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X-Ray Elastic Constants for Cubic Materials

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by

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ABSTRACT

The stress-strain relation to be used in X-ray stress measurements in anisotropic texture-free media is studied. The method for evaluation of appropriate elastic constants for a cubic medium is described. Some illustrative numerical examples have been worked out including line broadening due to elastic anisotropy. The elastic stress and strain compatibility at grain boundaries is taken into account using Kröner's method. These elastic constants obviously only apply when no internal stresses due to plastic deformation are present. The case of reorientation of free interstitials in the stress field can be taken into account.

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1. INTRODUCTION

When stresses are measured using X-rays the primary information obtained is the distance between a specific set of planes, for instance {310}, oriented in a known way relative to the specimen surface (see e g Macherauch [1]). Actually one obtains an average over grains with a specific normal but rotated around this normal. The problem is now to translate the measured distances between the planes into stresses. Due to the small penetration of X-rays, only tens of microns, surface boundary conditions can be assumed to hold in the measurement region which simplifies the analysis. The fact that single crystal response is anisotropic complicates the analysis as well as the constraint of stress and strain compatibility at grain boundaries. If the grain orientation distribution is not random, that is if there is texture, the translation becomes even more complicated.

The case of only elastic response seems to have a satisfactory solution due to Kröner [2] based on a theorem on inclusions by Eshelby [3]. The analysis has been extended by others (e g Kneer [4], Morris [5] and Faivre [6]) so that texture can also be treated although this necessitates the use of computer.

The particular elastic constant averages needed for X-ray stress determination have been evaluated for texture-free cubic materials (Bollenrath et al [7]) and hexagonal materials (Evenshor and Hauk [8]).

It has to be observed that stress variations can occur in a sample on different length scales (see e g Macherauch et al [9]). A classification scheme which is suitable for the analysis is division into three groups. First there are stresses with a typical wavelength much larger than the grain size, type I. These can be for instance thermal stresses or those due to external loads. Secondly there are stresses which vary from grain to grain: i e with a wavelength of the order of the grain size, type II. These can be due to different properties of different grains. Thirdly there are stresses which vary inside the grain: i e with a wavelength small compared to the grain size, type III. These can be the stress fields around single dislocations or point defects.

The main interest is usually in obtaining the type I stresses but the type II stresses complicate the analysis since a measurement yields an average over such stresses involving a region containing several grains. The type III stresses are of less importance in this context although stress fields from groups of dislocations or point defects might influence the X-ray stress measurements.

2. STRESS-STRAIN RELATIONS

Stresses and strains are related through Hooke's law (see e g Hirth and Lothe [10])

$$\sigma_{ij} = C_{ijk\ell}\, \epsilon_{k\ell} \tag{1}$$

and

$$\epsilon_{ij} = S_{ijk\ell}\, \sigma_{k\ell}, \tag{2}$$

where σ_{ij} are the stresses, ϵ_{ij} the strains and $C_{ijk\ell}$ and $S_{ijk\ell}$ elastic constants. Summation over repeated indices is implied. In an isotropic medium

$$C_{ijk\ell} = C_{12}\, \delta_{ij}\, \delta_{k\ell} + C_{44}(\delta_{ik}\, \delta_{j\ell} + \delta_{i\ell}\, \delta_{jk}), \tag{3}$$

where C_{12} and C_{44} are elastic constants and

$$\delta_{ij} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{else.} \end{cases} \tag{4}$$

Correspondingly

$$S_{ijk\ell} = S_{12}\, \delta_{ij}\, \delta_{k\ell} + S_{44}(\delta_{ik}\, \delta_{j\ell} + \delta_{i\ell}\, \delta_{jk}). \tag{5}$$

Thus

$$\epsilon_{ij} = S_{12}\, \delta_{ij}\, \sigma_{\ell\ell} + 2S_{44}\, \sigma_{ij}. \tag{6}$$

For the strain in the $\underline{n}$-direction one finds

$$\epsilon(\underline{n}) = n_i n_j \epsilon_{ij} = S_{12}\, \sigma_{\ell\ell} + 2S_{44}\, n_i n_j \sigma_{ij}. \tag{7}$$

