

SURFACE REPRESENTATION OF POLYCRYSTAL PHYSICAL PROPERTIES: ALL CRYSTAL CLASSES, SIMPLE AVERAGE APPROXIMATION

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Algorithms for polycrystal physical properties estimation are presented. Bunge's spherical harmonics treatment of surface representations, under simple average approximation, is applied. Specific formulae for so-called longitudinal magnitudes are given. Physical properties associated to tensors of second-, third- and fourth-rank are considered. All crystal and sample symmetries are covered.

KEY WORDS: Tensor properties, spherical harmonics, voigt average, crystal symmetry, sample symmetry.

INTRODUCTION

The calculation of physical properties in polycrystalline materials, starting from the corresponding properties of their constituent crystallites, is one of the important objectives in texture investigations. A general theoretical background for this problem has been given by Bunge (1982), who also wrote a pioneering work (1969) on ODF prediction of polycrystal mechanical properties. Recent developments in this field are associated to the use of orientation correlation and misorientation distribution functions, to self-consistent methods and presently to Matthies' (1994) geometrical mean approximation. The papers by Bunge (1989), Humbert (1991) and Mainprice (1994) may be representative of important moments in this working area.

A large number of specific studies have been performed in metallic (highly symmetric) systems. Special interest has been conferred to mechanical and magnetic properties. For the above mentioned cases, suitable algorithms and computer codes, ranging from simple averages to more sophisticated methods, have been established. However, in the case of low-symmetry materials, even for simple average estimations, we have not found a systematic presentation of such procedures.

Our purpose, with this work, is to contribute somewhat to a systematic treatment of polycrystal tensor properties. Specific algorithms for surface representation of properties associated to tensors of rank r ($2 \leq r \leq 4$) are presented. Simple average approximation and Bunge's spherical harmonics ODF expansions are used. All crystal and sample symmetries are considered.

THEORETICAL SUMMARY (for further details see Bunge, 1982)

Any macroscopic single-crystal tensor property $E = Y/X$ may be represented by one or more scalar functions $E(h)$ of the crystallographic direction h . This gives place to the so-called *surface representation* (Nye, 1957). X and Y are measured quantities. The mentioned functions may be described by expansions in series of surface spherical harmonics of the crystal symmetry $\dot{K}_l^\mu(h)$

$$E(h) = \sum_{l=0}^r \sum_{\mu=1}^{M(l)} e_l^\mu \dot{K}_l^\mu(h) \quad (1)$$

The coefficients e_l^μ characterize the property, r is the tensor's rank and $M(l)$ the number of linearly independent functions $\dot{K}_l^\mu(h)$.

The coefficients e_l^μ may be calculated by means of the integral

$$e_l^\mu = \oint E(h) \dot{K}_l^\mu(h) dh \quad (2)$$

Let us consider a macroscopically homogeneous polycrystalline sample with a texture described by the orientation distribution function (ODF)

$$f(g) = \sum_{l=0}^{\infty} \sum_{\mu=1}^{M(l)} \sum_{\nu=1}^{N(l)} C_l^{\mu\nu} \dot{T}_l^{\mu\nu}(g) \quad (3)$$

The ODF, or likewise the coefficients $C_l^{\mu\nu}$, characterize the volume fraction of crystallites in the neighborhood dg of the orientation g . $\dot{T}_l^{\mu\nu}(g)$ are symmetry-adapted three-dimensional spherical harmonics.

If the crystallites of the considered sample show the property $E(h)$, then the polycrystal simple average property \bar{E} will be a function of the sample direction y and may be calculated, in the so-called Voigt's approximation, by the general formula

$$\bar{E}(y) = \sum_{l=0}^r \sum_{\nu=1}^{N(l)} \bar{e}_l^\nu \dot{K}_l^\nu(y) \quad (4)$$

$N(l)$ is the number of linearly independent functions $\dot{K}_l^\nu(y)$ of the sample symmetry. The acceptance of the Voigt approximation is equivalent to the assumption of a constant value for the variable X over the entire polycrystal.

