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MOMENT POLE FIGURES IN RESIDUAL STRESS ANALYSIS

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The basic formulas (Reuss's approximation) for residual stress analysis are given in a revised form. All ODF-burdened information reduces to five "moment pole figures" simply to calculate using modern direct algorithms. The corresponding harmonic expressions are also more compact than other formulas known from literature. For texture components described by Standard Gaussian Functions the corresponding expressions can be given in an analytically closed form. The use of the concept of the geometrical mean approximation for calculating elastic constants (avoiding Reuss's limitations) will be explained in connection with the determination of residual stresses.

KEY WORDS: Stress analysis, moment pole figures, Reuss approximation, geometric mean.

INTRODUCTION

The new situation in Quantitative Texture Analysis (QTA) that follows from the high productivity of modern computer techniques, now available even on a personal level, was discussed in a special paper on ICOTOM-10 (Matthies, Vinel 1994).

Obviously there are no more limitations for the use of methods, "directly" considering the original analytical expressions, i.e. avoiding any transformations into the Fourier space. Moreover, the strategy of "working in the whole orientation (G) space" drastically simplifies the structure of the computer programs. Now they possess a "universal" character, i.e. may consider any crystal and sample symmetry without special libraries. The symmetries do practically not explicitly appear in the working expressions. They enter the problem by the numerical values of the ODF $f(g)$ and by the monocrystalline data of the property tensor components of interest.

As a rule the physical basic expressions in QTA are relatively simple. This holds also for the harmonic expressions in case of linear (bulk – i.e. considering all orientations) averaging procedures because of the orthogonality of the spherical functions (Bunge, 1982). The simplicity is lost for nonlinear problems or e.g. for the averaging integral typical in stress analysis. The last concerns only orientations along a one-dimensional path through the three-dimensional G space and leads to rather complicated working formulas (Brakman 1983; Schuman *et al.*, 1994).

For all these reasons the basic expressions of stress analysis were reanalysed. As it turns out, the structure of the working formulas can be simplified in a remarkable manner introducing so-called "moment pole figures".

2. THE BASIC EXPRESSIONS (REUSS'S APPROXIMATION)

The aim of stress analysis by diffraction experiments is the determination of the macroscopic (mean) stress field $\bar{\bar{\sigma}}$ from mean strain data $\bar{\varepsilon}$ measured for special subsets of grains in a polycrystalline sample (Van Houtte, De Buyser, 1993).

A subset "p" is characterized by the scattering vector $\mathbf{N}$ (given by $\mathbf{y} = [\varphi, \vartheta]$ in the sample coordinate system K_A), the normal $\mathbf{h}_i$ to the scattering plane ($\mathbf{h}_i = [\varphi_i, \vartheta_i]$ given in the crystal coordinate system K_B), and by the condition $\mathbf{y} \| \mathbf{h}_i$. The corresponding orientation path reads (Matthies *et al.*, 1994).

$$g_p(\tilde{\varphi}) = \{\mathbf{h}_i, \tilde{\varphi}\}^{-1}\{\mathbf{y}, 0\}; \; 0 \le \tilde{\varphi} \le 2\pi. \tag{1}$$

The shift of the Bragg angle Θ_i of a reflex $\mathbf{h}_i$ from its value Θ_i^0 for the stress free case leads to the experimental strain values

$$\bar{\varepsilon}^L_{33}(p) = \bar{\varepsilon}^L_{33}(\mathbf{h}_i, \mathbf{y}) = \frac{\sum \int_0^{2\pi} \varepsilon^L_{33}[g_p(\tilde{\varphi})] f(g_p(\tilde{\varphi}))\, d\tilde{\varphi}}{\sum \int_0^{2\pi} f(g_p(\tilde{\varphi}))\, d\tilde{\varphi}} \tag{2}$$