For the case of stresses at a surface, chosen to be the x_1x_2-plane this gives

$$\epsilon(\underline{n}) = S_{12}(\sigma_{11}+\sigma_{22}) + 2S_{44}(n_1^2\sigma_{11}+n_2^2\sigma_{22}+2n_1n_2\sigma_{12}), \tag{8}$$

since

$$\sigma_{3i} = \sigma_{i3} = 0 \qquad i = 1 \text{ to } 3. \tag{9}$$

For (see Fig 1)

$$\begin{aligned} n_1 &= -\sin\theta \sin\Psi \\ n_2 &= \cos\theta \\ n_3 &= \sin\theta \cos\Psi \end{aligned} \tag{10}$$

this leads to

$$\varepsilon(\theta, \Psi) = S_{12}(\sigma_{11}+\sigma_{22}) + 2S_{44}(\sin^2\theta \sin^2\Psi\, \sigma_{11}+\cos^2\theta\, \sigma_{22}- -2\sin\theta \cos\theta \sin\Psi\, \sigma_{12}). \tag{11}$$

For

$$\sigma_{12} = 0 \tag{12}$$

this gives

$$\frac{\partial\varepsilon(\theta,\Psi)}{\partial\sin^2\Psi} = 2S_{44} \sin^2\theta\, \sigma_{11} \tag{13}$$

$$\varepsilon(\theta, 0) = S_{12}(\sigma_{11}+\sigma_{22}) + 2S_{44} \cos^2\theta\, \sigma_{22}. \tag{14}$$

Since θ is to a good approximation determined by the choice of diffraction line corresponding to a certain reflecting plane σ_{11} can be found from a measurement of the difference in plane spacing between two values of Ψ. For another often employed choice for $\underline{n}$ (Fig 2) one finds, since $n_2 = 0$

$$\varepsilon(\underline{n}) = S_{12}(\sigma_{11}+\sigma_{22}) + 2S_{44}\, n_1^2\, \sigma_{11} \tag{15}$$

and thus

$$\frac{\partial\varepsilon(n)}{\partial n_1^2} = 2S_{44}\, \sigma_{11} \tag{16}$$

$$\varepsilon(n_1=0) = S_{12}(\sigma_{11}+\sigma_{22}) \tag{17}$$

that is the same method that can be used to find σ_{11} as in the previous case although σ_{12} can not be found. Notice however that in the first approach it was assumed that $\sigma_{12} = 0$. More measurements are needed if the principal stress directions are not known.

The above results were found using the assumption of isotropic elastic response. Unfortunately single crystal data show a markedly anisotropic elastic behaviour. For a cubic material the elastic constants are, in a coordinate system indicated by ^{o} with the axes parallel to the cubic axes of the material (see e g Dederichs and Leibfried [11])

$$C^o_{ijk\ell} = C_{12}\,\delta_{ij}\delta_{k\ell} + C_{44}(\delta_{ik}\delta_{j\ell}+\delta_{i\ell}\delta_{jk}) + d\,\delta_{ijk\ell} \tag{18}$$

where

$$d = C_{11} - C_{12} - 2C_{44} \tag{19}$$

and

$$\delta_{ijk\ell} = \begin{cases} 1 & \text{if } i = j = k = \ell \\ 0 & \text{else} \end{cases} \tag{20}$$

For an isotropic material one thus has

$$d = 0$$

or (21)

$$C_{44} = (C_{11} - C_{12})/2 \quad .$$

Similarly $S^o_{ijk\ell}$ contains an extra term $r\delta_{ijk\ell}$ where

$$r = S_{11} - S_{12} - 2S_{44}. \tag{22}$$

Further the transformation properties are (see e g Hirth and Lothe [10])

$$C_{ijk\ell} = T_{im}\,T_{jk}\,T_{ko}\,T_{\ell p}\,C^o_{mnop} \tag{23}$$

with

$$x_i = T_{im}\,x^o_m \tag{24}$$

and

$$x^o_m = T_{im}\, x_i. \tag{25}$$

T_{im} is the cosine for the angle between the x_i and x^o_m axes.