The coefficients \bar{e}_l^ν summarise the effects of both single crystal property and crystallite orientation distribution, characterized by e_l^μ and $C_l^{\mu\nu}$ respectively. They are calculated by

$$\bar{e}_l^\nu = \frac{1}{2l+1} \sum_{\mu=1}^{M(l)} C_l^{\mu\nu} e_l^\mu \quad (5)$$

The symmetric functions in (1), (3) and (4) used in this work are those real functions described by Raymond *et. al.*

If the orientation distribution is rotationally symmetric about the Z-axis of the sample coordinate system, then the expansion (3) coincides with that of the fibre axis inverse pole figure $R(h)$.

$$f(\mathbf{h}) = R(\mathbf{h}) = \sum_{l=0}^{\infty} \sum_{\mu=1}^{M(l)} C_l^\mu \dot{K}_l^\mu(\mathbf{h}) \quad (6)$$

C_l^μ characterizes the frequency distribution of crystal directions relative to the sample fibre axis. In this case, the property of the polycrystalline material is likewise rotationally symmetric about the Z-axis and

$$\bar{E}(\mathbf{y}) = \bar{E}(\phi) = \sum_{l=0}^r \bar{e}_l \bar{P}_l(\phi) \quad (7)$$

with

$$\bar{e}_l = \frac{1}{4\pi} \sqrt{\frac{2}{2l+1}} \sum_{\mu=1}^{M(l)} C_l^\mu e_l^\mu \quad (8)$$

TENSOR PROPERTIES OF SECOND RANK

Consider a physical property described by a symmetric tensor of second rank E. Examples of such properties are electric and magnetic susceptibilities, electric conductivity and thermal expansion. The so-called *longitudinal magnitude* of the analyzed property, in a given direction may always be described by a surface E(h). The analytical expression of E(h), relative to its principal axes, is

$$E(\mathbf{h}) = E_{11}h_1^2 + E_{22}h_2^2 + E_{33}h_3^2 \quad (9)$$

where h_i are the direction cosines of the crystal direction h.

With respect to such properties all crystals have at least orthorhombic symmetry. Equation (9) may be expressed, according to (1), by means of orthorhombic spherical surface harmonics. The coefficients e_l^μ and the functions $\dot{K}_l^\mu(\mathbf{h})$ are summarized in Table 1.

Table 2 shows the coefficients \bar{e}_l^ν and the functions $\dot{K}_l^\nu(\mathbf{y})$ corresponding to equations (4) and (5) for a polycrystal, with all common sample symmetries taken into account. Subindex t identifies triclinic coefficients and functions

For fibre textures, according to (7) and (8) one obtains

$$\bar{e}_0 = \frac{\sqrt{2}}{4\pi} C_0^1 e_0^1 = \frac{1}{\sqrt{2}\pi} e_0^1 \quad (10)$$

$$\bar{e}_2 = \frac{1}{4\pi} \sqrt{\frac{2}{5}} [C_2^1 e_2^1 + C_2^2 e_2^2]$$

TENSOR PROPERTIES OF THIRD RANK

Properties represented by symmetric tensors of third rank (specifically piezoelectricity) are exclusive of systems without centre of inversion. Here the *longitudinal surface* is described by

Table 1 Second-rank tensors. Single crystals.

l	μ	e_l^μ	$\dot{K}_l^\mu(h)^*$
0	1	$e_0^1 = \frac{2}{3} \sqrt{\pi} (E_{11} + E_{22} + E_{33})$	\bar{K}_0^0
2	1	$e_2^1 = \frac{2}{3} \sqrt{\frac{\pi}{5}} (2E_{33} - E_{11} - E_{22})$	\bar{K}_2^0
	2	$e_2^2 = \frac{2}{3} \sqrt{\frac{3\pi}{5}} (E_{11} - E_{22})$	\bar{K}_2^2

*The functions $\bar{K}_l^m(h)$ are the real spherical surface harmonics. (see Raymond *et al.*)

Table 2 Second-rank tensors. Polycrystals.

