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# Generalisation of the Vook-Witt and inverse Vook-Witt grain-interaction models to any loading state


## *Abstract*

Recently, the Vook-Witt and inverse Vook-Witt grain-interaction models have been developed and employed for the calculation of mechanical elastic constants and diffraction (X-ray) stress factors of, in particular, thin films. However, their applicability was limited to a planar, rotationally symmetric state of macroscopic, mechanical stress. For such a loading state (and an at least transversely elastically isotropic specimen), only two mechanical elastic constants suffice for describing the mechanical elastic behaviour and only the sum of two diffraction (X-ray) stress factors suffices for relating lattice strains to the single independent component of the mechanical stress tensor.

The restriction to a planar, rotationally symmetric state of mechanical stress will be lifted in this work, enabling the calculation of the full stiffness tensor and of all six diffraction (X-ray) stress factors.

The results of numerical calculations of mechanical elastic constants and diffraction (X-ray) stress factors on the basis of the Vook-Witt and inverse Vook-Witt models will be compared to corresponding results obtained employing the Eshelby-Kröner grain-interaction model considering ideal morphologic (grain-shape) textures.

## § 1. Introduction

For polycrystals, the macroscopic, mechanical elastic constants (relating mechanical strains to mechanical stresses) and the so-called diffraction (X-ray) stress factors (relating lattice strains to mechanical stresses) can be calculated from single-crystal elastic data of the individual grain composing the polycrystals. To this end, so-called elastic grain-interaction models, describing the distribution of stresses and strains over the differently oriented grains, can be employed (see, for example, Hauk 1997, Welzel and Mittemeijer, 2003).

Traditionally, so-called isotropic grain-interaction models (Welzel and Mittemeijer, 2003) are considered: in an isotropic grain-interaction model, the same grain-interaction assumptions are adopted for all directions in the specimen. A polycrystal presenting isotropic grain interaction is macroscopically elastically isotropic (sometimes termed quasi-isotropic) in the absence of crystallographic texture, whereas macroscopic elastic anisotropy occurs in the presence of crystallographic texture. The Voigt (1910), Reuss (1929), Neerfeld-Hill (Neerfeld 1942, Hill 1952) models and the Eshelby-Kröner model (for polycrystals consisting of, on the average, spherical grains, Kröner 1958) fall in this category.

However, even in the absence of crystallographic texture, polycrystals cannot generally be considered as being mechanically elastically isotropic. Thin films provide a possible example: due to their reduced dimensionality, thin films can exhibit transverse elastic isotropy (only) even in the absence of crystallographic texture. Recently, it has been demonstrated theoretically and experimentally by van Leeuwen *et al.* (1999) that the application of a new type of grain-interaction model, a so-called direction-dependent

grain-interaction model, is compatible with macroscopic anisotropic elastic behaviour even in the absence of crystallographic texture (see also Leoni *et al.* 2001 and Welzel *et al.* 2003). The notion 'direction-dependent grain interaction' signifies that different grain-interaction assumptions prevail along different directions in the specimen; in the so-called Vook-Witt model explored by van Leeuwen *et al.* (1999; cf. also Vook and Witt, 1965), as an example, a Reuss-type grain interaction (i.e. certain stress tensor components are identical for all crystallites) is adopted for the out-of-plane components of the stress tensor, whereas a Voigt-type grain interaction (i.e. certain strain tensor components are identical for all crystallites) is adopted for all in-plane components of the strain tensor. As extreme grain-interaction assumptions are adopted in the Vook-Witt model, it cannot be expected that this model is fully compatible with physical reality. To overcome this problem, the inverse Vook-Witt model, required for the construction of an effective grain-interaction model, has been recently proposed (Welzel *et al.* 2003).

In thin films, planar, rotationally symmetric states of residual stress are frequently met. However, other stress states may occur as well, in particular in cases of applied stress. So far, the Vook-Witt and inverse Vook-Witt models have only been applied for the case that the stress state is planar rotationally symmetric. This restriction will be lifted in this work by generalising the grain-interaction assumptions. This generalisation also enables the calculation of the full stiffness tensor (i.e., of five independent elastic constants) whereas previously, only two mechanical elastic constants could be calculated. Moreover, all six diffraction (X-ray) stress factors can now be calculated, whereas previously, only the sum of two diffraction stress factors was accessible.

The results obtained for mechanical elastic constants and lattice strains (diffraction stress factors) will be compared to results obtained from the Eshelby-Kröner model for morphologically textured specimens (see Koch *et al.* (2004) for a detailed discussion of the calculation scheme). In earlier studies (Welzel *et al.*, 2004) it has been shown that mechanical and diffraction elastic constants calculated employing the Vook-Witt model exhibit similarities with corresponding elastic constants calculated with the Eshelby-Kröner model for the case that flat-disk shaped grain are considered, whereas analogous similarities occur in comparing the inverse Vook-Witt model with the Eshelby-Kröner model for the case that needle shaped grain are considered. Similar findings are obtained in this work.

## *§ 2. Theoretical background*

### 2.1 Conventions

**Frames of reference and transformation of tensors from one frame of reference to another**

Stresses, strains, and elastic constants are tensorial quantities and it is thus necessary to define frames of reference. It is convenient to employ the following three Cartesian frames of reference: The crystal frame of reference (*C*), the specimen frame of reference (*S*) and the laboratory frame of reference (*L*). For details on the definition of these frames of reference, see, for example, Leoni *et al.* (2001) (for the definition of the crystal frame of reference in the case of non-cubic crystallites, see also Giacovazzo *et al.*, 1998). A superscript (*C*, *S* or *L*) will be attached to a tensor to indicate the reference frame adopted for the representation of the tensor. The absence of any superscript implies the validity of an equation independent of the reference frame used for tensor representation, but the same reference frame has to be adopted for all tensors in the equation. For the relative orientation of the specimen frame of reference and the laboratory frame of reference and a definition of the angles $\psi$ and $\varphi$, where $\psi$ is the inclination angle of the sample surface normal with respect to the diffraction vector and $\varphi$ denotes the rotation of the sample around the sample surface normal, see also Figure 1.

Transformations of tensors from one to another frame of reference can be performed employing rotation matrices. For a detailed description of the rotation matrices required for performing calculations described in this paper, see Leoni *et al.* (2001) for the case of cubic crystal symmetry and consider the Appendix of the work by Koch *et al.*

(2004) for cases of lower crystal symmetry. For a general introduction to the use of transformation matrices, see for example Hauk (1997).

**Calculation of averages**

In the following, it is useful to distinguish four types of averages of a tensor $\mathbf{\Omega}$ (as for example the strain tensor $\boldsymbol{\varepsilon}$):

- Averages of a tensor over all grains of a phase $\delta$ with a particular crystallographic orientation in the volume considered (the notion 'mesoscopic scale' is also used to denote such averages; Sprauel and Castex, 1991): this average will be denoted by the symbol $\mathbf{\Omega}_\delta(\mathbf{g})$, where $\mathbf{g}$ represents a vector in the three-dimensional crystallographic orientation (Euler) space *G* and defines the crystallographic orientation (for details, see, for example, Leoni *et al.*, 2001). $\mathbf{g} = \alpha, \beta, \gamma$ , where $\alpha$, $\beta$ and $\gamma$ are three Euler angles. The convention of Roe & Krigbaum (1964) for the definition of the Euler angles will be adopted (see also Leoni *et al.*, 2001). The phase indication will be omitted if an equation applies to all phases.
- Averages over all crystallographically differently oriented grains in the volume considered (so-called macroscopic, mechanical averages) this average will be denoted by angular brackets $\langle \mathbf{\Omega} \rangle$ and can be calculated as follows:

$$\langle \mathbf{\Omega} \rangle = \frac{1}{8\pi^2} \int_G \mathrm{f}(\mathbf{g}) \mathbf{\Omega}(\mathbf{g}) \; \mathrm{d}^3\mathrm{g} \,. \qquad (1)$$

where $\mathrm{f}(\mathbf{g})$, the crystallographic orientation distribution function (CODF), has to be employed as a weighing function in the case that crystallographic texture

occurs (Leoni et al., 2001). The factor $1/\left(8\pi^2\right)$ serves as a normalisation factor and is the volume of the Euler space $G$.