Since obviously the isotropic part of the elastic constants is not influenced by the coordinate transformation one finds

$$S_{ijk\ell} = S_{12}\,\delta_{ij}\delta_{k\ell} + S_{44}(\delta_{ik}\delta_{j\ell} + \delta_{i\ell}\,\delta_{jk}) + + r \sum_{m=1}^{3} T_{im}\,T_{jm}\,T_{km}\,T_{\ell m}. \tag{26}$$

This leads to

$$\varepsilon_{ij} = S_{12}\,\delta_{ij}\,\sigma_{\ell\ell} + 2S_{44}\,\sigma_{ij} + r \sum_{m=1}^{3} T_{im}\,T_{jm}\,T_{km}\,T_{\ell m}\,\sigma_{k\ell} \tag{27}$$

and

$$\varepsilon(\underline{n}) = S_{12}\,\sigma_{\ell\ell} + 2S_{44}\,n_i n_j \sigma_{ij} + r \sum_{m=1}^{3} (n_i T_{im})^2\,T_{km}\,T_{\ell m}\,\sigma_{k\ell}. \tag{28}$$

Notice that

$$n_i\,T_{im} = n^o_m \tag{29}$$

$$T_{km}\,T_{\ell m}\,\sigma_{k\ell} = \sigma^o_{mm} \qquad \text{(no summation over m)} \tag{30}$$

and

$$n_i n_j \sigma_{ij} = \sigma(\underline{n}). \tag{31}$$

$\underline{n}$ is given from the experimental situation to be the normal to a specific set of reflecting planes and $\underline{n}^o$ is thus also known. The orientation of the reflecting grain is however not known with regard to a rotation around $\underline{n}$. The transformation from x_i to an intermediate coordinate system x_i' where the x_3'-axis points in the $\underline{n}$-direction can be done by three successive rotations (see Fig 3). Take first a rotation Ψ around x_2, then a rotation κ around the new x_3 (the incident beam direction) and last a rotation $-(\frac{\pi}{2} - \theta)$ around the new x_1. For the first case studied above

(Fig 1) $\kappa = 0$ and for the second case (Fig 2) $\kappa = -\pi/2$. In order to transform from x_i' to x_i^o a rotation of an angle $-\kappa$ around $\underline{n} = x_3'$ is performed so that the new x_1- and x_2-axes are made to coincide with some suitably chosen directions in the x_i^o-system. Then a transformation is made from this particularly chosen coordinate system into x_i^o. The matrix for transformation from x_i^o to x_i' will be called T^o and from x_i' to x_i as T'.

Thus (T^T is the transpose of T and in this case is thus also the inverse of T)

$$(T')^T = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \sin\theta & -\cos\theta \\ 0 & \cos\theta & \sin\theta \end{pmatrix} \begin{pmatrix} \cos\kappa & \sin\kappa & 0 \\ -\sin\kappa & \cos\kappa & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \cos\Psi & 0 & \sin\Psi \\ 0 & 1 & 0 \\ -\sin\Psi & 0 & \cos\Psi \end{pmatrix} =$$

$$= \begin{pmatrix} 1 & 0 & 0 \\ 0 & \sin\theta & -\cos\theta \\ 0 & \cos\theta & \sin\theta \end{pmatrix} \begin{pmatrix} \cos\kappa\cos\Psi & \sin\kappa & \cos\kappa\sin\Psi \\ -\sin\kappa\cos\Psi & \cos\kappa & -\sin\kappa\sin\Psi \\ -\sin\Psi & 0 & \cos\Psi \end{pmatrix} =$$

$$= \begin{pmatrix} \cos\kappa\cos\Psi & \sin\kappa & \cos\kappa\sin\Psi \\ -\sin\kappa\sin\theta\cos\Psi+\cos\theta\sin\Psi & \cos\kappa\sin\theta & -\sin\kappa\sin\theta\sin\Psi-\cos\theta\cos\Psi \\ -\sin\kappa\cos\theta\cos\Psi-\sin\theta\sin\Psi & \cos\kappa\cos\theta & -\sin\kappa\cos\theta\sin\Psi+\sin\theta\cos\Psi \end{pmatrix} . \tag{32}$$

For $\kappa = 0$ this gives

$$T'(0) = \begin{pmatrix} \cos\Psi & 0 & -\sin\theta\sin\Psi \\ 0 & \sin\theta & \cos\theta \\ \sin\Psi & -\cos\theta\cos\Psi & \sin\theta\cos\Psi \end{pmatrix} . \tag{33}$$