given in a laboratory coordinate system K_L with $\mathbf{Z}_L \| \mathbf{N}$, and e.g. $\mathbf{X}_L$ inside the plane containing the incident and scattered beam. It holds $g^{AL} = (K_A \to K_L) = \{\mathbf{y}, 0\}$. The symbol $\sum$ means that a weighted sum over all physically equivalent $\mathbf{h}_i$ (depending on the crystal class $\mathcal{G}_B$ (Matthies, Helming, 1982)), also including Friedel's law $\pm\mathbf{h}_i$, is to be considered. The denominator in (2) describes (up to the factor $1/2\pi$) the well known reduced pole figure $\tilde{P}_{\mathbf{h}_i}(\mathbf{y})$ (below always denoted by "$\tilde{P}$").

By Hook's law of elasticity the local strains in (2) may be expressed by the local stresses and compliances S

$$\bar{\varepsilon}^L_{33}[g_p(\tilde{\varphi})] = S^L_{33mn}(g_p(\tilde{\varphi}))\sigma^L_{mn}(g_p(\tilde{\varphi})) = S^L_{33mn}(g_p(\tilde{\varphi}))[\{\mathbf{y}, 0\}_{mk}\{\mathbf{y}, 0\}_{nl}\sigma_{kl}(g_0(\tilde{\varphi}))]\,. \tag{3}$$

In stress analysis it is assumed that the mean strain corresponding to the path p can be related to the macroscopical stress $\bar{\bar{\sigma}}$ (does not depend on p) by

$$\bar{\varepsilon}^L_{33}(p) = \bar{\varepsilon}^L_{33}(\mathbf{h}_i, \mathbf{y}) = \tilde{S}^{L,p}_{33mn}\,\bar{\bar{\sigma}}^L_{mn} = [\tilde{S}^{L,p}_{33mn}\{\mathbf{y}, 0\}_{mk}\{\mathbf{y}, 0\}_{nl}]\bar{\bar{\sigma}}_{kl} \equiv \tilde{S}^{AL}_{33kl}(\mathbf{h}_i, \mathbf{y})\bar{\bar{\sigma}}_{kl} \tag{4}$$

The expression for the components of the p-specific mean compliance tensor $\tilde{S}$ is unknown. From (2) and (3) one can directly derive $\tilde{S}$ only by simplifying assumptions. The Reuss's approximation assumes that σ in (3) does not depend on p and is equal to the macroscopic $\bar{\bar{\sigma}}$.

S of a grain with orientation $g\,(= g^{AB})$ and the monocrystalline data S^0 (given in K_B) is described in K_L by

$$S^L_{33mn}(g) = (K_B \to K_L) = g^{BL}_{3r}\, g^{BL}_{3u}\, g^{BL}_{mv}\, g^{BL}_{nw}\, S^0_{ruvw}. \tag{5}$$

For $g^{BL} = g^{AL} \cdot g^{BA}$ with $g = g^{AB} = g_p(\tilde{\varphi})$ (1) it follows

$$g_p^{BL}(\tilde{\varphi}) = \{+\mathbf{h}_i, \tilde{\varphi}\} \equiv \{+\}. \tag{6}$$

Finally (using the symmetry properties of the ODF and compliances) for the Reuss's approximation the mathematical problem leads to the expression

$$\tilde{S}^{L_p}_{33mn} \equiv \bar{S}^{L}_{33mn}(\mathbf{h}_i, \mathbf{y}) = \frac{1}{4\pi\tilde{P}} \int_0^{2\pi} \left[\begin{array}{l} \{+\}_{3r}\{+\}_{3u}\{+\}_{mv}\{+\}_{nw} f(\{+\}^{-1} \cdot \{\mathbf{y}, 0\}) \\ + \{-\}_{3r}\{-\}_{3u}\{-\}_{mv}\{-\}_{nw} f(\{-\}^{-1} \cdot \{\mathbf{y}, 0\}) \end{array} \right] d\tilde{\varphi}\ S^0_{ruvw} \quad (7)$$

that has to be calculated using the given ODF $f(g)$ of the sample.
The relation (7) is valid for all crystal symmetries. Only in case of a crystal class of type III (mirror groups) the ODF must be symmetrized by an additional C_2 element due to the effect of uncorrectable ghosts (Matthies, Helming, 1982).