- Averages of a tensor over all grains of a phase $\delta$ (the notion 'pseudo-macroscopic scale' is also used to denote such averages (Noyan and Cohen, 1987; Sprauel and Castex, 1991): this average will be denoted by the symbol $\langle \mathbf{\Omega} \rangle_\delta$ and can be calculated as follows:

$$\langle \mathbf{\Omega} \rangle_\delta = \frac{1}{8\pi^2} \int_G \mathrm{f}\left(\mathbf{g}\right) \mathbf{\Omega}_\delta \;\; \mathrm{d}^3\mathrm{g} \tag{2}$$

- For diffraction averages of a phase $\delta$ only the diffracting crystallites have to be taken into account. As the orientation of the diffracting crystallites differs only by a rotation around the diffraction vector, the averaging has to be performed with respect to this degree of freedom, in the following called $\lambda$ (see, for example. Leoni *et al.* 2001):

$$^{hkl}\left\{\mathbf{\Omega}\right\}_\delta^{\varphi,\psi} = \frac{\int_0^{2\pi} \mathbf{\Omega}_\delta(hkl,\lambda,\varphi,\psi) \;\; f^*(hkl,\lambda,\varphi,\psi) d\lambda}{\int_0^{2\pi} f^*(hkl,\lambda,\varphi,\psi) d\lambda}. \tag{3}$$

$f^*(hkl,\lambda,\varphi,\psi)$ denotes the representation of the ODF in terms of the measurement parameters and the rotation angle with respect to the diffraction vector. The ODF as used in equation (2) cannot be directly used in equation (3) since the angles $\lambda,\varphi,\psi$ are *not* Euler angles representing a rotation of the *C* system with respect to the *S* system (they provide the rotation of the system *L* with respect to the system *S*). However, the values of $\alpha$, $\beta$, $\gamma$ and thus $f(\alpha,\beta,\gamma)$ at

every $\lambda$ can be calculated from *hkl*, $\lambda$, $\varphi$ and $\psi$, to be finally substituted for $f^*(hkl,\lambda,\varphi,\psi)$ in equation (3) (for a more detailed treatment of the necessary calculations, see Leoni *et al.* 2001).

## Lattice strains and diffraction stress factors

The diffraction strain measured for a particular reflection *hkl* at the orientation of the diffraction vector ($\varphi,\psi$) can be calculated according to (cf. equation (3)):

$$\varepsilon_\delta\left(hkl,\varphi,\psi\right) = {}^{hkl}\left\{\boldsymbol{\varepsilon}_{33}^{L}\right\}_\delta^{\varphi,\psi} = \frac{\int_0^{2\pi}\left(\boldsymbol{\varepsilon}_{33}^{L}\right)_\delta(hkl,\lambda,\varphi,\psi)\,f^*(hkl,\lambda,\varphi,\psi)d\lambda}{\int_0^{2\pi} f^*(hkl,\lambda,\varphi,\psi)d\lambda}. \qquad (4)$$

The $\varphi$, $\psi$ and *hkl*-dependent X-ray stress factors of the phase $\delta$, $F_{ij}^{\delta}(\psi,\varphi,hkl)$, relate the diffraction strain to mechanical stress expressed in the specimen frame of reference (the Einstein convention, i.e. summation over indices appearing twice in a formula, is adopted throughout the paper):

$$\varepsilon_\delta\left(hkl,\varphi,\psi\right) = F_{ij}^{\delta}(\psi,\varphi,hkl)\left\langle\boldsymbol{\sigma}_{ij}^{S}\right\rangle_\delta. \qquad (5)$$

Note that the $F_{ij}^{\delta}(\psi,\varphi,hkl)$ are not components of a tensor since they relate the lattice strain (a number) to the stress tensor (expressed in the *S*-system).

## Grain-shape / morphological texture

For the calculation of mechanical and diffraction elastic constants of polycrystals with a grain-shape texture employing the Eshelby-Kröner model, the treatment will be restricted

to polycrystals consisting of ellipsoidal grains[1]. It will be assumed that the ellipsoidal grains exhibit identical orientations of their principal axes in the specimen frame of reference, i.e. the ellipsoidal grains are aligned along common axes (an ideal grain-shape texture occurs). Only an ideal grain-shape texture is considered in the following, as only in this case unique mechanical elastic constants and X-ray stress factors can be calculated employing the Eshelby-Kröner model (for a more detailed discussion of the effect of a non-ideal morphological texture, see Koch *et al.*, 2004).

Note that the principal axes of a grain are only related to the *external* (geometrical) shape of the grain. Thereby nothing is prescribed regarding the crystallographic orientation of the grain (crystallite). In general, the (ellipsoidal) grains constituting the specimen will have different crystallographic orientations.

The shape of the grains will be described by a shape parameter $\eta$, which is defined as the ratio of the principal axis of the ellipsoid in the z-direction ($a_3$) of the specimen frame of reference to the principal axes of the ellipsoid in the x-direction ($a_1$) and the y-direction ($a_2$) in the specimen frame of reference, respectively:

$$\eta = \frac{a_3}{a_1} = \frac{a_3}{a_2} \tag{6}$$

Thus, the considered ellipsoidal grains present rotational symmetry with respect to the surface normal of the specimen.

[1] Of course, a real polycrystal cannot consist of ellispoidal grains (only). The ellipsoidal shape is an idealised shape, which is adopted in order to represent grains with (average) aspect ratios different from one, whereas a spherical shape is adopted for grains with an (average) aspect ratio of one.

## § 3. Generalisation of the Vook-Witt and inverse Vook-Witt models

### 3.1 The Vook-Witt model; grain-interaction assumptions

Traditionally, an at least transversely elastically isotropic specimen and a planar, rotationally symmetric state of stress are considered:

$$\left\langle \boldsymbol{\varepsilon}^s \right\rangle = \begin{pmatrix} \boldsymbol{\varepsilon}_{\|}^S & 0 & 0 \\ 0 & \boldsymbol{\varepsilon}_{\|}^S & 0 \\ 0 & 0 & \boldsymbol{\varepsilon}_{\|}^S \end{pmatrix}, \left\langle \boldsymbol{\sigma}^s \right\rangle = \begin{pmatrix} \boldsymbol{\sigma}_{\|}^s & 0 & 0 \\ 0 & \boldsymbol{\sigma}_{\|}^s & 0 \\ 0 & 0 & 0 \end{pmatrix} \qquad (7), (8)$$

The following grain-interaction assumptions are usually adopted: (i) the strain is rotationally symmetric in the plane of the film and (ii) equal for all crystallites and (iii) the stresses perpendicular to the layer are zero for all crystallites, i.e. the crystallites can deform freely in this direction. These assumptions fix parts of the stress and strain tensor for all crystallites:

$$\boldsymbol{\varepsilon}^s = \begin{pmatrix} \boldsymbol{\varepsilon}_{\|}^s & 0 & \Diamond \\ 0 & \boldsymbol{\varepsilon}_{\|}^s & \Diamond \\ \Diamond & \Diamond & \Diamond \end{pmatrix}, \boldsymbol{\sigma}^s = \begin{pmatrix} \Diamond & \Diamond & 0 \\ \Diamond & \Diamond & 0 \\ 0 & 0 & 0 \end{pmatrix}. \qquad (9),(10)$$

The tensor components marked by $\Diamond$ are not explicitly specified for every crystallite, but these components can be calculated from Hooke's law for every crystallite:

$$\boldsymbol{\varepsilon}_{ij}^S = \mathbf{s}_{ijkl}^S \boldsymbol{\sigma}_{kl}^S \qquad (11)$$

The $\mathbf{s}_{ijkl}^S$ are the single crystal elastic compliances expressed in the specimen frame of reference. Equation (11) represents a system of nine equations for eighteen unknowns, but as the strain and stress tensors are symmetric (i.e. $\boldsymbol{\varepsilon}_{ij} = \boldsymbol{\varepsilon}_{ji}$ and $\boldsymbol{\sigma}_{ij} = \boldsymbol{\sigma}_{ji}$), equation (11) is a short notation for six independent equations for twelve independent unknowns.

If six components of the twelve unknowns are known, as a consequence, the other components can be calculated by solving the system of equations (11).

In the following, it will still be assumed that the specimen is at least transversely elastically isotropic, but the restrictions with respect to the mechanical loading state will be lifted. A generalisation of the Vook-Witt model to arbitrary loading states can be achieved by adopting the following grain-interaction assumptions:

$$\boldsymbol{\varepsilon}^S = \begin{pmatrix} \langle \boldsymbol{\varepsilon}_{11}^S \rangle & \langle \boldsymbol{\varepsilon}_{12}^S \rangle & \Diamond \\ \langle \boldsymbol{\varepsilon}_{12}^S \rangle & \langle \boldsymbol{\varepsilon}_{22}^S \rangle & \Diamond \\ \Diamond & \Diamond & \Diamond \end{pmatrix}, \qquad \boldsymbol{\sigma}^s = \begin{pmatrix} \Diamond & \Diamond & \langle \boldsymbol{\sigma}_{13}^S \rangle \\ \Diamond & \Diamond & \langle \boldsymbol{\sigma}_{23}^S \rangle \\ \langle \boldsymbol{\sigma}_{13}^S \rangle & \langle \boldsymbol{\sigma}_{23}^S \rangle & \langle \boldsymbol{\sigma}_{33}^S \rangle \end{pmatrix}. \qquad (12),(13)$$

The tensor components marked by $\Diamond$ are not explicitly specified for every crystallite, but these components can be calculated from Hooke's law for every crystallite, equation (11) (see Appendix).