For $\kappa = -\frac{\pi}{2}$ one finds

$$T'(-\tfrac{\pi}{2}) = \begin{pmatrix} 0 & \sin\theta\cos\Psi+\cos\theta\sin\Psi & \cos\theta\cos\Psi-\sin\theta\sin\Psi \\ -1 & 0 & 0 \\ 0 & \sin\theta\sin\Psi-\cos\theta\cos\Psi & \cos\theta\sin\Psi+\sin\theta\cos\Psi \end{pmatrix} =$$

$$= \begin{pmatrix} 0 & \sin(\theta+\Psi) & \cos(\theta+\Psi) \\ -1 & 0 & 0 \\ 0 & -\cos(\theta+\Psi) & \sin(\theta+\Psi) \end{pmatrix} . \tag{34}$$

In order to evaluate the transformation from x_i^o to x_i' an intermediate coordinate system x_i'' is introduced with coordinate axes

$$\left.\begin{aligned} x_1'' &= \frac{1}{\sqrt{n_1^{o2}+n_2^{o2}}}\left(-n_3^o n_1^o,\ -n_3^o n_2^o,\ n_1^{o2}+n_2^{o2}\right) \\ x_2'' &= \frac{1}{\sqrt{n_1^{o2}+n_2^{o2}}}\left(n_2^o,\ -n_1^o,\ 0\right) \\ x_3'' &= \left(n_1^o,\ n_2^o,\ n_3^o\right) \end{aligned}\right\} \qquad (35)$$

where n_1^o, n_2^o and n_3^o are the coordinates of $\underline{n}$ in the x_i^o-system. With

$$x_i'' = T_{ij}'' x_i^o \qquad (36)$$

one finds

$$T_{ij}'' = \begin{pmatrix} -\frac{n_3^o n_1^o}{\sqrt{n_1^{o2}+n_2^{o2}}} & -\frac{n_3^o n_2^o}{\sqrt{n_1^{o2}+n_2^{o2}}} & \sqrt{n_1^{o2}+n_2^{o2}} \\ \frac{n_2^o}{\sqrt{n_1^{o2}+n_2^{o2}}} & -\frac{n_1^o}{\sqrt{n_1^{o2}+n_2^{o2}}} & 0 \\ n_1^o & n_2^o & n_3^o \end{pmatrix}. \qquad (37)$$

The above choice of the x_i''-system can in the case of cubic symmetry always be done since at least one of n_1^o, n_2^o and n_3^o is different from zero and all permutations of n_1^o, n_2^o and n_3^o represent the same type of planes.

For T^o it is found that

$$T_{ij}^o = T_{ik}^{\varphi}\, T_{kj}'' \qquad (38)$$

with

$$T^{\varphi} = \begin{pmatrix} \cos\varphi & \sin\varphi & 0 \\ -\sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{pmatrix}. \qquad (39)$$

Finally

$$T_{ij} = T_{ik}{}' \; T_{k\ell}{}^{\varphi} \; T_{\ell j}{}''. \tag{40}$$

The anisotropic contribution to the strain $\epsilon(\underline{n})$ is thus found to be

$$\epsilon^{A}(\underline{n}) = r \sum_{m=1}^{3} (n_i T_{im})^2 \; T_{km} T_{\ell m} \sigma_{k\ell} = r \sum_{m=1}^{3} T_{km} n_m{}^{o} T_{\ell m} n_m{}^{o} \sigma_{k\ell} =$$

$$= r \; \sigma_{k\ell} \sum_{m=1}^{3} T_{ko}{}' T_{op}{}^{\varphi} T_{pm}{}'' \, n_m{}^{o} \; T_{\ell q}{}' T_{qr}{}^{\varphi} T_{rm}{}'' \, n_m{}^{o} \tag{41}$$

Since the X-ray measurement yields an average over φ this average has to be worked out.

If, according to the model of Reuss, the stresses in all grains are considered to be the same then the average of $\epsilon^{A}(\underline{n})$ over φ is

$$\overline{\epsilon^{A}(\underline{n})}^{\varphi,\,\mathrm{Reuss}} = r \; \sigma_{k\ell} \{ \tfrac{1}{2} (T_{k1}{}' T_{\ell 1}{}' + T_{k2}{}' T_{\ell 2}{}') \sum_{m=1}^{3} [(T_{1m}{}'' n_m{}^{o})^2 +$$

$$+ (T_{2m}{}'' n_m{}^{o})^2] + T_{k3}{}' T_{\ell 3}{}' \sum_{m=1}^{3} (T_{3m}{}'' n_m{}^{o})^2 + \tfrac{1}{2} (T_{k1}{}' T_{\ell 2}{}' -$$

$$- T_{k2}' T_{\ell 1}') \sum_{m=1}^{3} T_{1m}{}'' n_m{}^{o} T_{2m}'' n_m{}^{o} \}. \tag{42}$$