The fourfold product of elements of the rotation matrix $g_p^{BL}(\tilde{\varphi})$ leads to rather complicated expressions if (7) is calculated in the given form or trying to combine the $\mathbf{h}_i$ (as well as $\mathbf{y}$) dependence (Brakman, 1983; Schuman *et al.*, 1994). The extraction of the pure $\tilde{\varphi}$-dependence from this product results in drastic simplifications.

3. MOMENT POLE FIGURES

According to $\{\mathbf{h}_i, \tilde{\varphi}\} = \{\tilde{\varphi}, 0, 0\}\{\mathbf{h}_i, 0\}$ the $\tilde{\varphi}$- and $\mathbf{h}_i$-dependence in $\{+\}$ or $\{-\}$ of (7) can be separated. The $\mathbf{h}_i$-parts we combine with the monocrystalline compliances S^0 that leads to the $\mathbf{h}_i$-specific quantities U

$$U_{cd}(\mathbf{h}_i) \equiv S_{33cd}(\mathbf{h}_i) = \{\mathbf{h}_i, 0\}_{3r}\{\mathbf{h}_i, 0\}_{3u}\{\mathbf{h}_i, 0\}_{cv}\{\mathbf{h}_i, 0\}_{dw} S^0_{ruvw} \quad (8)$$

possessing the parities

$$U_{cd}(-\mathbf{h}_i) = \begin{array}{l} +U_{cd}(\mathbf{h}_i) \text{ for } cd = 11, 22, 33, 23 \\ -U_{cd}(\mathbf{h}_i) \text{ for } cd = 12, 13 \end{array} \quad (9)$$

From the explicit form of the rotation matrix $\{\tilde{\varphi}, 0, 0\}$

$$\{\tilde{\varphi}, 0, 0\} = \begin{pmatrix} \cos\tilde{\varphi} & \sin\tilde{\varphi} & 0 \\ -\sin\tilde{\varphi} & \cos\tilde{\varphi} & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad (10)$$

it follows that the $\{\ \}_{3r}$ and $\{\ \}_{3u}$ factors in (7) do not depend on $\tilde{\varphi}$.

Moreover, all $\tilde{\varphi}$-related integrals can obviously be reduced to the five "moments" of the orientation distribution density of the projection path g_p (1):

$$\begin{array}{l} J_0(\mathbf{h}_i, \mathbf{y}) \\ J_1(\mathbf{h}_i, \mathbf{y}) \\ J_2(\mathbf{h}_i, \mathbf{y}) \\ J_3(\mathbf{h}_i, \mathbf{y}) \\ J_4(\mathbf{h}_i, \mathbf{y}) \end{array} = \frac{1}{2\pi\tilde{P}} \int_0^{2\pi} \begin{array}{l} 1 \\ \cos\tilde{\varphi} \\ \sin\tilde{\varphi} \\ \cos 2\tilde{\varphi} \\ \sin 2\tilde{\varphi} \end{array} f(\{\mathbf{h}_i, \tilde{\varphi}\}^{-1}\{\mathbf{y}, 0\}) d\tilde{\varphi}. \quad (11)$$