Sample symmetry	l	ν	\bar{e}_l^ν	$\dot{K}_l^\nu(y)$	
C_i	0	1	$\bar{e}_{-0}^{-1} = C_0^{11} e_0^1 = e_0^1$	\bar{K}_0^0	
	2	1	$\bar{e}_2^{-1} = \frac{1}{5} [C_2^{11} e_2^1 + C_2^{21} e_2^2]$	\bar{K}_2^{-2}	
		2	$\bar{e}_2^{-2} = \frac{1}{5} [C_2^{12} e_2^1 + C_2^{22} e_2^2]$	\bar{K}_2^{-1}	
		3	$\bar{e}_2^{-3} = \frac{1}{5} [C_2^{13} e_2^1 + C_2^{23} e_2^2]$	\bar{K}_2^0	
		4	$\bar{e}_2^{-4} = \frac{1}{5} [C_2^{14} e_2^1 + C_2^{24} e_2^2]$	\bar{K}_2^1	
		5	$\bar{e}_2^{-5} = \frac{1}{5} [C_2^{15} e_2^1 + C_2^{25} e_2^2]$	\bar{K}_2^2	
C_{2h}	2 Z	0	$\bar{e}_0^1 = \bar{e}_{0r}^1$	\dot{K}_{0r}^1	
		2	1	$\bar{e}_2^1 = \bar{e}_{2r}^1$	\dot{K}_{2r}^1
			2	$\bar{e}_2^2 = \bar{e}_{2r}^2$	\dot{K}_{2r}^3
	3		$\bar{e}_2^3 = \bar{e}_{2r}^3$	\dot{K}_{2r}^5	
	2 Y	0	$\bar{e}_0^1 = \bar{e}_{0r}^1$	\dot{K}_{0r}^1	
		2	1	$\bar{e}_2^1 = \bar{e}_{2r}^1$	\dot{K}_{2r}^3
			2	$\bar{e}_2^2 = \bar{e}_{3r}^2$	\dot{K}_{2r}^4
			3	$\bar{e}_2^3 = \bar{e}_{2r}^3$	\dot{K}_{2r}^5

Table 2 Cont'd.

Sample symmetry	l	ν	\bar{e}_l^ν	$\dot{K}_l^\nu(y)$
D_{2h}	0	1	$\bar{e}_0^1 = \bar{e}_{0t}^1$	\dot{K}_{0t}^1
	2	1	$\bar{e}_2^1 = \bar{e}_{2t}^1$	\dot{K}_{2t}^3
		2	$\bar{e}_2^2 = \bar{e}_{2t}^2$	\dot{K}_{2t}^5

(In the present paper, subindex t means *triclinic*.)

$$d'_{111} = \sum_{i,j,k}^l a_{1i} a_{1j} a_{1k} d_{ijk} \quad (11)$$

where the transformation components a_{li} are the direction cosines of the orientation $h = OX'_1$ relative to the coordinate axes OX_i .

e_l^μ coefficients and $\dot{K}_l^\mu(h)$ functions for expansion (1) corresponding to triclinic crystal symmetry are shown in Table 3. So-called reduced (matrix) notation of the independent components d_{ij} is used. The non-centrosymmetric nature of the considered property implies that only odd- l coefficients are non-null.

Table 4 gives e_l^μ for other crystal systems, with reference to those reported in Table 3. $\dot{K}_l^\mu(h)$ functions follow the same relationship.

Table 3 Third-rank tensors. Single crystals. Triclinic symmetry.

l	μ	e_l^μ	$\dot{K}_l^\mu(h)$
1	1	$e_1^1 = \frac{2}{5} \sqrt{\frac{\pi}{3}} [3d_{22} + d_{21} + d_{23} + d_{16} + d_{34}]$	\bar{K}_1^{-1}
	2	$e_1^2 = \frac{2}{5} \sqrt{\frac{\pi}{3}} [3d_{33} + d_{32} + d_{31} + d_{15} + d_{24}]$	\bar{K}_1^0
	3	$e_1^3 = \frac{2}{5} \sqrt{\frac{\pi}{3}} [3d_{11} + d_{12} + d_{13} + d_{26} + d_{35}]$	\bar{K}_1^1
3	1	$e_3^1 = \sqrt{\frac{2\pi}{35}} [d_{16} + d_{21} - d_{22}]$	\bar{K}_3^{-3}
	2	$e_3^2 = 2 \sqrt{\frac{\pi}{105}} [d_{14} + d_{25} + d_{36}]$	\bar{K}_3^{-2}
	3	$e_3^3 = \frac{2}{5} \sqrt{\frac{\pi}{42}} [4(d_{23} + d_{34}) - (3d_{22} + d_{21} + d_{16})]$	\bar{K}_3^{-1}
	4	$e_3^4 = \frac{2}{5} \sqrt{\frac{\pi}{7}} [2d_{33} - (d_{32} + d_{31} + d_{24} + d_{15})]$	\bar{K}_3^0

