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# Calculation of X-ray stress factors using vector parameterization and irreducible representations for SO(3) group

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**Abstract.** In the presence of texture, the concept of X-ray elastic constants as well as $\mathrm{Sin}^2\psi$ law is inapplicable and the X-ray stress factors (XSF) connecting average strain and stress have to be used [1-2]. The SO(3) vector parameterization with smart composition law [3-4] proved to be a powerful tool for handling transformations between reference systems used in XSF calculation. Decomposition of the 4-th rank elastic constant tensor on the SO(3) irreducible representations (IR) allows one to highlight the symmetry properties and to separate isotropic and anisotropic parts. Joint use of the vector parameterization and IR decomposition enables to obtain transparent analytical expressions for XSF in case of textures described by preferred spherical/fiber components.

## Introduction

The X-ray residual stress analysis (XSA) is a widespread technique for determination residual stresses present in polycrystalline material [1]. X-ray diffraction enables to find strain state in terms of variation of the interplane space averaged over diffracting crystallites. In order to find residual stress, additional assumptions about grain-interaction model and information about texture present in the sample have to be taken into consideration. The connection between measured strain and stress follows from the Hooke's law [1]:

$$\varepsilon^{L}_{33}(\mathbf{h},\mathbf{y}) = F_{ij}(\mathbf{h},\mathbf{y}) < \sigma^{S}_{ij} >, \tag{1}$$

$$\mathbf{y} = \{\mathrm{Sin}(\psi)\mathrm{Cos}(\varphi), \mathrm{Sin}(\psi)\mathrm{Sin}(\varphi), \mathrm{Cos}(\psi)\}, \tag{2}$$

$$\mathbf{h} = \{\mathrm{Sin}(\varphi_B)\mathrm{Cos}(\beta_B), \mathrm{Sin}(\varphi_B)\mathrm{Sin}(\beta_B), \mathrm{Cos}(\varphi_B)\}, \tag{3}$$

where $\mathbf{y}$ is the unit vector defining direction of the measurement, given in the sample reference system (S), $\psi$ is the angle between specimen surface normal and the direction of measurement $\mathbf{y}$, $\varphi$ is the rotation angle of the specimen around the specimen surface normal; $\mathbf{h}$ is the unit vector directed along the reciprocal lattice vector (*hkl*) of considered reflection, angles $\varphi_B, \beta_B$ are given in the crystallographic reference system (C); $\varepsilon^{L}_{33}(\mathbf{h},\mathbf{y})$ is the measured strain in direction $\mathbf{y}$ of reflection (*hkl*), the strain is defined in the laboratory reference system (L), the z axis of which is directed along $\mathbf{y}$; $\sigma^{S}_{ij}$ is the residual stress tensor defined in (S) system; $F_{ij}(\mathbf{h},\mathbf{y})$ are XSF of interest. If the sample is untextured and macroscopically elastically isotropic the X-ray elastic constants $S_1(\mathbf{h}), 1/2S_2(\mathbf{h})$ can be used instead of XSF:

$$F_{ij}(\mathbf{h},\mathbf{y}) = 1/2\, S_2(\mathbf{h})\, y_i y_j + S_1(\mathbf{h})\delta_{ij}, \tag{4}$$

and conventional $\mathrm{Sin}^2\psi$ techniques can be applied. However, in the presence of texture the complete fit based on XSF dependence on measuring direction $\boldsymbol{y}$ should be performed [1]. For that purpose analytical expressions for XSF are of importance. The calculation of XSF requires the averaging based on texture information of polycrystalline tensor $a_{ijkl}$, found according to adopted grain-interaction model ($a_{ijkl} = s_{ijkl}$ for Reuss model, or $a_{ijkl} = c^{-1}{}_{ijkl}$ for Voigt model). The averaging procedure requires the knowledge of the sample orientation distribution function (ODF) and in the most cases is performed numerically [2]. In the present paper for the case of texture described by fiber or spherical components analytical expressions for XSF are obtained with help of SO(3) vector parameterization and 4th rank elastic constant tensor IR decomposition. These techniques proved to be useful for handling transformations between (S), (C), (L) systems used in XSA.