Now

$$T_{k3}{}' = n_k \tag{43}$$

$$T_{3m}{}'' = n_k{}^{o} \tag{44}$$

$$T_{k1}{}' T_{\ell 1}{}' + T_{k2}{}' T_{\ell 2}{}' = T_{ki}{}' T_{\ell i}{}' - T_{k3}{}' T_{\ell 3}{}' = \delta_{k\ell} - n_k n_\ell \tag{45}$$

$$T_{1m}{}'' T_{1n}{}'' + T_{2m}{}'' T_{2n}{}'' = \delta_{mn} - n_m{}^{o} n_n{}^{o} \tag{46}$$

and

$$\sigma_{k\ell} = \sigma_{\ell k}. \tag{47}$$

Thus

$$\overline{\epsilon^{A}(\underline{n})}^{\varphi,\mathrm{Reuss}} = r\,\sigma_{k\ell}\{\tfrac{1}{2}(\delta_{k\ell}-n_k n_\ell)(1-\sum_{m=1}^{3} n_m^{o4}) + n_k n_\ell \sum_{m=1}^{3} n_m^{o4} =$$

$$= r\,\tfrac{1}{2}(1-\sum_{m=1}^{3} n_m^{o4})\sigma_{\ell\ell} - r\,\tfrac{1}{2}(1-3\sum_{m=1}^{3} n_m^{o4}) n_k n_\ell\,\sigma_{k\ell}\}. \qquad (48)$$

This can be rewritten in terms of

$$\Gamma^{o} = \tfrac{1}{2}(1-\sum_{m=1}^{3} n_m^{o4}) = \sum_{m=1}^{3} n_m^{o2} n_{m+1}^{o2} = \frac{h^2k^2+k^2\ell^2+\ell^2k^2}{(h^2+k^2+\ell^2)^2} \qquad (49)$$

where h, k and ℓ are the Miller indices of the reflecting plane.

Adding the isotropic contribution gives finally

$$\overline{\epsilon(\underline{n})}^{\varphi,\mathrm{Reuss}} = (S_{12}+r\Gamma^{o})\sigma_{\ell\ell} + (2S_{44}+r-3r\Gamma^{o}) n_k n_\ell \sigma_{k\ell} =$$

$$= (S_{12}+r\Gamma^{o})\sigma_{\ell\ell} + (S_{11}-S_{12}-3r\Gamma^{o}) n_k n_\ell \sigma_{k\ell}, \qquad (50)$$

which is the result given by for instance Macherauch [1]. The result can also be expressed in terms of the unnormalized cubic harmonic

$$K^{(4)}(\underline{n}^{o}) = 3 - 5\sum_{m=1}^{3} n_m^{o4} = 10\,\Gamma^{o} - 2 \qquad (51)$$

Since the average over all $\underline{n}^{o}$ of the cubic harmonic is zero one finds for the average over all angles, the ordinary Reuss average

$$\overline{\epsilon(\underline{n})}^{\mathrm{Reuss}} = (S_{12}+r/5)\sigma_{\ell\ell} + (2S_{44}+2r/5) n_k n_\ell \sigma_{k\ell}. \qquad (52)$$

This result is given for instance by Hirth and Lothe [10].

Notice that the Voigt average elastic constants, where the strain is assumed to be the same in all grains, is obtained if ϵ_{ij}, σ_{ij} and $S_{ijk\ell}$ are replaced by σ_{ij}, ϵ_{ij} and $C_{ijk\ell}$ respectively.

3. AVERAGE STRESS-STRAIN RELATION

The assumptions of constant strain (Voigt) or constant stress (Reuss) are obviously not correct. Hill [12] showed, however, that these values give upper and lower limits. Kröner [2] used the solution to the ellipsoidal inclusion problem given by Eshelby [3] and determined elastic constants so that both stress and strain compatibility is obtained. These constants were derived in a self-consistent manner and were given in explicit form by Kröner when the average crystal is istotropic (that is with a random distribution of grain orientations). Solutions for non-isotropic average crystals have been worked out later [4, 5]. These solutions require quite a lot of computer calculation but the influence of texture can be estimated. The case of a heterogenous material has also been studied [6]. Most of these mentioned treatments have been interested in average polycrystal elastic constants and not the ones relevant for X-ray stress determination. For the X-ray elastic constants the average searched for is over the orientation range determined by rotations around the chosen reflection normal. Equations for X-ray elastic constants have been given for average isotropic crystals where the single crystals have cubic [7] or hexagonal [8] symmetry. The stress-strain relation can be written as

$$\epsilon_{ij}(\Omega) = (s_{ijk\ell} + T_{ijk\ell}(\Omega))\sigma_{k\ell}. \tag{53}$$