Finally with

$$\tilde{J}_q(\mathbf{h}_i, \mathbf{y}) = [J_q(\mathbf{h}_i, \mathbf{y}) + J_q(-\mathbf{h}_i, \mathbf{y})]/2$$

and

$$\tilde{\tilde{J}}_q(\mathbf{h}_i, \mathbf{y}) = [J_q(\mathbf{h}_i, \mathbf{y}) - J_q(-\mathbf{h}_i, \mathbf{y})]/2 \quad (12)$$

the expression (7) can be represented in the very compact form ($\tilde{J}_0 \equiv 1$; $\bar{S}^L_{33mn} = \bar{S}^L_{33nm}$):

$$\begin{aligned}
\bar{S}^L_{3311}(\mathbf{h}_i, \mathbf{y}) &= (U_{11} + U_{22})\tilde{J}_0/2 + (U_{11} - U_{22})\tilde{J}_3/2 + U_{12}\tilde{\tilde{J}}_4 \\
\bar{S}^L_{3322}(\mathbf{h}_i, \mathbf{y}) &= (U_{11} + U_{22})\tilde{J}_0/2 - (U_{11} - U_{22})\tilde{J}_3/2 - U_{12}\tilde{\tilde{J}}_4 \\
\bar{S}^L_{3333}(\mathbf{h}_i, \mathbf{y}) &= U_{33}\tilde{J}_0 \\
\bar{S}^L_{3323}(\mathbf{h}_i, \mathbf{y}) &= U_{23}\tilde{J}_1 - U_{13}\tilde{\tilde{J}}_2 \\
\bar{S}^L_{3313}(\mathbf{h}_i, \mathbf{y}) &= U_{13}\tilde{\tilde{J}}_1 + U_{23}\tilde{J}_2 \\
\bar{S}^L_{3312}(\mathbf{h}_i, \mathbf{y}) &= U_{12}\tilde{\tilde{J}}_3 - (U_{11} - U_{22})\tilde{J}_4/2 \ .
\end{aligned} \tag{13}$$

The key quantities are the moments J and the U-values simplifying the analysis of the properties of the "X-ray elastic constants" $\bar{S}^L$.

For direct methods the calculation of the moments (11) is straightforward. Using the harmonic approach the corresponding working expression will be somewhat more complex. But, on the other hand, it gives a better transparency for analytical questions of practical interest.

Representing the ODF by the symmetrized (rotation groups G_A and G_B) real tesseral functions $\bar{D}^l_{\mu,\nu}(g)$ (Matthies, 1988; Matthies *et al.*, 1988)

$$f(g) = \sum_{l=0}^{\infty} \sum_{\nu=1}^{\mathcal{L}(G_A,\, l)} \sum_{\mu=1}^{\mathcal{L}(G_B,\, l)} C_l^{\mu,\nu} \bar{D}^l_{\mu,\nu}(g^{-1})$$

it follows for the moments (11)

$$J_q(\mathbf{h}_i, \mathbf{y}) = \frac{1}{\tilde{P}} \sum_{l=0}^{\infty} \sum_{\nu=1}^{\mathcal{L}(G_A,\, l)} \sum_{\mu=1}^{\mathcal{L}(G_B,\, l)} \sum_{\bar{s},\bar{p}=-l}^{l} C_l^{\mu,\nu} \bar{D}^l_{\mu,\bar{s}}(\{\mathbf{h}_i, 0\}) \bar{D}^l_{\nu,\bar{p}}(\{\mathbf{y}, 0\}) T_q(\bar{s}, \bar{p}), \tag{15}$$

with

$$\begin{aligned}
T_0 &= \delta_{\bar{s},\bar{p}} \quad \delta_{\bar{p},0} \\
T_1 &= \delta_{\bar{s},\bar{p}} \quad [\delta_{\bar{p},1} + \delta_{\bar{p},-1}] \\
T_2 &= \delta_{\bar{s},-\bar{p}} \quad [\delta_{\bar{p},1} - \delta_{\bar{p},-1}] \\
T_3 &= \delta_{\bar{s},\bar{p}} \quad [\delta_{\bar{p},2} + \delta_{\bar{p},-2}] \\
T_4 &= \delta_{\bar{s},-\bar{p}} \quad [\delta_{\bar{p},2} - \delta_{\bar{p},-2}] \ .
\end{aligned} \tag{16}$$

As can be seen from (15) there are not any limitations for l. Except for $q = 0$ (these terms are connected with the common pole figures) there are not l-depending parity relations according to $\pm\mathbf{h}_i$. Therefore the problem needs the C-coefficients with even and odd l.