## SO(3) vector parameterization and IR decomposition

**Vector-parameter.** There are numerous ways to describe the orientation of one coordinate system with respect to another, i.e. there are numerous ways of SO(3) parameterization. The most widespread one for XSA is the parameterization via Euler angles since it is closely connected to the goniometer rotations [2]. From the theoretical point of view the most favorable parameterization is that one for which the expression for rotation matrix via parameterization parameters and the composition law have the simplest form. These criteria are satisfied by the vector parameterization, which was first introduced by J.W.Gibbs and was explicitly worked by F.I.Fedorov who rediscovered it in the frame of reference-free covariant approach to rotation group and Lorentz group [3-4].

In this approach the rotation is described by three components of the vector-parameter $\mathbf{c} = \{c_1, c_2, c_3\}$, the direction of $\mathbf{c}$ defines the axis of rotation, its length is equal to $\mathrm{Tan}\,\varphi/2$, where $\varphi$ is angle of rotation. The rotation matrix is expressed via $\mathbf{c}$ as

$$T_{ij}(\mathbf{c}) = \frac{(1-\mathbf{c}^2)\delta_{ij} + 2\mathbf{c}_i\mathbf{c}_j + 2\varepsilon_{ikj}\mathbf{c}_k}{1+\mathbf{c}^2}, \tag{5}$$

where $\varepsilon_{ikj}$ is the antisymmetric Levi-Cevita pseudotensor, summation convention is used throughout this paper. The vector parameterization is outstanding among other parameterizations because of its elegant composition law, which enables to express two successive rotations with parameters $\mathbf{c}^{(1)}$ and $\mathbf{c}^{(2)}$ as a single rotation with parameter $\mathbf{c}^{(12)}$:

$$T_{ij}(\mathbf{c}^{(2)})T_{jk}(\mathbf{c}^{(1)}) = T_{ik}(\langle \mathbf{c}^{(2)}, \mathbf{c}^{(1)} \rangle) = T_{ik}(\mathbf{c}^{(12)}), \qquad \langle \mathbf{c}^{(2)}, \mathbf{c}^{(1)} \rangle = \frac{\mathbf{c}^{(1)} + \mathbf{c}^{(2)} + \mathbf{c}^{(2)} \times \mathbf{c}^{(1)}}{1 - \mathbf{c}^{(1)}\mathbf{c}^{(2)}}. \tag{6}$$

Also the vector parameterization has following convenient properties:

$$T_{ij}(\{0,0,0\}) = \delta_{ij}; \qquad T(\mathbf{c})^{-1} = T(-\mathbf{c}). \tag{7}$$

**IR for 4th rank elasticity tensor.** The transformation of arbitrary 4th rank tensor under the rotation can be found by convolution with 4 transformation matrices: $a_{i'j'k'l'} = T_{i'i}T_{j'j}T_{k'k}T_{l'l}a_{ijkl}$. However, this approach is too bulky and doesn't utilize the symmetry properties of the elasticity tensor. From the group theory point of view, the 4th rank tensors form the representation space of the rotation group, and it can be decomposed on irreducible representation spaces [5]. In the case of lowest triclinic symmetry the compliance tensor is decomposed on

$$\begin{aligned}
&2 \text{ IR with weight } l = 0 \text{ (scalars) } \sigma^{(s)}_{ijkl}, s = 1,2 - \text{isotropic part;}\\
&4 \text{ IR with weight } l = 2 \text{ (deviators) } \delta^{(d)\,m}_{ijkl}, d = 1...4,\ m = \text{-}2,..,2; \qquad (8)\\
&1 \text{ IR with weight } l = 4 \text{ (nonor) } \eta^{m}_{ijkl}, m = \text{-}4,...,4.
\end{aligned}$$