## 3.2 The inverse Vook-Witt model; grain-interaction assumptions

In the inverse Vook-Witt model, the traditionally adopted grain-interaction assumptions for a transversely isotropic film subjected to a plane, rotationally symmetric state of stress are as follows: (i) the in-plane stress is rotationally symmetric and (ii) equal for all crystallites and (iii) the strain perpendicular to the film surface is equal for all crystallites. Like in the (regular) Vook-Witt model, these assumptions fix certain strain and stress tensor components for all crystallites:

$$\boldsymbol{\varepsilon}^S = \begin{pmatrix} \Diamond & \Diamond & 0 \\ \Diamond & \Diamond & 0 \\ 0 & 0 & \boldsymbol{\varepsilon}_{\perp}^S \end{pmatrix}, \qquad \boldsymbol{\sigma}^S = \begin{pmatrix} \boldsymbol{\sigma}_{\parallel}^S & 0 & \Diamond \\ 0 & \boldsymbol{\sigma}_{\parallel}^S & \Diamond \\ \Diamond & \Diamond & \Diamond \end{pmatrix}. \qquad (14),(15)$$

The missing strain and stress tensor components for each crystallite, marked by $\Diamond$, can be calculated from Hooke's law analogous to the Vook-Witt model (cf. discussion in Section 2.2.1 above).

In the following, it will still be assumed that the specimen is at least transversely elastically isotropic, but the restrictions with respect to the mechanical loading state will be lifted. A generalisation of the inverse Vook-Witt model to arbitrary loading states can be achieved by adopting the following grain-interaction assumptions:

$$\boldsymbol{\varepsilon}^S = \begin{pmatrix} \Diamond & \Diamond & \left\langle \boldsymbol{\varepsilon}_{13}^S \right\rangle \\ \Diamond & \Diamond & \left\langle \boldsymbol{\varepsilon}_{23}^S \right\rangle \\ \left\langle \boldsymbol{\varepsilon}_{13}^S \right\rangle & \left\langle \boldsymbol{\varepsilon}_{23}^S \right\rangle & \left\langle \boldsymbol{\varepsilon}_{33}^S \right\rangle \end{pmatrix}, \quad \boldsymbol{\sigma}^S = \begin{pmatrix} \left\langle \boldsymbol{\sigma}_{11}^S \right\rangle & \left\langle \boldsymbol{\sigma}_{12}^S \right\rangle \Diamond & \Diamond \\ \left\langle \boldsymbol{\sigma}_{12}^S \right\rangle & \left\langle \boldsymbol{\sigma}_{22}^S \right\rangle \Diamond & \Diamond \\ \Diamond & \Diamond & \Diamond \end{pmatrix}. \qquad (16),(17)$$

The tensor components marked by $\Diamond$ are not explicitly specified for every crystallite, but these components can be calculated from Hooke's law for every crystallite, equation (11) (see Appendix).

## 3.3 Calculation of the mechanical elastic constants

In thin films, plane, rotationally symmetric states of mechanical stress are frequently met (cf. equations (7), (8)). Under such loading conditions, which were so far considered for the Vook-Witt and the inverse Vook-Witt models, two mechanical elastic constants A and B suffice, as only three independent non-zero stress and strain tensor components occur:

$$\boldsymbol{\varepsilon}_{\parallel}^S = A\boldsymbol{\sigma}_{\parallel}^S , \qquad (18)$$

$$\boldsymbol{\varepsilon}_{\perp}^S = B\boldsymbol{\sigma}_{\parallel}^S . \qquad (19)$$

A calculation of the full mechanical stiffness tensor is possible by considering a set of different hypothetical mechanical loading states as follows:

(i) uniaxial strain along the $S_1$-axis:

$$\left\langle \boldsymbol{\varepsilon}^S \right\rangle = \begin{pmatrix} \boldsymbol{\varepsilon}_1^S & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \left\langle \boldsymbol{\sigma}^S \right\rangle = \begin{pmatrix} \boldsymbol{\sigma}_1^S & 0 & 0 \\ 0 & \boldsymbol{\sigma}_2^S & 0 \\ 0 & 0 & \boldsymbol{\sigma}_3^S \end{pmatrix} . \qquad (20), (21)$$

For the Vook-Witt model, the grain-interaction assumptions read,

$$\boldsymbol{\varepsilon}^S = \begin{pmatrix} \boldsymbol{\varepsilon}_1^S & 0 & \Diamond \\ 0 & 0 & \Diamond \\ \Diamond & \Diamond & \Diamond \end{pmatrix}, \boldsymbol{\sigma}^s = \begin{pmatrix} \Diamond & \Diamond & 0 \\ \Diamond & \Diamond & 0 \\ 0 & 0 & \boldsymbol{\sigma}_3^S \end{pmatrix} . \qquad (22), (23)$$

To ensure that $\left\langle \boldsymbol{\varepsilon}_{33}^S \right\rangle = 0$ the following procedure can be followed: starting from arbitrary values for the strain $\boldsymbol{\varepsilon}_1^S$ and $\boldsymbol{\sigma}_3^S$, the mechanical averages of the strain and stress tensors can be calculated. In general, the strain perpendicular to the surface, $\left\langle \boldsymbol{\varepsilon}_{33}^S \right\rangle$ , will then not be zero. However, by changing the mechanical stress perpendicular to the surface $\boldsymbol{\sigma}_3^S = \left\langle \boldsymbol{\sigma}_{33}^S \right\rangle$ (keeping $\boldsymbol{\varepsilon}_1^S$ fixed), $\left\langle \boldsymbol{\varepsilon}_{33}^S \right\rangle$ can be made zero, so that a uniaxial strain state is achieved. To this end, the above described calculation has to be repeated for another value $\boldsymbol{\sigma}_3^S$. As $\left\langle \boldsymbol{\varepsilon}_{33}^S \right\rangle$ is linearly related to $\boldsymbol{\sigma}_3^S$,

$$\left\langle \boldsymbol{\varepsilon}_{33}^S \right\rangle = m \cdot \boldsymbol{\sigma}_3^S + c \qquad (24)$$

The stress making $\left\langle \boldsymbol{\varepsilon}_{33}^S \right\rangle$ equal to zero can be determined from equation (24) once the constants *m* and *c* have been calculated from the two (arbitrary) values of the stress

$\left(\boldsymbol{\sigma}_3^S\right)_1$, $\left(\boldsymbol{\sigma}_3^S\right)_2$ and the corresponding stresses perpendicular to the film surface $\left\langle \boldsymbol{\varepsilon}_{33}^S \right\rangle_1$ and $\left\langle \boldsymbol{\varepsilon}_{33}^S \right\rangle_2$.

For the inverse Vook-Witt model, the grain-interaction assumptions read:

$$\boldsymbol{\varepsilon}^s = \begin{pmatrix} \Diamond & \Diamond & 0 \\ \Diamond & \Diamond & 0 \\ 0 & 0 & 0 \end{pmatrix}, \ \boldsymbol{\sigma}^s = \begin{pmatrix} \boldsymbol{\sigma}_1^S & 0 & \Diamond \\ 0 & \boldsymbol{\sigma}_2^S & \Diamond \\ \Diamond & \Diamond & \Diamond \end{pmatrix}. \qquad (25), (26)$$

To ensure that $\left\langle \boldsymbol{\varepsilon}_{22}^S \right\rangle = 0$, a procedure analogous to the procedure described below equations (22) and (23) can be followed in order to find an appropriate value for $\sigma_2^s$.

Once a mechanical loading state specified in equations (20) and (21) has been achieved, three components of the reduced stiffness tensor can be calculated from:

$$\mathbf{C}_{11}^S = \boldsymbol{\sigma}_1^s / \boldsymbol{\varepsilon}_1^s, \ \mathbf{C}_{12}^S = \boldsymbol{\sigma}_2^S / \boldsymbol{\varepsilon}_1^S, \ \mathbf{C}_{13}^S = \boldsymbol{\sigma}_3^S / \boldsymbol{\varepsilon}_1^S. \qquad (27),(28),(29)$$

(ii) Uniaxial strain along the $S_3$-axis:

$$\left\langle \boldsymbol{\varepsilon}^S \right\rangle = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \boldsymbol{\varepsilon}_3^S \end{pmatrix}, \ \left\langle \boldsymbol{\sigma}^S \right\rangle = \begin{pmatrix} \boldsymbol{\sigma}_1^S & 0 & 0 \\ 0 & \boldsymbol{\sigma}_1^S & 0 \\ 0 & 0 & \boldsymbol{\sigma}_3^S \end{pmatrix}. \qquad (30), (31)$$

For the Vook-Witt model, the grain-interaction assumptions read,

$$\boldsymbol{\varepsilon}^S = \begin{pmatrix} 0 & 0 & \Diamond \\ 0 & 0 & \Diamond \\ \Diamond & \Diamond & \Diamond \end{pmatrix}, \ \boldsymbol{\sigma}^S = \begin{pmatrix} \Diamond & \Diamond & 0 \\ \Diamond & \Diamond & 0 \\ 0 & 0 & \boldsymbol{\sigma}_3^S \end{pmatrix}. \qquad (32), (33)$$

whereas for the inverse Vook-Witt model, the grain-interaction assumptions read:

$$\boldsymbol{\varepsilon}^S = \begin{pmatrix} \Diamond & \Diamond & 0 \\ \Diamond & \Diamond & 0 \\ 0 & 0 & \boldsymbol{\varepsilon}_3^S \end{pmatrix}, \ \boldsymbol{\sigma}^S = \begin{pmatrix} \boldsymbol{\sigma}_1^S & 0 & \Diamond \\ 0 & \boldsymbol{\sigma}_1^S & \Diamond \\ \Diamond & \Diamond & \Diamond \end{pmatrix}. \qquad (34), (35)$$