The so-called $\sin^2\Psi$-law plays a remarkable role in residual stress analysis. It appears for the ϑ-dependence ($\Psi \hat{=} \vartheta$) of $\bar{\varepsilon}^L_{33}(\mathbf{h}_i, \mathbf{y})$, i.e. of the $\tilde{S}^{AL}$-values from (4) for Reuss's approximation (7), if the $\tilde{S}^{L,p}_{33mn}$ components do not depend on $\mathbf{y} = [\varphi, \vartheta]$, additionally assuming $\bar{\bar{\sigma}}_{k3} = 0$ (Van Houtte, De Buyser, 1993).

A trivial solution is the case of the random distribution $f(g) = 1$ with $C_l^{\mu,\nu} \equiv 0$ for $l \neq 0$. This gives $J_q = 0$ ($q \neq 0$) – cf. (11), (15), (16).

The effect is also known for any $f(g)$, $\mathbf{h}_i = (001)$ and cubic crystal symmetry ($G_B = O, T$). That the $q \neq 0$ moments also disappear in the case $G_B = O$ it directly follows from (15) using

$$\bar{D}^l_{\mu,\bar{s}}(\{\mathbf{h}_i, 0\}) = \sum_{\bar{m}=-l}^{l} {}^{G_B}A_l^{\mu,\bar{m}} \bar{D}^l_{\bar{m},\bar{s}}(\{\mathbf{h}_i, 0\}) \quad , \tag{17}$$

$\bar{D}^l_{\bar{m},\bar{s}}(0, 0, 0) = \delta_{\bar{m},\bar{s}}$, and $\bar{s} = \pm 1, \pm 2$ for $q \neq 0$ (cf. (16) also). Because of the cubic fourfold rotation axis the symmetry coefficients ${}^{G_B}A_l^{\mu,\bar{m}}$ are not equal to zero only for $\bar{m} = 0, \pm 4, \pm 8, \ldots$

Analogical effects appear for $\mathbf{h}_i = (001)$ and all crystal classes with the rotation parts $G_B = C_3, D_3, C_4, D_4, C_6, D_6$, as well as for the (111) direction and cubic symmetry ($G_B = O, T$).

It is remarkable that in all these cases (except $\mathbf{h}_i = (001)$, $G_B = T$, with J_4, $J_5 \neq 0$) the ODF- and **y**-independence of (13) is "twice-covered" due to the arising connections $U_{11} = U_{22}$, $U_{12} = U_{13} = U_{23} = 0$.

4. PATH MOMENTS FOR STANDARD COMPONENTS

The Gaussian standard distribution at g_0 with the halfwidth (FWHM) b is given by (Matthies *et al.*, 1987; Matthies, 1980).

$$F^G(b, g_0; g) = N(S)e^{S\cos\tilde{\omega}}, \qquad \cos\tilde{\omega} = [\mathrm{SPUR}(g_0^{-1}g) - 1]/2; \tag{18}$$

$$N(S) = 1/[I_0(S) - I_1(S)]; \qquad S = \ln 2/[2\sin^2(b/4)],$$

with $I_m(x)$ – modified Bessel functions.
Using F^G for $f(g)$ the right side of (11) (without $\tilde{P}$) is denoted by $P_q(b, g_0 \mid \mathbf{h}_i, \mathbf{y}) \equiv P_q$ and can exactly be resolved:

$$P_0 = P_0(S, z), \qquad P_1 = \cos\varepsilon^* \, P_1(S, z), \qquad P_2 = \sin\varepsilon^* \, P_1(S, z),$$