The basis tensors $\sigma^{(s)}_{ijkl}, \delta^{(d)\,m}_{ijkl}, \eta^{m}_{ijkl}$ can be calculated with help of the Clebsch-Gordan coefficients $C^{j,m}_{j_1,m_1;j_2,m_2}$ starting from circular vectors $e^{-1} = (1/\sqrt{2}, i/\sqrt{2}, 0), e^{0} = (0,0,\text{-}1), e^{1} = (1/\sqrt{2}, i/\sqrt{2}, 0)$, the IR of weight l=1. E.g.:

$$\sigma^{(1)}_{pqrs} = C^{0,0}_{1,i'';1,m'} C^{1,m'}_{1,i';0,0} C^{0,0}_{1,i;1,j} e^{i}_{p} e^{j}_{q} e^{i'}_{r} e^{i''}_{s} = \delta_{pq}\delta_{rs}, \qquad i, j, i', i'', m' = \ 1,0,1; \qquad p,q,r,s = 1,2,3. \qquad (9)$$

The IR decomposition highlights the symmetry properties of compliance tensor and separates its isotropic and anisotropic part, e.g. for cubic system

$$S^{(cub.)}_{ijkl} = \underbrace{(S_{11} + 2S_{12})\sigma^{(1)}_{ijkl} + \frac{4(S_{11} - S_{12}) + 3S_{44}}{2\sqrt{5}} \sigma^{(2)}_{ijkl}}_{\text{isotropic part}} + \underbrace{(A - 1)S_{44}\left(\frac{1}{4}(\eta^{-4}_{ijkl} + \eta^{4}_{ijkl}) + \frac{1}{2}\sqrt{\frac{7}{10}}\eta^{0}_{ijkl}\right)}_{\text{anisotropic part}},$$

where $A = \dfrac{2(S_{11} - S_{12})}{S_{44}}$ is the Zener's anisotropy ratio.

The rotation transformation in the subspace of IR of weight l is performed with help of angular momentum matrices. For the rotation described by the vector parameter **c** the expression is following [3]:

$$T^{(l)}_{n\,n'} = \sum_{m=-l}^{l} e^{-2\,i\,m\,\mathrm{ArcTan}(|\mathbf{c}|)} \frac{P^{l}_{m}\left(-\,i\,\mathbf{c}\,\mathbf{J}^{(l)}_{n\,n'}/|\mathbf{c}|\right)}{P^{l}_{m}\left(-\,i\,m\right)}, \qquad (10)$$

where $\mathbf{J}^{(l)}_{n\,n'}$ are the angular momentum matrices, $P^{l}_{m}(x) = \prod_{m' \neq m}^{m'=-l..l} (x + i\,m')$.

**Vector parameters for transformations between (S), (L), (C) reference systems.** If in two reference systems the components of unit vector are $\mathbf{p}$ and $\mathbf{p}'$, the vector parameter for transformation from $\mathbf{p}$ to $\mathbf{p}'$ is

$$\mathbf{c} = \frac{\mathrm{Tan}(\alpha/2)(\mathbf{p} + \mathbf{p}') + \mathbf{p} \times \mathbf{p}'}{1 + \mathbf{p}\mathbf{p}'}, \qquad (11)$$

where $\alpha$ is an arbitrary angle since the transformation has a degree of freedom left [3]. Since the unit vector directed along the diffraction vector is $\mathbf{y}$ in (S) and $\mathbf{e_z} = \{0,0,1\}$ in (L) system, the vector parameter for transformation from (S) to (L) is

$$ {}^{LS}\mathbf{c} = \frac{\mathbf{y}\times\mathbf{e_z}}{1+\mathbf{y}\mathbf{e_z}}. \qquad (12)$$