For the inverse Vook-Witt model, to ensure that $\left\langle \boldsymbol{\varepsilon}_{11}^{S} \right\rangle = \left\langle \boldsymbol{\varepsilon}_{22}^{S} \right\rangle = 0$, a procedure analogous to the procedure described below equations (22) and (23) can be followed in order to find an appropriate value for $\sigma_1^s$ (note that no such procedure is required for the Vook-Witt model for the loading state considered). Once a mechanical loading state specified in equations (30) and (31) has been achieved, two components of the reduced stiffness tensor can be calculated from:

$$\mathbf{C}_{13}^{S} = \boldsymbol{\sigma}_1^S / \boldsymbol{\varepsilon}_3^S, \ \mathbf{C}_{33}^{S} = \boldsymbol{\sigma}_3^S / \boldsymbol{\varepsilon}_3^S . \qquad (36),(37)$$

(iii) pure shear-strain loading:

$$\left\langle \boldsymbol{\varepsilon}^S \right\rangle = \begin{pmatrix} 0 & \boldsymbol{\varepsilon}_{s1}^S & 0 \\ \boldsymbol{\varepsilon}_{s1}^S & 0 & \boldsymbol{\varepsilon}_{s2}^S \\ 0 & \boldsymbol{\varepsilon}_{s2}^S & 0 \end{pmatrix}, \ \left\langle \boldsymbol{\sigma}^S \right\rangle = \begin{pmatrix} 0 & \boldsymbol{\sigma}_{s1}^S & 0 \\ \boldsymbol{\sigma}_{s1}^S & 0 & \boldsymbol{\sigma}_{s2}^S \\ 0 & \boldsymbol{\sigma}_{s2}^S & 0 \end{pmatrix}. \qquad (38), (39)$$

For the Vook-Witt model, the grain-interaction assumptions read,

$$\boldsymbol{\varepsilon}^S = \begin{pmatrix} 0 & \boldsymbol{\varepsilon}_{s1}^S & \Diamond \\ \boldsymbol{\varepsilon}_{s1}^S & 0 & \Diamond \\ \Diamond & \Diamond & \Diamond \end{pmatrix}, \ \boldsymbol{\sigma}^S = \begin{pmatrix} \Diamond & \Diamond & 0 \\ \Diamond & \Diamond & \boldsymbol{\sigma}_{s2}^S \\ 0 & \boldsymbol{\sigma}_{s2}^S & 0 \end{pmatrix}. \qquad (40), (41)$$

To ensure that $\left\langle \boldsymbol{\varepsilon}_{33}^S \right\rangle = 0$, a procedure analogous to the procedure described below equations (22) and (23) can be followed in order to find an appropriate value for $\boldsymbol{\sigma}_{s2}^S$.

For the inverse Vook-Witt model, the grain-interaction assumptions read:

$$\boldsymbol{\varepsilon}^S = \begin{pmatrix} \Diamond & \Diamond & 0 \\ \Diamond & \Diamond & \boldsymbol{\varepsilon}_{s2}^S \\ 0 & \boldsymbol{\varepsilon}_{s2}^S & 0 \end{pmatrix}, \ \boldsymbol{\sigma}^S = \begin{pmatrix} 0 & \boldsymbol{\sigma}_{s1}^S & \Diamond \\ \boldsymbol{\sigma}_{s1}^S & 0 & \Diamond \\ \Diamond & \Diamond & \Diamond \end{pmatrix}. \qquad (42), (43)$$

To ensure that $\left\langle \boldsymbol{\varepsilon}_{11}^S \right\rangle = \left\langle \boldsymbol{\varepsilon}_{22}^S \right\rangle = 0$, a procedure analogous to the procedure described below equations (22) and (23) can be followed in order to find an appropriate value for $\boldsymbol{\sigma}_{s1}^S$.

Once a mechanical loading state specified in equations (38) and (39) has been achieved, two components of the reduced stiffness tensor can be calculated from:

$$\mathbf{C}_{44}^{S} = \boldsymbol{\sigma}_{\mathbf{s}2}^{S} / 2\boldsymbol{\varepsilon}_{\mathbf{s}2}^{S}\,,\ \mathbf{C}_{66}^{S} = \boldsymbol{\sigma}_{\mathbf{s}1}^{s} / \boldsymbol{\varepsilon}_{\mathbf{s}1}^{s}\,. \qquad (44),(45)$$

Note that other sets of hypothetical loading states can be conceived, which also allow the evaluation of all components of the stiffness tensor.

## 3.4 Calculation of lattice strains and diffraction stress factors

Lattice strains can, in principle, be straightforwardly calculated following equation (4). In the following, a procedure will be outlined for calculating lattice strains for a given mechanical state of stress $\left\langle \boldsymbol{\sigma}^{S} \right\rangle$.

(i) The mechanical elastic constants, i.e. the full stiffness tensor and its inverse, the mechanical compliance tensor $\mathbf{S}$, should be calculated first following the procedure outlined in Section 3.3.

(ii) From the mechanical stress tensor $\left\langle \boldsymbol{\sigma}^{S} \right\rangle$ the full mechanical strain tensor $\left\langle \boldsymbol{\varepsilon}^{S} \right\rangle$ can be calculated from Hooke's law:

$$\left\langle \boldsymbol{\varepsilon}^{S} \right\rangle = \mathbf{S} \left\langle \boldsymbol{\sigma}^{S} \right\rangle . \qquad (46)$$

(iii) Employing the grain-interaction assumptions (cf. equations (12), (13) for the Vook-Witt model and equations (16) and (17) for the inverse Vook-Witt model), the strain tensor $\boldsymbol{\varepsilon}^{S}(\mathbf{g})$ and its projection on the diffraction vector (i.e. $\boldsymbol{\varepsilon}_{33}^{L}(\mathbf{g})$) can be calculated.

(iv) The diffraction stress factors, if at all required, can be obtained by imposing simple mechanical stress states, where only one stress tensor component is non-zero from:

$$F_{ij}(\psi,\varphi,hkl) = \varepsilon(\psi,\varphi,hkl) \;/\; \left\langle \boldsymbol{\sigma}_{ij}^{S} \right\rangle . \tag{47}$$

## *4. Results and discussion*

Mechanical and diffraction elastic constants of polycrystals are presented in the following. Single-crystal elastic data of materials employed in the calculations have been listed in Table 1. For cubic crystallites, an anisotropy factor $A_i$ can be defined as:

$$A_i = \frac{s_{11}^C - s_{12}^C}{2s_{44}^C} = \frac{2c_{44}^C}{c_{11}^C - c_{12}^C} \tag{48}$$

$A_i < 1$ indicates that the <*hhh*> direction is softer than the <00*l*> direction, whereas $A_i > 1$ indicates that the <*hhh*> direction is stiffer than the <00*l*> direction. Values for $A_i$ have also been given in Table 1.

### 4.1 Mechanical elastic constants

**TUNGSTEN**

The components of the mechanical stiffness tensor of a tungsten polycrystal, as calculated according to the Vook-Witt model, inverse Vook-Witt model and Eshelby-Kröner model involving two extreme grain morphologies (flat-disk shaped grains, $\eta = 0.1$, and needle-shaped grains, $\eta = 10$) have been gathered in Table 2.

[Insert Table 2 about here]

Tungsten is an intrinsically (practically) elastically isotropic material. As a consequence, the mechanical elastic properties are insensitive to the grain interaction. Hence, the same isotropic mechanical stiffness tensor is obtained for all types of grain-interaction.

**COPPER AND IRON**

The components of the mechanical stiffness tensor of copper and iron polycrystals, as calculated according to the Vook-Witt model, inverse Vook-Witt model and Eshelby-Kröner model involving two extreme grain morphologies (flat-disk shaped grains, $\eta = 0.1$, and needle-shaped grains, $\eta = 10$) have been gathered in Tables 3 and 4.

[Insert Tables 3 & 4 about here]

Copper and iron exhibit pronounced single-crystal elastic anisotropy and as a consequence, the components of the mechanical stiffness tensor are also sensitive to grain interaction. For the Eshelby-Kröner model with a spherical grain shape ($\eta = 1$), an obviously isotropic stiffness tensor, with only two independent components ($\mathbf{C}_{11}^{S}, \mathbf{C}_{12}^{S}$), is obtained. It holds that:

$$\mathbf{C}_{44}^{S} = \tfrac{1}{2}\ \mathbf{C}_{11}^{S} - \mathbf{C}_{12}^{S} \quad , \tag{49}$$

thus $\mathbf{C}_{44}^{S}$ is not an independent component in this case.