Table 3 Cont'd.

l	μ	e_l^μ	$\dot{K}_l^\mu (h)$
	5	$e_3^5 = \frac{2}{5} \sqrt{\frac{\pi}{42}} [4(d_{13} + d_{35}) - (3d_{11} + d_{12} + d_{26})]$	\bar{K}_3^1
	6	$e_3^6 = 2 \sqrt{\frac{\pi}{105}} [d_{15} + d_{31} - d_{24} - d_{32}]$	\bar{K}_3^2
	7	$e_3^7 = \sqrt{\frac{2\pi}{35}} [d_{11} - d_{12} - d_{26}]$	\bar{K}_3^3

Table 4 Third-rank tensors. Single crystals, Other symmetries.

Crystalline symmetry	Class		e_l^μ	
			$l = 1$	$l = 3$
Monoclinic	C_2	$2 \parallel x_3$	$e_1^1 = e_{1t}^2$	$e_3^1 = e_{3t}^2$ $e_3^2 = e_{3t}^4$ $e_3^3 = e_{3t}^6$
		$2 \parallel x_2$	$e_1^1 = e_{1t}^1$	$e_3^1 = e_{3t}^1$ $e_3^2 = e_{3t}^2$ $e_3^3 = e_{3t}^3$
	C_s	$m \perp x_3$	$e_1^1 = e_{1t}^1$ $e_1^2 = e_{1t}^3$	$e_3^1 = e_{3t}^1$ $e_3^2 = e_{3t}^3$ $e_3^3 = e_{3t}^5$ $e_3^4 = e_{3t}^7$
		$m \perp x_2$	$e_1^1 = e_{1t}^2$ $e_1^2 = e_{1t}^3$	$e_3^1 = e_{3t}^4$ $e_3^2 = e_{3t}^5$ $e_3^3 = e_{3t}^6$ $e_3^4 = e_{3t}^7$
Orthorhombic	D_2			$e_3^1 = e_{3t}^2$
	C_{2v}		$e_1^1 = e_{1t}^2$	$e_3^1 = e_{3t}^4$ $e_3^2 = e_{3t}^6$
Tetragonal	C_4 and C_{4v}		$e_1^1 = e_{1t}^2$	$e_3^1 = e_{3t}^4$ $e_3^2 = e_{3t}^6$
	S_4			$e_3^1 = e_{3t}^2$ $e_3^2 = e_{3t}^6$
	D_4		$d'_{111} \equiv 0$	
	D_{2d}	$m \perp x_1$		$e_3^1 = e_{3t}^6$
$2 \parallel x_1$			$e_3^1 = e_{3t}^2$	

Table 4 Cont'd.

Crystalline symmetry	Class		e_l^μ	
			$l = 1$	$l = 3$
Trigonal	C_3		$e_1^1 = e_{1r}^2$	$e_3^1 = e_{3r}^1$ $e_3^2 = e_{3r}^4$ $e_3^3 = e_{3r}^7$
	D_3			$e_3^1 = e_{3r}^7$
	C_{3v}	$m \perp x_2$	$e_1^1 = e_{1r}^2$	$e_3^1 = e_{3r}^4$ $e_3^2 = e_{3r}^7$
		$m \perp x_1$	$e_1^1 = e_{1r}^2$	$e_3^1 = e_{3r}^4$ $e_3^2 = e_{3r}^1$
Hexagonal	C_6 and C_{6v}		$e_1^1 = e_{1r}^2$	$e_3^1 = e_{3r}^4$
	D_6		$d'_{111} \equiv 0$	
	C_{3h}			$e_3^1 = e_{3r}^1$ $e_3^2 = e_{3r}^7$
	D_{3h}	$m \perp x_2$		$e_3^1 = e_{3r}^7$
		$m \perp x_1$		$e_3^1 = e_{3r}^1$
Cubic	O		$d_{ij} \equiv 0$	
	T and T_d			$e_3^1 = e_{3r}^2$