$$P_3 = \cos 2\varepsilon^* \, P_2(S, z), \qquad P_4 = \sin 2\varepsilon^* \, P_2(S, z), \tag{19}$$

with

$$P_m(S, z) = N(S)e^{-S(1-z)/2} I_m(S(1 + z)/2), \tag{20}$$

and

$$g^* = \{\alpha^*, \beta^*, \gamma^*\} = \{\mathbf{y}, 0\}g_0^{-1} \{\mathbf{h}_i, 0\}, \; z = \cos\beta^* = \mathbf{h}_i \cdot g_0 \cdot \mathbf{y}, \tag{21}$$

$$\varepsilon^* = \alpha^* + \gamma^* \; .$$

For $\mathbf{h}_i \to -\mathbf{h}_i$ it follows $z \to -z$ and $\varepsilon^* \to \varepsilon^* + \pi - 2\alpha^*$. The "ellipsoidal" generalization (Eschner, 1993) of the central Gaussian standard function (18) also leads to closed expressions of the form (19), (20).

5. THE GEOMETRIC MEAN OF ELASTIC CONSTANTS

The arithmetic mean ("$\overline{\quad}^{a}$") over all orientations is the simplest approximation in order to describe the macroscopic property $\bar{E}$ of a polycrystalline sample using the microscopic values E^0 and the ODF $f(g)$. For the elastic compliances in Reuss's approximation it reads

$$\bar{S}^{a}_{i_1 i_2, j_1 j_2} = \int_G g_{i'_1 i_1} g_{i'_2 i_2} g_{j'_1 j_1} g_{j'_2 j_2} f(g)\, dg\, S^0_{i'_1 i'_2, j'_1 j'_2} \,. \tag{22}$$

Introducing effective matrices W with elements $W_{II'}$ combining the i as well as the j indexes of the product of two g elements the relation (22) can be written as (Matthies, Humbert, 1993)

$$\bar{S}^{a} = \overline{WW}^{a} : S^0 \,. \tag{23}$$

The stiffness is given in Voigt's approximation by

$$\bar{C}^{a} = \overline{WW}^{a} : C^0 \,. \tag{24}$$

The well known complication is that the symmetry of the "inverse properties" ($S \equiv C^{-1}$), also valid on the macroscopic level,

$$\bar{S} = (\bar{C})^{-1} \tag{25}$$

is not obeyed by the arithmetic mean. $\bar{S}^{a}$ and $(\bar{C}^{a})^{-1}$ may remarkably differ.

However, in the frame of $\overline{WW}^{a}$ the condition (25) can exactly be realized with the help of the so-called "geometric mean" (Matthies, Humbert, 1993; Moraviec, 1989).

$$\bar{S}^{\,\mathrm{GEO}} = e^{\overline{Ln S}^{a}} = e^{\overline{WW}^{a} \,:\, Ln S^0} \,. \tag{26}$$

For not strong orientation correlations between neighbouring grains or except extremely nonspherical grain forms the simple geometric mean leads to results quite close to those of much more complicated self-consistent schemes (Kröner, 1986; Matthies, Humbert, 1994; Matthies, Humbert in the press).

6. THE GEOMETRIC MEAN IN STRESS ANALYSIS

Comparing (22) and (7) there are some analogies not only concerning the chosen Reuss's approximation but also the complications in connection with the physical property (25). Therefore it may be useful to consider a geometric path mean (Matthies *et al.*, 1994) interpreting (7) as

$$\bar{S}^{L}(\mathbf{h}_i, \mathbf{y}) = {}^{BL}\overline{WW}^{p} : S^0 \tag{27}$$

generalized now for all (not only the 33mn) tensor components:

$${}^{L}S^{\,p,\mathrm{GEO}} = e^{{}^{L}\overline{Ln S}^{p}} = e^{{}^{BL}\overline{WW}^{p} :\, Ln S^0} \,. \tag{28}$$

The integrals connected with the ${}^{BL}\overline{WW}^{p}$-values will now contain four $\tilde{\varphi}$-depending factors, i.e. (cf. (10), (11)) at the end four additional moments (for $\cos 3\tilde{\varphi}$, $\sin 3\tilde{\varphi}$, $\cos 4\tilde{\varphi}$, $\sin 4\tilde{\varphi}$) are to be calculated yet.