For the Vook-Witt and inverse Vook-Witt models, transverse elastic isotropy occurs and in this case the macroscopic stiffness tensor consists of five independent components ($\mathbf{C}_{11}^{S}, \mathbf{C}_{12}^{S}, \mathbf{C}_{13}^{S}, \mathbf{C}_{33}^{S}, \mathbf{C}_{44}^{S}$). The transverse isotropy reflects the rotational symmetry of the grain-interaction assumptions (cf. equations (12), (13) for the Vook-witt model and equations (16), (17) for the inverse Vook-Witt model).

Also for non-spherical shapes ($\eta \neq 1$), transverse elastic isotropy occurs. The transverse isotropy reflects the rotational symmetry of the grain-shape texture with respect to the surface normal of the specimen. Hence, an isotropic grain interaction

occurs for the case of spherical inclusions, but a direction-dependent grain interaction occurs if a grain-shape texture is present.

As the grain shape approaches the limit of a flat-disk shaped grains $\eta \to 0$ , the components of the stiffness tensor tend to the corresponding VW values, whereas in the limit of needle-shaped grains $\eta \to \infty$ , the components tend towards the corresponding iVW values. These findings can be summarised as follows:

$$\lim_{\eta \to 0} \mathbf{C}^S{}_{EK} \approx \mathbf{C}^S{}_{VW} , \tag{50}$$

$$\lim_{\eta \to \infty} \mathbf{C}^S{}_{EK} \approx \mathbf{C}^S{}_{iVW} . \tag{51}$$

Subscripts have been attached to the stiffness tensor in order to specify the grain-interaction model. The symbol '$\simeq$' ('approximately equal') has been preferred over the symbol '=' in order to express that no convergence in the strict mathematical sense occurs. Similar (numerical) findings have been obtained in an earlier work and also a mathematical explanation and an explanation based on intuition of these similarities has been given (see Welzel *et al.*, 2004).

## 4.2 Diffraction (X-ray) stress factors

The effect of the grain shape on the diffraction (X-ray) stress factors will be demonstrated in the following using plots of $\varepsilon\left(hkl,\varphi,\psi\right)$ versus $\sin^2\psi$ (so-called $\sin^2\psi$-plots) assuming that the polycrystal considered is subjected to a uniaxial state of stress:

$$\left\langle \boldsymbol{\sigma}^S \right\rangle = \begin{pmatrix} \boldsymbol{\sigma}_{11} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{52}$$

with $\boldsymbol{\sigma}_{11} = 100\text{MPa}$. In this case, equation (5) can be simplified to

$$\varepsilon\ \left(hkl, \varphi, \psi\right) = \left(F_{11}\left(\varphi, \psi, hkl\right)\right)\boldsymbol{\sigma}_{11}. \tag{53}$$

For the plots, the angle $\varphi$ will be set to zero.

## TUNGSTEN

A $\sin^2\psi$-plot for a tungsten polycrystal is shown in figure 2.

[Insert figure 2 about here]

The same straight line obtained in the $\sin^2\psi$-plot is independent of the type of grain interaction or *hkl* reflection chosen. This is a consequence of the intrinsic elastic isotropy, which makes the diffraction stress factors (as well as the mechanical elastic constants; cf. Section 4.1) insensitive to grain interaction.

## COPPER AND IRON

Figures 3and 4 gather $\sin^2\psi$-plots calculated according to the VW, iVW and EK (for morphological textures with $\eta = 0.1$ and $\eta = 10$, cf. Section 2) models for crystallographically untextured copper and iron polycrystals subjected to uniaxial states of stress (100MPa).

[Insert figure 3 and 4 about here]

For spherical grain shape, linear $\sin^2\psi$-plots are obtained for all reflections, reflecting the occurrence of macroscopic/mechanical isotropy. However, for the case of the Vook-Witt model, inverse Vook-Witt model and a grain-shape texture, distinct curvature occurs in the $\sin^2\psi$-plots, most pronouncedly for the 200 reflections. Figures 3 and 4 also demonstrate that the effect of the grain-interaction on the diffraction elastic

constants can be stronger than the effect on the mechanical elastic constants (cf. Section 4.1).

The occurrence of non-linear $\sin^2\psi$-plots corresponds to the occurrence of macroscopic elastic anisotropy. This is well known in the context of the diffraction stress analysis of crystallographically textured specimens, where the occurrence of texture leads to mechanical anisotropy and non-linear $\sin^2\psi$-plots. It was shown very recently by Welzel and Mittemeijer (2003) that non-linear $\sin^2\psi$-plots could occur in general for macroscopically elastically anisotropic specimens, independent of the occurrence of crystallographic texture.

Striking similarities among the $\sin^2\psi$-plots calculated with the different grain-interaction models can be observed: the Vook-Witt model results in similar $\sin^2\psi$-plots as the EK model for flat-disk shaped grains ($\eta = 0.1$), whereas the $\sin^2\psi$-plots obtained from the inverse Vook-Witt model exhibit similarities with the corresponding plots obtained from the Eshelby-Kröner model for needle-shaped inclusions ($\eta = 10$). These findings parallel the results obtained for the mechanical elastic constants (cf. Section 4.1). Similar (numerical) findings have been obtained in an earlier work and also a mathematical explanation and an explanation based on intuition of these similarities has been given (see Welzel *et al.*, 2004).

## *5. Summary*

- Generalisations of the grain-interaction assumptions of the Vook-Witt and inverse Vook-Witt models allow the calculation of the full mechanical stiffness (and compliance) tensors and of all diffraction stress factors, whereas previously only two mechanical elastic constants and only the sum of two diffraction (X-ray) could have been calculated.
- The direction-dependent grain-interaction assumptions employed in the Vook-Witt and inverse Vook-Witt models are reflected by the occurrence of transverse isotropy for the mechanical compliance tensor, i.e. five independent components occur. The effect of the elastic grain interaction on the mechanical elastic constants is generally weak.
- The direction-dependent grain-interaction assumptions employed in the Vook-Witt and inverse Vook-Witt models are also reflected by the occurrence of non-linear $\sin^2\psi$-plots.
- The effect of elastic grain interaction on the diffraction stress factors can be large: distinct curvature can occur in $\sin^2\psi$-plots, as has been demonstrated for the case of a uniaxial stress state. Diffraction stress analysis is therefore a sensitive tool to investigate elastic grain interaction.
- The mechanical elastic constants and diffraction stress factors (represented in the form of $\sin^2\psi$-plots) have been compared with corresponding values calculated employing the Eshelby-Kröner model considering a morphological (grain-shape) texture: Similarities among the Vook-Witt and the Eshelby-Kröner models occur for

the case that a polycrystal consisting of needle-shaped grains with their principal axes aligned along common directions in the specimen is considered for the Eshelby-Kröner model. These similarities concern the diffraction and mechanical elastic constants. Such similarities among the inverse Vook-Witt and the Eshelby-Kröner model also occur for the case that a polycrystal consisting of flat disk-shaped grains with their principal axes aligned along common directions in the specimen is considered for the Eshelby-Kröner model. These findings are in line with previously obtained results ().

- Even though the Vook-Witt and inverse Vook-Witt models have been developed in order to deal with the effect of elastic surface anisotropy of bulk polycrystals and thin films, they are capable of modelling the effect of an ideal morphological texture on the elastic grain-interaction. In this context, they can be used as substitutes for the mathematically much more tedious Eshelby-Kröner model.

Welzel, U., **Fréour, S.** (2007) Extension of the Vook-Witt and inverse Vook-Witt elastic grain-interaction models to general loading states, *Philosophical Magazine*, **87**, 3921-3943.

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## *Appendix*

### Vook-Witt model

From the stress and strain tensor components equal to the mechanical averages (cf. equations (12), (13)), the unknown components can be calculated as follows:

After defining the vector $\mathbf{x}$ of which the components are the unknown components of the stress tensor $\boldsymbol{\sigma}^S$:

$$\mathbf{x} = \begin{pmatrix} \boldsymbol{\sigma}_{11}^S \\ \boldsymbol{\sigma}_{12}^S \\ \boldsymbol{\sigma}_{22}^S \end{pmatrix}, \tag{A1}$$

the unknown stress tensor components ($\boldsymbol{\sigma}_{11}^S, \boldsymbol{\sigma}_{12}^S, \boldsymbol{\sigma}_{22}^S$) can be obtained from:

$$\mathbf{x} = \mathbf{A}^{-1}\mathbf{b} \tag{A2}$$

with:

$$\mathbf{A}_{11} = 1 - \mathbf{c}_{1133}^S \mathbf{s}_{3311}^S - 4\mathbf{c}_{1113}^S \mathbf{s}_{1311}^S - 4\mathbf{c}_{1123}^S \mathbf{s}_{2311}^S \tag{A3}$$

$$\mathbf{A}_{12} = -2\mathbf{c}_{1133}^S \mathbf{s}_{3312}^S - 4\mathbf{c}_{1113}^S \mathbf{s}_{1312}^S - 4\mathbf{c}_{1123}^S \mathbf{s}_{2312}^S \tag{A4}$$

$$\mathbf{A}_{13} = -\mathbf{c}_{1133}^S \mathbf{s}_{3322}^S - 2\mathbf{c}_{1113}^S \mathbf{s}_{1322}^S - 2\mathbf{c}_{1123}^S \mathbf{s}_{2322}^S \tag{A5}$$