For polycrystal average piezoelectricity one obtains, if sample symmetry is triclinic:

$$\begin{aligned} \bar{d}'_{111}(y) = & \bar{e}_1^1 \dot{K}_1^1(y) + \bar{e}_1^2 \dot{K}_1^2(y) + \bar{e}_1^3 \dot{K}_1^3(y) + \bar{e}_3^1 \dot{K}_3^1(y) + \bar{e}_3^2 \dot{K}_3^2(y) + \bar{e}_3^3 \dot{K}_3^3(y) \\ & + \bar{e}_3^4 \dot{K}_3^4(y) + \bar{e}_3^5 \dot{K}_3^5(y) + \bar{e}_3^6 \dot{K}_3^6(y) + \bar{e}_3^7 \dot{K}_3^7(y) \end{aligned} \quad (12)$$

with \bar{e}_l^v coefficients calculated from (5). For example, if the crystal symmetry is C_3 or D_3 , then these coefficients are given in Table 5.

The functions $\dot{K}_l^v(y)$ in (12) are the same as those reported in Table 3, with $v = \mu$. For other sample symmetries the average value of the property may be obtained from (12), using Table 6. In these cases, the number of linearly independent functions depends on symmetry requirements (see Raymond *et al.*).

For fibre texture and any crystal symmetry one obtains

$$\bar{d}'_{111}(\phi) = \bar{e}_1 \bar{P}_1(\phi) + \bar{e}_3 \bar{P}_3(\phi) \quad (13)$$

Table 5 Third-rank tensors. Coefficients of the equation (12) for C_s and D_3 symmetry.

	C_3	D_3
$\bar{e}_1^v (v = 1, 2, 3)$	$\frac{1}{3} [C_1^{1v} e_1^1 + C_1^{2v} e_1^2]$	0
$\bar{e}_3^v (v = 1, 2, \dots, 7)$	$\frac{1}{7} [C_3^{1v} e_3^1 + C_3^{2v} e_3^2 + C_3^{3v} e_3^3 + C_3^{4v} e_3^4]$	$\frac{1}{7} C_3^{1v} e_3^1$

Table 6 Third-rank tensors. Polycrystals.

Sample symmetry		$\dot{K}_l^v(y)$	
		$l = 1$	$l = 3$
C_2	$2 \parallel Z$	$\dot{K}_1^1 = \dot{K}_{1r}^2$	$\dot{K}_3^1 = \dot{K}_{3r}^2$ $\dot{K}_3^2 = \dot{K}_{3r}^4$ $\dot{K}_3^3 = \dot{K}_{3r}^6$
	$2 \parallel Y$	$\dot{K}_1^1 = \dot{K}_{1r}^1$	$\dot{K}_3^1 = \dot{K}_{3r}^1$ $\dot{K}_3^2 = \dot{K}_{3r}^2$ $\dot{K}_3^3 = \dot{K}_{3r}^3$
C_s	$m \perp Z$	$\dot{K}_1^1 = \dot{K}_{1r}^1$ $\dot{K}_1^2 = \dot{K}_{1r}^3$	$\dot{K}_3^1 = \dot{K}_{3r}^1$ $\dot{K}_3^2 = \dot{K}_{3r}^3$ $\dot{K}_3^3 = \dot{K}_{3r}^5$ $\dot{K}_3^4 = \dot{K}_{3r}^7$
	$m \perp Y$	$\dot{K}_1^1 = \dot{K}_{1r}^2$ $\dot{K}_1^2 = \dot{K}_{1r}^3$	$\dot{K}_3^1 = \dot{K}_{3r}^4$ $\dot{K}_3^2 = \dot{K}_{3r}^5$ $\dot{K}_3^3 = \dot{K}_{3r}^6$ $\dot{K}_3^4 = \dot{K}_{3r}^7$
D_2			$\dot{K}_3^1 = \dot{K}_{3r}^2$
C_{2v}		$\dot{K}_1^1 = \dot{K}_{1r}^2$	$\dot{K}_3^1 = \dot{K}_{3r}^4$ $\dot{K}_3^2 = \dot{K}_{3r}^6$