However, it is apparent, that not only the grains belonging to a given path will influence the result, but also all other grains considered e.g. by the bulk geometric mean (26). For the final "bulk path geometric mean" ${}^{L}\tilde{S}^{p}$ an equation was derived (Matthies *et al.*, 1994) once more applying the connection (25):

$$ {}^{L}\tilde{S}^{p} = {}^{L}S^{\mathrm{GEO}}\,[{}^{L}\tilde{S}^{p}]^{-1}\;{}^{L}S^{p,\mathrm{GEO}}, \tag{29}$$

with ${}^{L}S^{\mathrm{GEO}}$ the $\bar{S}^{\mathrm{GEO}}$ described in K_L ($g^{AL} = \{\mathbf{y}, 0\}$). Equation (29) can be resolved iteratively. It shows a quick convergence.

7. CONCLUSION

The introduction of the moment pole figures remarkable simplifies the working expressions for the *X*-ray elastic constants in Reuss's approximation. The moments can simply be calculated by direct algorithms. The corresponding harmonic expressions are also more compact than other formulas known from literature. All *l*-tems are important. A reduction to only *l*-even terms is impossible.

The appearance of the $\sin^2\psi$-law in Reuss's approximation is quite apparent using the moments. The ODF independence of the moments for $\mathbf{h}_i = (001)$ immediately follows for a series of noncubic crystal symmetries also.

Using Gaussian standard distributions for ODF models the moments can be given in an analytical closed form. The concept of the geometric mean, exactly obeying the "principle of the inverse experiment" (Lichtenecker, Rother, 1931) can be generalized for path integrals too.

There exist universal PC-adapted FORTRAN programs for any crystal symmetries calculating residual stress data using Reuss's, the path geometric as well as the bulk path geometric mean approximation. Hereby the ODF can be given numerically or by a parameter set of Gaussian texture components.

Comparing the three approximations (7), (28) and (29) for the *X*-ray elastic constants $\tilde{S}^{L,p}$ (or $\tilde{S}^{AL}$ ($\mathbf{h}_i$, $\mathbf{y}$)) in (4) differences can be seen concerning the form of the $\sin^2\psi$-curves as well as the $\bar{\bar{\sigma}}$ values fitted from the experimental strain data.

For the "Santa Fe like" test distribution (Matthies, 1988) (cubic/orthorhombic symmetry; *S*-position ($g_0 = \{123\}\ \langle 634\rangle$); Gaussian, $b = 17^0$, Phon = 0.2), and using the copper S^0-data, it follows for instance with $\mathbf{h}_i = (011)$, $\mathrm{y} = [\varphi, \vartheta] = [90^0, 40^0]$: $\tilde{P}_{\mathbf{h}_i}(\mathbf{y}) = 1.72$ and $\bar{S}^{AL}_{33mn}(\mathbf{h}_i, \mathbf{y})$ [100*GPa*] given in the Table below.

(mn)	*Reuss*	*Path Geo*	*Bulk Path Geo*
11	–0.51 E-03	–0.67 E-03	–0.14 E-02
22	0.40 E-03	0.61 E-03	0.99 E-03
33	0.25 E-02	0.25 E-02	0.28 E-02
23	0.61 E-02	0.54 E-02	0.54 E-02
13	0	0	0
12	0	0	0

The publication of more analytical details concerning the sometimes comprehensive derivation of the working formulas given above is in preparation. This also concerns other numerical results including the analysis of experimental data.

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