$$\mathbf{A}_{21} = -\mathbf{c}_{1233}^S \mathbf{s}_{3311}^S - 4\mathbf{c}_{1213}^S \mathbf{s}_{1311}^S - 4\mathbf{c}_{1223}^S \mathbf{s}_{2311}^S \tag{A6}$$

$$\mathbf{A}_{22} = 1 - 2\mathbf{c}_{1233}^S \mathbf{s}_{3312}^S - 4\mathbf{c}_{1213}^S \mathbf{s}_{1312}^S - 4\mathbf{c}_{1223}^S \mathbf{s}_{2312}^S \tag{A7}$$

$$\mathbf{A}_{23} = -\mathbf{c}_{1233}^S \mathbf{s}_{3322}^S - 2\mathbf{c}_{1213}^S \mathbf{s}_{1322}^S - 2\mathbf{c}_{1223}^S \mathbf{s}_{2322}^S \tag{A8}$$

$$\mathbf{A}_{31} = -\mathbf{c}_{2233}^S \mathbf{s}_{3311}^S - 4\mathbf{c}_{2213}^S \mathbf{s}_{1311}^S - 4\mathbf{c}_{2223}^S \mathbf{s}_{2311}^S \tag{A9}$$

$$\mathbf{A}_{32} = -2\mathbf{c}_{2233}^S \mathbf{s}_{3312}^S - 4\mathbf{c}_{2213}^S \mathbf{s}_{1312}^S - 4\mathbf{c}_{2223}^S \mathbf{s}_{2312}^S \tag{A10}$$

$$\mathbf{A}_{33} = 1 - \mathbf{c}^S_{2233}\mathbf{s}^S_{3322} - 2\mathbf{c}^S_{2213}\mathbf{s}^S_{1322} - 2\mathbf{c}^S_{2223}\mathbf{s}^S_{2322} \tag{A11}$$

and

$$\mathbf{b} = \begin{pmatrix} \mathbf{c}^S_{1111}\left\langle \boldsymbol{\varepsilon}^S_{11} \right\rangle + \mathbf{c}^S_{1122}\left\langle \boldsymbol{\varepsilon}^S_{22} \right\rangle + 2\mathbf{c}^S_{1112}\left\langle \boldsymbol{\varepsilon}^S_{12} \right\rangle + \mathbf{c}^S_{1133}\boldsymbol{\xi}_1 + 2\mathbf{c}^S_{1113}\boldsymbol{\xi}_2 + 2\mathbf{c}^S_{1123}\boldsymbol{\xi}_3 \\ \mathbf{c}^S_{1211}\left\langle \boldsymbol{\varepsilon}^S_{11} \right\rangle + \mathbf{c}^S_{1211}\left\langle \boldsymbol{\varepsilon}^S_{22} \right\rangle + 2\mathbf{c}^S_{1212}\left\langle \boldsymbol{\varepsilon}^S_{12} \right\rangle + \mathbf{c}^S_{1233}\boldsymbol{\xi}_1 + 2\mathbf{c}^S_{1213}\boldsymbol{\xi}_2 + 2\mathbf{c}^S_{1223}\boldsymbol{\xi}_3 \\ \mathbf{c}^S_{2211}\left\langle \boldsymbol{\varepsilon}^S_{11} \right\rangle + \mathbf{c}^S_{2222}\left\langle \boldsymbol{\varepsilon}^S_{22} \right\rangle + 2\mathbf{c}^S_{2212}\left\langle \boldsymbol{\varepsilon}^S_{12} \right\rangle + \mathbf{c}^S_{2233}\boldsymbol{\xi}_1 + 2\mathbf{c}^S_{2213}\boldsymbol{\xi}_2 + 2\mathbf{c}^S_{2223}\boldsymbol{\xi}_3 \end{pmatrix} \tag{A12}$$

with:

$$\boldsymbol{\xi}_1 = \mathbf{s}^S_{3333}\left\langle \boldsymbol{\sigma}^S_{33} \right\rangle + 2\mathbf{s}^S_{3313}\left\langle \boldsymbol{\sigma}^S_{13} \right\rangle + \mathbf{s}^S_{3323}\left\langle \boldsymbol{\sigma}^S_{23} \right\rangle, \tag{A13}$$

$$\boldsymbol{\xi}_2 = \mathbf{s}^S_{1333}\left\langle \boldsymbol{\sigma}^S_{33} \right\rangle + 2\mathbf{s}^S_{1313}\left\langle \boldsymbol{\sigma}^S_{13} \right\rangle + \mathbf{s}^S_{1323}\left\langle \boldsymbol{\sigma}^S_{23} \right\rangle, \tag{A14}$$

$$\boldsymbol{\xi}_3 = \mathbf{s}^S_{2333}\left\langle \boldsymbol{\sigma}^S_{33} \right\rangle + 2\mathbf{s}^S_{2313}\left\langle \boldsymbol{\sigma}^S_{13} \right\rangle + \mathbf{s}^S_{2323}\left\langle \boldsymbol{\sigma}^S_{23} \right\rangle. \tag{A15}$$

Then, the unknown strain tensor components can be obtained employing Hooke's law (equation (11)).

## Inverse Vook-Witt model

From the stress and strain tensor components equal to the mechanical averages (cf. equations (16), (17)), the unknown components can be calculated as follows:

After defining the vector $\mathbf{x}$ of which the components are the unknown components of the stress tensor $\boldsymbol{\sigma}^S$:

$$\mathbf{x} = \begin{pmatrix} \boldsymbol{\sigma}^S_{13} \\ \boldsymbol{\sigma}^S_{23} \\ \boldsymbol{\sigma}^S_{33} \end{pmatrix}, \tag{A16}$$

the unknown stress tensor components ($\boldsymbol{\sigma}^S_{13}, \boldsymbol{\sigma}^S_{23}, \boldsymbol{\sigma}^S_{33}$) can be obtained from:

$$\mathbf{x} = \mathbf{A}^{-1}\mathbf{b} \tag{A17}$$

with:

$$\mathbf{A}_{11} = 1 - 2\mathbf{c}^S_{1311}\mathbf{s}^S_{1113} - 2\mathbf{c}^S_{1322}\mathbf{s}^S_{2213} - 4\mathbf{c}^S_{1312}\mathbf{s}^S_{1213} \tag{A18}$$

$$\mathbf{A}_{12} = -2\mathbf{c}^S_{1311}\mathbf{s}^S_{1123} - 2\mathbf{c}^S_{1322}\mathbf{s}^S_{2223} - 4\mathbf{c}^S_{1312}\mathbf{s}^S_{1223} \tag{A19}$$

$$\mathbf{A}_{13} = -\mathbf{c}^S_{1311}\mathbf{s}^S_{1133} - 2\mathbf{c}^S_{1322}\mathbf{s}^S_{2233} - 2\mathbf{c}^S_{1312}\mathbf{s}^S_{1233} \tag{A20}$$

$$\mathbf{A}_{21} = -2\mathbf{c}^S_{2311}\mathbf{s}^S_{1113} - 2\mathbf{c}^S_{2322}\mathbf{s}^S_{2213} - 4\mathbf{c}^S_{2312}\mathbf{s}^S_{1213} \tag{A21}$$

$$\mathbf{A}_{22} = 1 - 2\mathbf{c}^S_{2311}\mathbf{s}^S_{1123} - 2\mathbf{c}^S_{2322}\mathbf{s}^S_{2223} - 4\mathbf{c}^S_{2312}\mathbf{s}^S_{1223} \tag{A22}$$

$$\mathbf{A}_{23} = -\mathbf{c}^S_{2311}\mathbf{s}^S_{1133} - \mathbf{c}^S_{2322}\mathbf{s}^S_{2233} - 2\mathbf{c}^S_{2312}\mathbf{s}^S_{1233} \tag{A23}$$

$$\mathbf{A}_{31} = -2\mathbf{c}^S_{3311}\mathbf{s}^S_{1113} - 2\mathbf{c}^S_{3322}\mathbf{s}^S_{2213} - 4\mathbf{c}^S_{3312}\mathbf{s}^S_{1213} \tag{A24}$$

$$\mathbf{A}_{32} = -2\mathbf{c}^S_{3311}\mathbf{s}^S_{1123} - 2\mathbf{c}^S_{3322}\mathbf{s}^S_{2223} - 4\mathbf{c}^S_{3312}\mathbf{s}^S_{1233} \tag{A25}$$

$$\mathbf{A}_{33} = 1 - \mathbf{c}^S_{3311}\mathbf{s}^S_{1133} - \mathbf{c}^S_{3322}\mathbf{s}^S_{2223} - 2\mathbf{c}^S_{3312}\mathbf{s}^S_{1233} \tag{A26}$$