with \bar{e}_l triclinic coefficients:

$$\bar{e}_1 = \frac{1}{4\pi} \sqrt{\frac{2}{3}} \sum_{\mu=1}^3 C_1^\mu e_1^\mu \quad (14)$$

$$\bar{e}_3 = \frac{1}{4\pi} \sqrt{\frac{2}{7}} \sum_{\mu=1}^7 C_3^\mu e_3^\mu \quad (15)$$

The number of terms in (14) and (15) for other symmetries will depend on the non-null e_l^μ reported in Table 4.

TENSOR PROPERTIES OF FOURTH RANK

Elasticity is the characteristic property associated to fourth rank tensors. It may also be described by longitudinal surfaces according to the transformation law:

$$S'_{llll} = \sum_{ijkl} a_{li} a_{lj} a_{lk} a_{ll} S_{ijkl} \quad (16)$$

If S_{ijkl} is the compliance tensor, then the surface S'_{llll} gives the inverse of Young's modulus or eventually elasticity modulus. Expressions for e_l^μ – coefficients and $\bar{K}_l^\mu(h)$ – functions are shown in Tables 7 and 8 for all crystal symmetries, excluding the cubic case. The reduced notation S_{ij} is used. Due to centrosymmetric nature of the considered property, all odd- l coefficients in (1) and (4) are null.

Table 7 Fourth-rank tensors. Single crystals. Triclinic symmetry.

l	μ	e_l^μ	$\bar{K}_l^\mu(h)$
0	1	$e_0^1 = \frac{2}{5} \sqrt{\pi} [S_{11} + S_{22} + S_{33} + \frac{2}{3} (S_{12} + S_{13} + S_{23}) + \frac{1}{3} (S_{44} + S_{55} + S_{66})]$	\bar{K}_0^0
2	1	$e_2^1 = \frac{4}{35} \sqrt{15\pi} [S_{16} + S_{26} + \frac{1}{3} (S_{36} + S_{45})]$	\bar{K}_2^{-2}
	2	$e_2^2 = \frac{4}{105} \sqrt{15\pi} [S_{14} + S_{56} + 3(S_{24} + S_{34})]$	\bar{K}_2^{-1}
	3	$e_2^3 = \frac{3}{105} \sqrt{5\pi} [2(S_{66} + 6S_{33} + S_{13} + S_{23}) - (6S_{11} + 6S_{22} + S_{44} + S_{55} + 4S_{12})]$	\bar{K}_2^0
	4	$e_2^4 = \frac{4}{105} \sqrt{15\pi} [S_{25} + S_{46} + 3(S_{15} + S_{35})]$	\bar{K}_2^1
	5	$e_2^5 = \frac{4}{35} \sqrt{15\pi} [S_{11} - S_{22} + \frac{1}{3} (S_{13} - S_{23}) - \frac{1}{6} (S_{44} - S_{55})]$	\bar{K}_2^2
4	1	$e_4^1 = \frac{4}{105} \sqrt{35\pi} [S_{16} - S_{26}]$	\bar{K}_4^{-4}
	2	$e_4^2 = \frac{3}{105} \sqrt{70\pi} [S_{14} + S_{56} - S_{24}]$	\bar{K}_4^{-3}
	3	$e_4^3 = \frac{4}{105} \sqrt{5\pi} [2(S_{36} + S_{45}) - (S_{16} + S_{26})]$	\bar{K}_4^{-2}
	4	$e_4^4 = \frac{6}{315} \sqrt{10\pi} [4S_{34} - (S_{14} + 3S_{24} + S_{56})]$	\bar{K}_4^{-1}