The unit diffraction vector in (C) system is $\mathbf{h}$, in (L) it is $\mathbf{e_z} = \{0,0,1\}$; however, the orientation of (C) has a degree of freedom since all crystallites with $\mathbf{h}$ in (C) system directed along $\mathbf{e_z}$ in (L) system and rotated by arbitrary angle $\alpha$ around the $\mathbf{e_z}$ direction in (L) satisfy the Bragg condition:

$$ {}^{LC}\mathbf{c} = \left\langle \mathrm{Tan}(\alpha/2)\mathbf{e_z}, \frac{\mathbf{h}\times\mathbf{e_z}}{1+\mathbf{h}\mathbf{e_z}} \right\rangle = \frac{\mathrm{Tan}(\alpha/2)(\mathbf{h}+\mathbf{e_z})+\mathbf{h}\times\mathbf{e_z}}{1+\mathbf{h}\mathbf{e_z}}. \qquad (13)$$

The same considerations lead to

$$ {}^{CS}\mathbf{c} = \frac{-\mathrm{Tan}((\alpha+\delta)/2)(\mathbf{y}+\mathbf{h})+\mathbf{y}\times\mathbf{h}}{1+\mathbf{y}\mathbf{h}}. \qquad (14)$$

and since ${}^{CS}\mathbf{c} = \left\langle -{}^{LC}\mathbf{c}, {}^{LS}\mathbf{c} \right\rangle$ using Eq. 6, Eq. 12 and Eq. 13 and comparing to Eq. 14, we obtain

$$ \delta = 2\,\mathrm{ArcTan}\frac{\mathrm{Sin}(\beta_B - \varphi)\mathrm{Sin}(\varphi_B/2)\mathrm{Sin}(\psi/2)}{\mathrm{Cos}(\varphi_B/2)\mathrm{Cos}(\psi/2)+\mathrm{Cos}(\beta_B - \varphi)\mathrm{Sin}(\varphi_B/2)\mathrm{Sin}(\psi/2)}. \qquad (15)$$

**Texture approximation by spherical/fiber components**

The complete description of texture is given in terms of ODF $f(g)$, $f(g)dg$ defines the fraction of crystallites the (C) system of which can be obtained from (S) by transformation described by parameters of group volume dg in the vicinity of g [6]. Since ODF is the function of 3 variables its complete description requires large massive of data. However, often ODF can be sufficiently accurately approximated by model functions with several parameters, the model of spherical or fiber components being one of them [6].

**Spherical component.** In the spherical component model ODF is modeled by sum of functions concentrated around preferred orientation $g^p$. The function has the following form in Euler parameterization [6]:

$$ f(g, g^p) = N e^{S\,\mathrm{Cos}(\omega)}, $$
$$ \mathrm{Cos}(\omega/2) = \mathrm{Cos}\frac{\varphi_1-\varphi_1^p}{2}\mathrm{Cos}\frac{\varphi_2-\varphi_2^p}{2}\mathrm{Cos}\frac{\Phi-\Phi^p}{2} - \mathrm{Sin}\frac{\varphi_1-\varphi_1^p}{2}\mathrm{Sin}\frac{\varphi_2-\varphi_2^p}{2}\mathrm{Cos}\frac{\Phi+\Phi^p}{2}. \qquad (16)$$

The expression for $\mathrm{Cos}(\omega/2)$ has covariant nature and we can expect that it should have simple form in the vector parameterization. With help of relations between the vector and Euler parameters [3]

$$\{c_1,c_2,c_3\} = \{-\frac{\mathrm{Tan}\frac{\Phi}{2}\mathrm{Cos}\frac{\varphi_1-\varphi_2}{2}}{\mathrm{Cos}\frac{\varphi_1+\varphi_2}{2}}, \frac{\mathrm{Tan}\frac{\Phi}{2}\mathrm{Sin}\frac{\varphi_1-\varphi_2}{2}}{\mathrm{Cos}\frac{\varphi_1+\varphi_2}{2}}, -\mathrm{Tan}\frac{\varphi_1+\varphi_2}{2}\}, \tag{17}$$

we get

$$\mathrm{Cos}(\omega/2) = \frac{1+\mathbf{c}\mathbf{c}^p}{\sqrt{1+\mathbf{c}^2}\sqrt{1+\mathbf{c}^{p2}}}. \tag{18}$$