and

$$\mathbf{b} = \begin{pmatrix} \mathbf{c}^S_{1333}\left\langle \boldsymbol{\varepsilon}^S_{33} \right\rangle + 2\mathbf{c}^S_{1313}\left\langle \boldsymbol{\varepsilon}^S_{13} \right\rangle + 2\mathbf{c}^S_{1323}\left\langle \boldsymbol{\varepsilon}^S_{23} \right\rangle + \mathbf{c}^S_{1311}\boldsymbol{\xi}_1 + \mathbf{c}^S_{1322}\boldsymbol{\xi}_2 + 2\mathbf{c}^S_{1312}\boldsymbol{\xi}_3 \\ \mathbf{c}^S_{2333}\left\langle \boldsymbol{\varepsilon}^S_{33} \right\rangle + 2\mathbf{c}^S_{2313}\left\langle \boldsymbol{\varepsilon}^S_{13} \right\rangle + 2\mathbf{c}^S_{2323}\left\langle \boldsymbol{\varepsilon}^S_{23} \right\rangle + \mathbf{c}^S_{3211}\boldsymbol{\xi}_1 + \mathbf{c}^S_{2322}\boldsymbol{\xi}_2 + 2\mathbf{c}^S_{2312}\boldsymbol{\xi}_3 \\ \mathbf{c}^S_{3311}\left\langle \boldsymbol{\varepsilon}^S_{33} \right\rangle + 2\mathbf{c}^S_{3322}\left\langle \boldsymbol{\varepsilon}^S_{13} \right\rangle + 2\mathbf{c}^S_{3323}\left\langle \boldsymbol{\varepsilon}^S_{23} \right\rangle + \mathbf{c}^S_{3311}\boldsymbol{\xi}_1 + \mathbf{c}^S_{3322}\boldsymbol{\xi}_2 + 2\mathbf{c}^S_{3312}\boldsymbol{\xi}_3 \end{pmatrix} \tag{A27}$$

with:

$$\boldsymbol{\xi}_1 = \mathbf{s}^S_{1111}\left\langle \boldsymbol{\sigma}^S_{11} \right\rangle + \mathbf{s}^S_{1122}\left\langle \boldsymbol{\sigma}^S_{22} \right\rangle + 2\mathbf{s}^S_{1112}\left\langle \boldsymbol{\sigma}^S_{12} \right\rangle, \tag{A28}$$

$$\boldsymbol{\xi}_2 = \mathbf{s}^S_{2211}\left\langle \boldsymbol{\sigma}^S_{11} \right\rangle + \mathbf{s}^S_{2222}\left\langle \boldsymbol{\sigma}^S_{22} \right\rangle + 2\mathbf{s}^S_{2212}\left\langle \boldsymbol{\sigma}^S_{12} \right\rangle, \tag{A29}$$

$$\boldsymbol{\xi}_3 = \mathbf{s}^S_{1211}\left\langle \boldsymbol{\sigma}^S_{11} \right\rangle + \mathbf{s}^S_{1222}\left\langle \boldsymbol{\sigma}^S_{22} \right\rangle + 2\mathbf{s}^S_{1212}\left\langle \boldsymbol{\sigma}^S_{12} \right\rangle. \tag{A30}$$

Then, the unknown strain tensor components can be obtained employing Hooke's law (equation (11)).

## *Tables*

Table 1

| | $\mathbf{s}_{11}$ (TPa$^{-1}$) | $\mathbf{s}_{12}$ (TPa$^{-1}$) | $\mathbf{s}_{44}$ (TPa$^{-1}$) | $A_i$ (TPa$^{-1}$) |
|---|---|---|---|---|
| W (bcc) | 2.57 | -0.73 | 6.60 | 1.00 |
| Cu (fcc)* | 14.995 | -6.2822 | 13.263 | 3.21 |
| Fe (bcc) | 7.62 | -2.79 | 8.58 | 2.43 |

* calculated from stiffness tensor components

Table 2

| **W** | $\mathbf{C}_{11}^{S}$ (GPa) | $\mathbf{C}_{33}^{S}$ (GPa) | $\mathbf{C}_{44}^{S}$ (GPa) | $\mathbf{C}_{12}^{S}$ (GPa) | $\mathbf{C}_{13}^{S}$ (GPa) |
|---|---|---|---|---|---|
| all models | 502.32 | 502.32 | 151.51 | 199.29 | 199.29 |

Table 3

| **Cu** | $\mathbf{C}_{11}^{S}$ (GPa) | $\mathbf{C}_{33}^{S}$ (GPa) | $\mathbf{C}_{44}^{S}$ (GPa) | $\mathbf{C}_{12}^{S}$ (GPa) | $\mathbf{C}_{13}^{S}$ (GPa) |
|---|---|---|---|---|---|
| VW | 202.39 | 198.88 | 47.16 | 102.65 | 106.16 |
| EK (disk) | 202.16 | 199.43 | 47.41 | 103.15 | 105.89 |
| EK (sphere) | 201.30 | 201.30 | 48.17 | 104.95 | 104.95 |
| EK (needle) | 200.84 | 202.15 | 48.49 | 105.84 | 104.52 |
| IVW | 200.80 | 204.08 | 49.56 | 106.84 | 103.56 |

Table 4

| **Fe** | $\mathbf{C}_{11}^{S}$ (GPa) | $\mathbf{C}_{33}^{S}$ (GPa) | $\mathbf{C}_{44}^{S}$ (GPa) | $\mathbf{C}_{12}^{S}$ (GPa) | $\mathbf{C}_{13}^{S}$ (GPa) |
|---|---|---|---|---|---|
| VW | 274.30 | 270.54 | 81.24 | 106.06 | 109.83 |
| EK (disk) | 274.06 | 271.12 | 81.49 | 106.60 | 109.54 |
| EK (sphere) | 273.12 | 273.12 | 82.29 | 108.54 | 108.54 |
| EK (needle) | 272.62 | 274.08 | 82.64 | 109.52 | 108.06 |
| IVW | 272.77 | 276.32 | 83.91 | 110.50 | 106.94 |

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## *Figures*

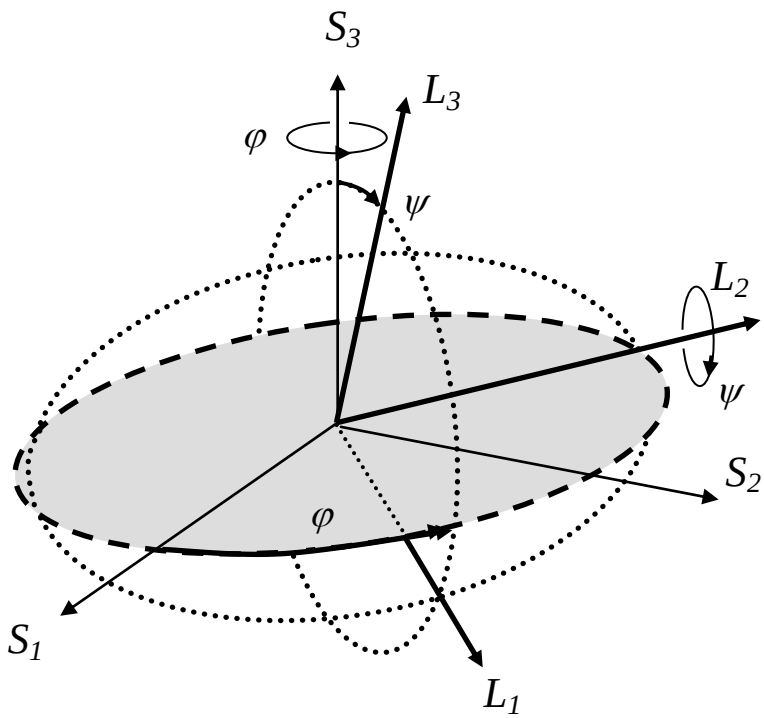


Figure 1.

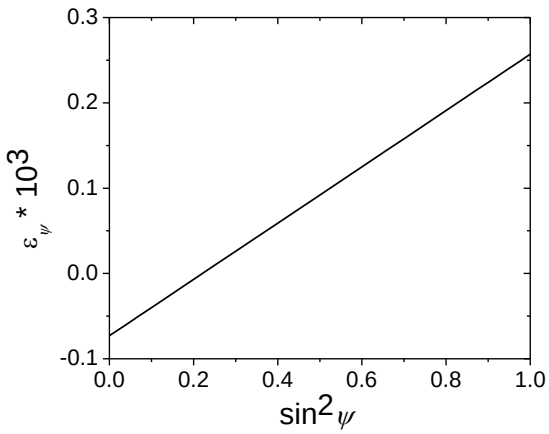


Figure 2.