Table 7 Cont'd

l	μ	e_l^μ	$\bar{K}_4^{\mu}(h)$
5		$e_4^5 = \frac{2}{105} \sqrt{\pi} [3(S_{11} + S_{22}) + 8(S_{33} - S_{13} - S_{22}) - 4(S_{44} + S_{55} + S_{66} + S_{12})]$	\bar{K}_4^0
6		$e_4^6 = \frac{6}{315} \sqrt{10\pi} [4S_{35} - (3S_{15} + S_{25} + S_{46})]$	\bar{K}_4^1
7		$e_4^7 = \frac{4}{105} \sqrt{5\pi} [2S_{13} + S_{22} + S_{55} - S_{11} - S_{44} - 2S_{23}]$	\bar{K}_4^2
8		$e_4^8 = \frac{2}{105} \sqrt{70\pi} [S_{15} - (S_{25} + S_{46})]$	\bar{K}_4^3
9		$e_4^9 = \frac{4}{105} \sqrt{35\pi} [S_{11} + S_{22} - S_{66} - 2S_{12}]$	\bar{K}_4^4

Table 8 Fourth-rank tensors. Single crystals. Other symmetries.

Crystalline system	Class		e_l^μ		
			$l = 0$	$l = 2$	$l = 4$
Monoclinic	all	$2 \parallel x_3$	$e_0^1 = e_{0t}^1$	$e_2^1 = e_{2t}^1$ $e_2^2 = e_{2t}^3$ $e_2^3 = e_{2t}^5$	$e_4^1 = e_{4t}^1$ $e_4^2 = e_{4t}^3$ $e_4^3 = e_{4t}^5$ $e_4^4 = e_{4t}^7$ $e_4^5 = e_{4t}^9$
		$2 \parallel x_2$	$e_0^1 = e_{0t}^1$	$e_2^1 = e_{2t}^3$ $e_2^2 = e_{2t}^4$ $e_2^3 = e_{2t}^5$	$e_4^1 = e_{4t}^5$ $e_4^2 = e_{4t}^6$ $e_4^3 = e_{4t}^7$ $e_4^4 = e_{4t}^8$ $e_4^5 = e_{4t}^9$
Orthorhombic	all		$e_0^1 = e_{0t}^1$	$e_2^1 = e_{2t}^3$ $e_2^2 = e_{2t}^5$	$e_4^1 = e_{4t}^5$ $e_4^2 = e_{4t}^7$ $e_4^3 = e_{4t}^9$
Tetragonal	C_4, S_4, C_{4h}		$e_0^1 = e_{0t}^1$	$e_2^1 = e_{2t}^3$	$e_4^1 = e_{4t}^1$ $e_4^2 = e_{4t}^5$ $e_4^3 = e_{4t}^9$
	$D_4, C_{4v}, D_{2d}, D_{4h}$		$e_0^1 = e_{0t}^1$	$e_2^1 = e_{2t}^3$	$e_4^1 = e_{4t}^5$ $e_4^2 = e_{4t}^9$

Table 8 Cont'd.

Crystalline symmetry	Class		e_l^μ		
			$l = 0$	$l = 2$	$l = 4$
Trigonal	C_3, C_{3i}		$e_0^1 = e_{0r}^1$	$e_2^1 = e_{2r}^3$	$e_4^1 = e_{4r}^2$ $e_4^2 = e_{4r}^5$ $e_4^3 = e_{4r}^8$
	D_3, C_{3v}, D_{3d}	$m \perp x_1$	$e_0^1 = e_{0r}^1$	$e_2^1 = e_{2r}^3$	$e_4^1 = e_{4r}^5$ $e_4^2 = e_{4r}^2$
	C_{3v}, D_{3d}	$m \perp x_2$	$e_0^1 = e_{0r}^1$	$e_2^1 = e_{2r}^3$	$e_4^1 = e_{4r}^5$ $e_4^2 = e_{4r}^8$
Hexagonal	all		$e_0^1 = e_{0r}^1$	$e_2^1 = e_{2r}^3$	$e_4^1 = e_{4r}^5$