For $\mathbf{c} = \overset{CS}{\mathbf{c}}$ and preferred orientation $\mathbf{c}^p$ it can be shown that

$$\mathrm{Cos}(\omega) = \mathrm{Cos}^2(\theta^*/2)\mathrm{Cos}\big(\alpha+\delta+2\mathrm{ArcTan}(b/a)\big) - \mathrm{Sin}^2(\theta^*/2),\ \mathrm{Cos}(\theta^*) = \mathbf{h}_i \mathrm{T}(\mathbf{c}^p)_{ij}\mathbf{y}_j,$$

$$a = \frac{1+\mathbf{hy}-\mathbf{c}^p\mathbf{hy}}{\sqrt{1+\mathbf{c}^{p2}}\sqrt{(\mathbf{h}+\mathbf{y})^2}}, \qquad b = \frac{\mathbf{c}^p(\mathbf{h}+\mathbf{y})}{\sqrt{1+\mathbf{c}^{p2}}\sqrt{(\mathbf{h}+\mathbf{y})^2}}, \qquad \mathrm{Cos}^2(\theta^*/2) = a^2+b^2. \tag{19}$$

**Fiber component.** ODF in the fiber component method is determined by the angle between the fiber axis $\mathbf{f}^p$ in (S) system and the vector $\mathbf{h}^p$ in (C) system:

$$f(g) = \mathrm{N}e^{\mathrm{S}\mathrm{Cos}(\omega)}, \qquad \mathrm{Cos}(\omega) = \mathbf{h}^p{}_i \overset{CS}{\mathrm{T}}_{ij}\mathbf{f}^p{}_j. \tag{20}$$

Expressing $\overset{CS}{\mathrm{T}}$ with help of Eq. 14 we get $f(g)$ as a function of $\alpha$ introduced in Eq. 13:

$$\mathrm{Cos}(\omega) = \mathrm{Cos}(\theta_y)\mathrm{Cos}(\theta_h) + \mathrm{Sin}(\theta_y)\mathrm{Sin}(\theta_h)\mathrm{Cos}(\alpha+\delta_{fh}),$$

$$\mathrm{Cos}(\theta_h) = \mathbf{h}^p\mathbf{h},\ \mathrm{Cos}(\theta_y) = \mathbf{f}^p\mathbf{y},\ \delta_{fh} = \mathrm{ArcTan}\frac{\mathbf{f}_{pr}\mathbf{h}_{pr}}{\mathbf{f}_{pr}\mathbf{h}_{pr}\mathbf{e}_z}, \tag{21}$$

$$\mathbf{h}_{pr_i} = (\delta_{ij}-\mathbf{e}_{z_i}\mathbf{e}_{z_j})\mathrm{T}_{jk}\Big(\frac{\mathbf{h}\times\mathbf{e}_z}{1+\mathbf{h}\mathbf{e}_z}\Big)\mathbf{h}^p{}_k, \mathbf{f}_{pr_i} = (\delta_{ij}-\mathbf{e}_{z_i}\mathbf{e}_{z_j})\overset{LS}{\mathrm{T}}_{jk}\mathbf{f}^p{}_k.$$

**XSF calculation.**

The general expression for XSF has the following form:

$$\mathrm{F}_{ij}(\mathbf{h},\mathbf{y}) = \frac{\int_0^{2\pi} d\alpha\, \overset{LC}{\mathrm{T}}_{3i'}(\alpha)\overset{LC}{\mathrm{T}}_{3j'}(\alpha)\overset{LC}{\mathrm{T}}_{kk'}(\alpha)\overset{LC}{\mathrm{T}}_{ll'}(\alpha)\overset{C}{a}_{i'j'k'l'}f\big(g^{CS}(\alpha)\big)\overset{LS}{\mathrm{T}}_{ki}\overset{LS}{\mathrm{T}}_{lj}}{\int_0^{2\pi} d\alpha\, f\big(g^{CS}(\alpha)\big)}. \tag{22}$$

Here the $\overset{LS}{\mathrm{T}}$ matrices convert the stress tensor defined in (S) from (S) to (L) system; the integration over $\alpha$ takes into account contributions from all crystallites contributing to Bragg peak weighted with corresponding ODF.