Here $\epsilon_{ij}(\Omega)$ is the strain in a single crystal grain with the orientation determined by Ω and where $\sigma_{k\ell}$ is the externally applied stress. $s_{ijk\ell}$ are the elastic compliance constants of the average isotropic crystal. These have to be calculated from the single crystal elastic constants. $T_{ijk\ell}(\Omega)$ are extra elastic constants which account for a correction due to the constraining effect of the surrounding matrix on the grain of interest. Equation (53) can be interpreted in terms of elastic polarization in much the same way as is done in a dielectric.

The results for an average isotropic crystal composed of single crystals of cubic symmetry were given by Bollenrath et al [7]. Due to the symmetry one can write

$$s_{ijk\ell} = s_{44}(\delta_{ik}\delta_{j\ell} + \delta_{i\ell}\,\delta_{jk}) + s_{12}\,\delta_{ij}\delta_{k\ell} \tag{54}$$

$$T_{ijk\ell} = T_{44}(\delta_{ik}\delta_{j\ell} + \delta_{i\ell}\delta_{jk}) + T_{12}\,\delta_{ij}\delta_{k\ell} + T_o\,\delta_{ijk\ell} \tag{55}$$

with

$$T_o \equiv T_{11} - T_{12} - 2T_{44} \tag{56}$$

The evaluation of the constants is most easily done from expressions for the tensor invariants.

From the given single crystal data C_{ij} is first evaluated

$$3K \equiv C_{11} + 2C_{12} \tag{57}$$

$$\mu \equiv C_{44} \tag{58}$$

$$2\nu \equiv C_{11} - C_{12}. \tag{59}$$

From this follows directly, due to the cubic symmetry, that the bulk modulus for the isotropic average crystal is

$$3(s_{11} + 2s_{12}) = \frac{1}{K}. \tag{60}$$

Further the average shear modulus G is found from

$$G^3 + \alpha G^2 + \beta G + \gamma = 0 \tag{61}$$

with

$$\alpha = \frac{9K + 4\nu}{8} \tag{62}$$

$$\beta \doteq - \frac{(3K + 12\nu)\mu}{8} \tag{63}$$

$$\gamma = - 3K\mu\nu/4. \tag{64}$$

s_{11} and s_{12} can be determined from equation (60) and

$$2(s_{11} - s_{12}) = \frac{1}{G}. \tag{65}$$

Further, due to isotropy

$$s_{44} = \frac{1}{2}(s_{11} - s_{12}) \equiv \frac{1}{4G}. \tag{66}$$

The T_{ij}-s are evaluated from

$$T_{44} = \frac{(G-\mu)(3K+6G)}{2G[8G^2+G(9K+12\mu) + 6K\mu]} \tag{67}$$

$$T_{12} = T_{44} \tag{68}$$

$$T_{11} = -2T_{44}. \tag{69}$$

As a check one can use

$$T_{11} - T_{12} = \frac{(G-\nu)(3K+6G)}{G[8G^2+G(9K+12\nu)+6\nu K]}. \tag{70}$$

The average values for the elastic X-ray constants are found in a similar way as was used for the modified Reuss averages. That is,

$$\bar{\epsilon}(\underline{n}^o) = [s_{12}+T_{12}+T_o\Gamma^o]\sigma_{\ell\ell} + [2s_{44}+2T_{44}+T_o-3T_o\Gamma^o]n_k n_\ell \sigma_{k\ell} \equiv$$

$$\equiv (s_{12}+T_{12}+T_o\Gamma^o)\sigma_{\ell\ell} + (s_{11}-s_{12}+T_{11}-T_{12}-3\Gamma^o T_o)n_k n_\ell \sigma_{k\ell}. \tag{71}$$