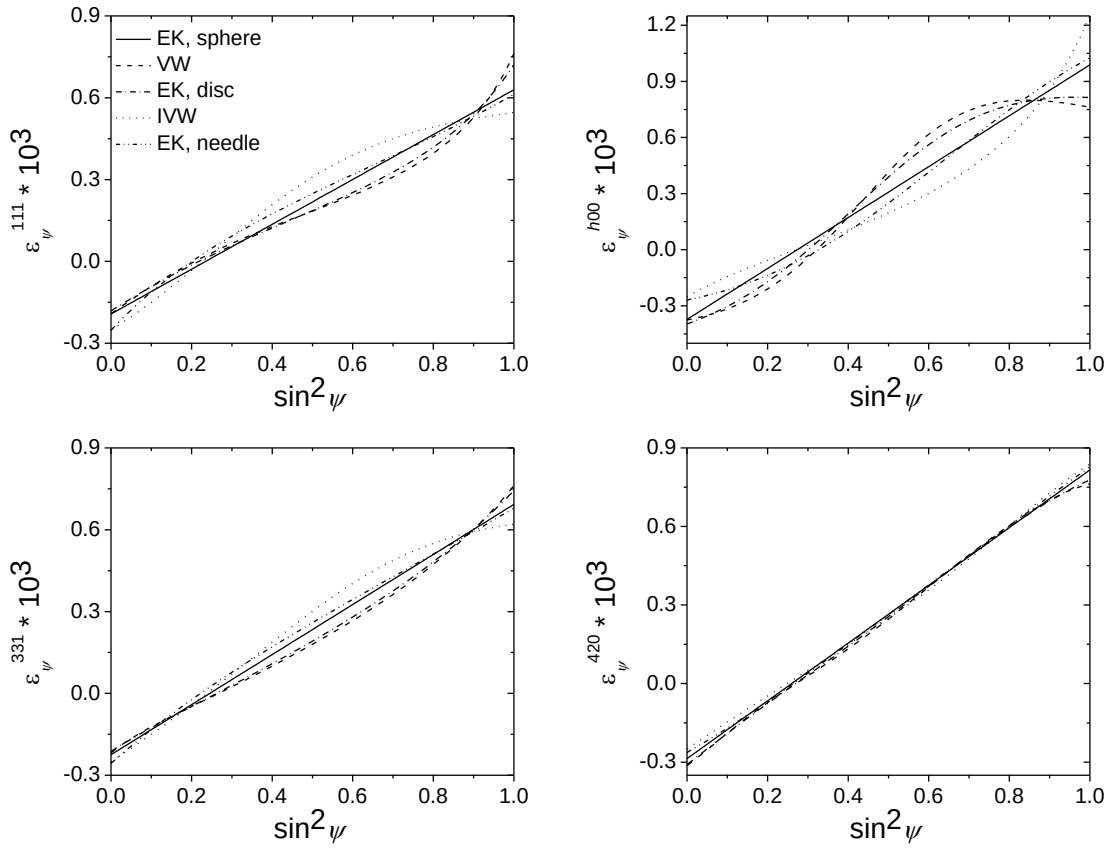
EK, sphere
VW
EK, disc
IVW
EK, needle
$\varepsilon_{\psi}^{111} * 10^3$
$\varepsilon_{\psi}^{h00} * 10^3$
$\varepsilon_{\psi}^{331} * 10^3$
$\varepsilon_{\psi}^{420} * 10^3$
$\sin^2\psi$

Figure 3.

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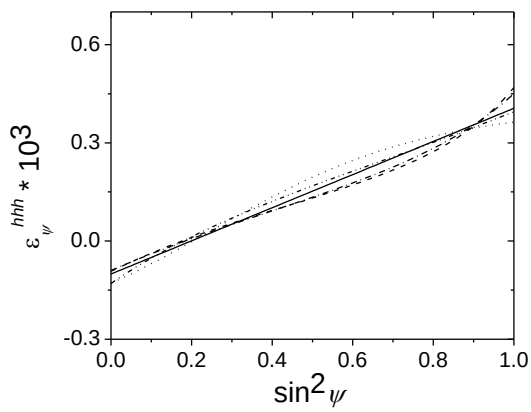

Welzel, U., **Fréour, S.** (2007) Extension of the Vook-Witt and inverse Vook-Witt elastic grain-interaction models to general loading states, *Philosophical Magazine*, **87**, 3921-3943.

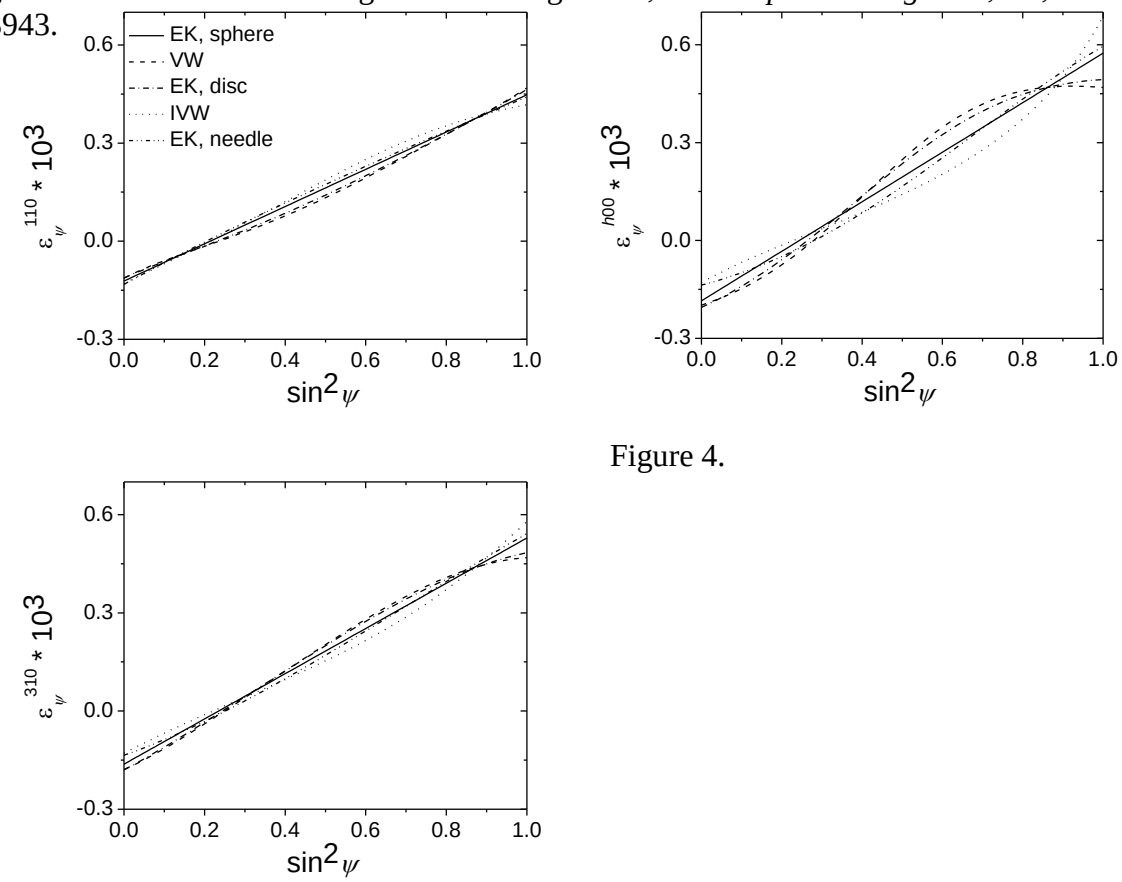


Figure 4.

## *Table captions*

Table 1: Single crystal elastic stiffnesses for cubic materials (Meyers and Chawla 1984).

Table 2: Stiffness tensor components of a tungsten polycrystal calculated according to different grain-interaction models. The same results are obtained for all grain-interaction models.

Table 3: Stiffness tensor components of a copper polycrystal calculated according to different grain-interaction models.

Table 4: Stiffness tensor components of a iron polycrystal calculated according to different grain-interaction models.

## *Figure captions*

Figure 1. Definition of and relations between the crystal (*C*), sample (*S*) and laboratory (*L*) reference frames.

Figure 2. $\sin^2\psi$-plot for a tungsten polycrystal subjected to a uniaxial tensile stress calculated according to different grain-interaction models: Vook-Witt model, inverse Vook-Witt model, Eshelby-Kroener model (with $\eta = 0.1$ (discs), $\eta = 1$(spheres), $\eta = 10$ (needles)). The same result is obtained for all models and all reflections.

Figure 3. $\sin^2\psi$-plot for a copper polycrystal subjected to a uniaxial tensile stress calculated according to different grain-interaction models: Vook-Witt model, inverse Vook-Witt model, Eshelby-Kroener model (with $\eta = 0.1$ (‘discs’), $\eta = 1$(‘spheres’), $\eta = 10$ (‘needles’)).

Figure 3. $\sin^2\psi$-plot for a copper polycrystal subjected to a uniaxial tensile stress calculated according to different grain-interaction models: Vook-Witt model, inverse Vook-Witt model, Eshelby-Kroener model (with $\eta = 0.1$ (‘discs’), $\eta = 1$(‘spheres’), $\eta = 10$ (‘needles’)).

Figure 4. $\sin^2\psi$-plot for a copper polycrystal subjected to a uniaxial tensile stress calculated according to different grain-interaction models: Vook-Witt model, inverse

Welzel, U., **Fréour, S.** (2007) Extension of the Vook-Witt and inverse Vook-Witt elastic grain-interaction models to general loading states, *Philosophical Magazine*, **87**, 3921-3943.

Vook-Witt model, Eshelby-Kroener model (with $\eta = 0.1$ ('discs'), $\eta = 1$('spheres'),

$\eta = 10$ ('needles')).