If ODF depends on $\alpha$ as $e^{S\,\mathrm{Cos}(\alpha+\delta)}$ (it is true for spherical and fiber component model functions, Eq. 19 and Eq. 21) the integration can be executed analytically. Let us consider transformation of $\overset{C}{a}_{i'j'k'l'}$ with help of IR decomposition and apply Eq. 10. From Eq. 6, Eq. 13 it follows that $T^{(1)}_{nn'}(\overset{LC}{\mathbf{c}}) = T^{(1)}_{nn''}(\mathrm{Tan}(\alpha/2)\mathbf{e_z})T^{(1)}_{n''n'}(\frac{\mathbf{h}\times\mathbf{e_z}}{1+\mathbf{he_z}})$ and the only term depended on $\alpha$ can be expressed as:

$$T^{(1)}_{nn'}(\mathrm{Tan}(\alpha/2)\mathbf{e}_z) = \delta_{nn'}\,e^{-in\alpha}. \tag{23}$$

Taking into account that $\int_0^{2\pi} d\alpha\, e^{S\,\mathrm{Cos}(\alpha+\delta)-im\alpha} = 2\pi e^{im\delta} I_m(S)$, $I_m(S)$ is the modified m-th order Bessel function, we arrive at the final expression:

$$F_{ij}(\mathbf{h},\mathbf{y}) = \Big( \sum_{s=1,2} \sigma^{(s)}_{33kl}\sigma^{(s)}_{i'j'k'l'}\overset{C}{a}_{i'j'k'l'} + \sum_{d=1}^{4} \delta^{(d)m}_{33kl} \frac{I_m(S\omega)e^{im\varphi}}{I_0(S\omega)}\delta_{mm'}T^{(2)}_{m'n}\Big(\frac{\mathbf{h}\times\mathbf{e}_z}{1+\mathbf{he}_z}\Big)\delta^{(d)n}_{i'j'k'l'}\overset{C}{a}_{i'j'k'l'} + \eta^{m}_{33kl}\frac{I_m(S\omega)e^{im\varphi}}{I_0(S\omega)}\delta_{mm'}T^{(4)}_{m'n}\Big(\frac{\mathbf{h}\times\mathbf{e}_z}{1+\mathbf{he}_z}\Big)\eta^{n}_{i'j'k'l'}\overset{C}{a}_{i'j'k'l'}\Big)\overset{LS}{T}_{ki}\overset{LS}{T}_{lj}, \tag{24}$$

where $\omega = \mathrm{Cos}^2(\theta^*/2)$, $\varphi = \delta + 2\mathrm{ArcTan}(b/a)$ for spherical and $\omega = \mathrm{Sin}(\theta_y)\mathrm{Sin}(\theta_h), \varphi = \delta_{fh}$ for fiber texture model functions.

## Summary

The rotation group vector parameterization proved to be useful for treating transformations between (S), (L), (C) reference systems used in XSA, the explicit expressions are given in Eq. 12, Eq. 13 and Eq. 14. The $4^{th}$ rank elasticity tensor IR decomposition and transformation according to Eq. 10 together with utilization of explicit dependence of $\overset{LC}{c}$ and $\overset{CS}{c}$ on angle $\alpha$ describing the rotation of the crystallites contributing to Bragg peak enabled to obtain analytical expression Eq. 24 for the cases of ODF described by the spherical or fiber model functions.

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