round depressions along [001] and $[00\bar{1}]$ directions and four non-round depressions along [100], [010], $[\bar{1}00]$ and $[0\bar{1}0]$ directions.

(3) For nickel sulfate and tin, Young's modulus surface has two round protuberances along [001] and $[00\bar{1}]$ directions but four depressed grooves along [100], [010], $[\bar{1}00]$ and $[0\bar{1}0]$ directions.

(4) For all nine tetragonal crystals considered, only in (001) plane Poisson's ratio is not direction dependent. In (100), (110), (101) and (111) planes, however, Poisson's ratio depends strongly on the direction, but the maximum and the minimum values of Poisson's ratio are found along two orthogonal symmetry directions in each plane.

(5) For all nine tetragonal crystals considered, only in (111) plane, the values of Poisson's ratio are always positive. However, the negative values of Poisson's ratio are found in some ranges of the angle θ for (100), (001), (110) and (101) planes of tetragonal crystals ammonium dihydrogen phosphate, indium, nickel sulfate, potassium dihydrogen arsenate and potassium dihydrogen phosphate. This implies that if a crystal is elongated in uniaxial tension direction, it will not contract but elongate in those directions perpendicular to the tension direction.

References

[1] Lee D N 1999 *J. Mater. Sci.* **34** 2575
[2] Lee D N 2002 *Mater. Sci. Forum* **408–412** 75
[3] Zhou W M and Wang C Y 2004 *Acta Phys. Sin.* **53** 4308 (in Chinese)
[4] Ding Z B, Yao S D, Wang K and Cheng K 2006 *Acta Phys. Sin.* **55** 2977 (in Chinese)
[5] Gu P F, Zheng Z R, Zhao Y J and Liu X 2006 *Acta Phys. Sin.* **55** 6459 (in Chinese)
[6] Zhou W M, Wang C Y, Chen Y H and Wang Z G 2006 *Chin. Phys.* **15** 1315
[7] Li R B 2007 *Acta Phys. Sin.* **56** 3428 (in Chinese)
[8] Wang Q, Ding J N, He Y L, Xue W and Fan Z 2007 *Acta Phys. Sin.* **56** 4834 (in Chinese)
[9] Zhang J M and Xu K W 2002 *Acta Phys. Sin.* **51** 2562 (in Chinese)
[10] Zhang J M and Xu K W 2004 *Acta Phys. Sin.* **53** 176 (in Chinese)
[11] Zhang J M, Zhang Y and Xu K W 2005 *Chin. Phys.* **14** 1862
[12] Zhang J M, Zhang Y, Xu K W and Ji V 2006 *Appl. Surf. Sci.* **253** 2432
[13] Cheng B W, Yao F, Xue C L, Zhang J G, Li C B, Mao R W, Zuo Y H, Luo L P and Wang Q M 2005 *Acta Phys. Sin.* **54** 4350 (in Chinese)
[14] Ni X G and Yin J W 2006 *Acta Phys. Sin.* **55** 6522 (in Chinese)
[15] Liu H, Ke F J, Pan H and Zhou M 2007 *Acta Phys. Sin.* **56** 407 (in Chinese)
[16] Chen C B, Liu Z M, Ma Y M, Cui T, Liu B B and Zou G T 2007 *Acta Phys. Sin.* **56** 2828 (in Chinese)
[17] Ohmi T, Saito T, Otsuki M and Shibata T 1991 *J. Electrochem. Soc.* **138** 1089
[18] Harase J 1992 *Mater. Sci. Forum* **94–96** 419
[19] Choi J H, Kang S Y and Lee D N 2000 *J. Mater. Sci.* **35** 4055
[20] Zhang J M, Xu K W and Ji V 2001 *J. Cryst. Growth* **226** 168
[21] Zhang J M and Xu K W 2003 *Acta Phys. Sin.* **52** 145 (in Chinese)
[22] Zhang J M, Xu K W and Zhang M R 2003 *Acta Phys. Sin.* **52** 1207 (in Chinese)
[23] Dölle H 1979 *J. Appl. Cryst.* **12** 489
[24] Murarka S P 1997 *Mater. Sci. Eng.* R **19** 87
[25] Nye J F 1985 *Physical Properties of Crystals* (Oxford: Clarendon) Chapter 8
[26] Gray D E 1972 *American Institute of Physics Handbook* (New York: McGraw-Hill) pp2–54
[27] Milstein F and Huang K 1979 *Phys. Rev.* B **19** 2030
[28] Kitagawa K, Ueda M and Miyamoto H 1980 *Acta Metall.* **28** 1505
[29] Milstein F and Rasky D 1982 *Phil. Mag.* A **45** 49
[30] Milstein F and Marschall J 1988 *Phil. Mag.* A **58** 365
[31] Milstein F and Marschall J 1992 *Acta Metall. Mater.* **40** 1229