For cubic symmetry we obtain:

$$\begin{aligned}
 e_0^1 &= \frac{2}{5} \sqrt{\pi} (3S_{11} + 2S_{12} + S_{44}) \\
 e_4^1 &= \frac{4}{105} \sqrt{2\pi} [2S_{11} - (2S_{12} + S_{44})]
 \end{aligned} \quad (17)$$

with symmetric functions (see Raymond *et al.*):

$$\dot{\bar{K}}_0^1(\mathbf{h}) = \bar{K}_0^0(\mathbf{h}) \quad (18)$$

$$\dot{\bar{K}}_4^1(\mathbf{h}) = \sqrt{\frac{7}{24}} [\sqrt{2} \bar{K}_4^0(\mathbf{h}) + \frac{\sqrt{70}}{7} \bar{K}_4^4(\mathbf{h})] \quad (19)$$

For a polycrystal, it is possible to express the average elasticity in the form (12). For sample triclinic symmetry, then the expansion of function $\bar{S}'_{11}(\mathbf{y})$ will have one term for $l = 0$, five for $l = 2$ and nine for $l = 4$. Other sample symmetries are solved by the same method as that leading to Table 6, taking into account Tables 7 and 8 and using equations (4)–(5). For example, if crystal-sample symmetry is D_{4h} – D_{2h} one obtains:

$$\begin{aligned}
 \bar{S}'_{11}(\mathbf{y}) &= \bar{e}_0^1 \dot{\bar{K}}_{0r}^1(\mathbf{y}) + \bar{e}_2^1 \dot{\bar{K}}_{2r}^3(\mathbf{y}) + \bar{e}_2^2 \dot{\bar{K}}_{2r}^5(\mathbf{y}) + \bar{e}_4^1 \dot{\bar{K}}_{4r}^5(\mathbf{y}) + \bar{e}_4^2 \dot{\bar{K}}_{4r}^7(\mathbf{y}) \\
 &+ \bar{e}_4^3 \dot{\bar{K}}_{4r}^9(\mathbf{y})
 \end{aligned} \quad (20)$$

with

$$\bar{e}_0^1 = C_0^{11} \quad e_0^1 = e_0^1 \quad \bar{e}_4^1 = \frac{1}{9} [C_4^{11} e_{4r}^5 + C_4^{21} e_{4r}^9]$$

$$\begin{aligned}\bar{e}_2^1 &= \frac{1}{5} C_2^{11} e_{2t}^3 & \bar{e}_4^2 &= \frac{1}{9} [C_4^{12} e_{4t}^5 + C_4^{22} e_{4t}^9] \\ \bar{e}_2^2 &= \frac{1}{5} C_2^{12} e_{2t}^3 & \bar{e}_4^3 &= \frac{1}{9} [C_4^{13} e_{4t}^5 + C_4^{23} e_{4t}^9]\end{aligned}\quad (21)$$

Function $\bar{K}_{it}^v(y)$ in (20) are the same as those reported in Table 7 for $v = \mu$.

Finally, for fibre textures

$$\bar{S}'_{11}(y) = \bar{e}_0 \bar{P}_0(\phi) + \bar{e}_2 \bar{P}_2(\phi) + \bar{e}_4 \bar{P}_4(\phi) \quad (22)$$

where \bar{e}_i for triclinic crystal symmetry are given by:

$$\bar{e}_0 = \frac{\sqrt{2}}{4\pi} C_0^1 e_0^1 = \frac{1}{\sqrt{2}\pi} e_0^1 \quad (23)$$

$$\bar{e}_2 = \frac{1}{4\pi} \sqrt{\frac{2}{5}} \sum_{\mu=1}^5 C_2^\mu e_2^\mu \quad (24)$$

$$\bar{e}_4 = \frac{1}{4\pi} \sqrt{\frac{2}{9}} \sum_{\mu=1}^9 C_4^\mu e_4^\mu \quad (25)$$

The number of terms in (24)–(25) will depend, for the other crystal symmetries, on the non-null coefficients e_i^μ reported in Table 8.

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