Since

$$2s_{44} = s_{11} - s_{12} \tag{72}$$

due to isotropy and

$$T_o \equiv T_{11} - T_{12} - 2T_{44}. \tag{73}$$

This thus gives the best choice for X-ray elastic constants - in the elastic range. With a customary notation (for instance Macherauch [1])

$$s_1 = s_{12} + T_{12} + \Gamma^o T_o \tag{74}$$

$$\frac{1}{2}s_2 = s_{11}-s_{12}+T_{11}-T_{12}-3\Gamma^o T_o = 2s_{44}+2T_{44}+(1-3\Gamma^o)T_o \tag{75}$$

A computer program has been written which evaluates these elastic constants. As an example data are given for Fe and UO_2 in Fig 4.

In order to investigate the line broadening due to elastic anisotropy a computer program was written which evaluates the strains in grains with different angles of rotation around the diffraction plane normal. Data are given for one case in Fig 5. The broadening is found to be small and is further reduced if Kröner's elastic constants are used in stead of single crystal elastic constants.

4. INFLUENCE OF FREE INTERSTITIALS

Free interstitials which can change to new positions when acted upon by an applied stress influence the elastic response of the medium. Examples are free carbon or nitrogen interstitials in steel. This effect can be taken into account through a change in the single crystal elastic constants used to evaluate the polycrystal line response.

For the case of tetragonal point defects in a cubic medium one has (see for instance Kröner [13] or Nowick and Heller [14])

$$\delta C_{ijk\ell} = - \frac{n}{9kT} (\Delta P)^2 (3\delta_{ijk\ell} - \delta_{ij}\delta_{k\ell}) \tag{76}$$

where $\delta C_{ijk\ell}$ is the change in the elastic constants, n the number per unit volume of free interstitials, k Boltzmann's constant, T the absolute temperature and ΔP the difference in dipole moment between the two types of sites. Thus for instance with $P_{11} \neq P_{22} = P_{33}$ and all other zero

$$\Delta P = P_{11} - P_{22} \tag{77}$$

Also

$$\delta S_{ijk\ell} = \frac{n}{9kT} (\Delta P)^2 (S_{11} - S_{12})^2 (3\delta_{ijk\ell} - \delta_{ij}\delta_{k\ell}) \tag{78}$$

The dipole moments can be evaluated from the change in lattice parameter with concentration of interstitials (Kröner [15])

$$P_{ij} = \frac{1}{n} C_{ijk\ell} \epsilon_{k\ell}^{G} \tag{79}$$

where $\epsilon_{k\ell}^{G}$ is the strain measured as a change in lattice constant due to n interstitials per unit volume.

As an example consider C in Fe. Kröner [15] gives

$$\left.\begin{aligned} P_{11} &= 11.2 \text{ eV} \\ P_{22} = P_{33} &= 4.6 \text{ eV} \end{aligned}\right\} \tag{80}$$

For 1 w% C ($n^{-1} = 2.58 \cdot 10^{-22}$ cm^3) at room temperature (kT = 0.025 eV) one finds

$$\delta C_{ijk\ell} = -12.0 \cdot 10^{11} (3\delta_{ijk\ell} - \delta_{ij}\delta_{k\ell}) \text{ dyn/cm}^2 \tag{81}$$

For Fe the elastic constants are, in units of 10^{11} dyn/cm^2 (ref [16])

$$C_{11} = 22.9 \\ C_{12} = 13.4 \\ C_{44} = 11.5 \tag{82}$$

and the changes found are (in 10^{11} dyn/cm^2)

$$\delta C_{11} = -24.0 \cdot \alpha \\ \delta C_{12} = 12.0 \cdot \alpha \\ \delta C_{44} = \delta C_{1212} = 0 \tag{83}$$

where α is the concentration of free carbon interstitials in w%. The influence is thus negligible for concentrations less than 0.01 w%.

5. SUMMARY

The elastic constants to be used in X-ray stress measurements have been studied. In a cubic texture-free medium the strain $\varepsilon(\underline{n})$ related to the measured change in plane spacing for planes with normal $\underline{n}$ is

$$\varepsilon(\underline{n}) = (s_{12}+T_{12}+\Gamma^o T_o)(\sigma_{11}+\sigma_{22}) + \\ + (2s_{44}+2T_{44}+(1-3\Gamma^o)T_o)(n_1{}^2\sigma_{11}{}^2+n_2{}^2\sigma_{22}{}^2+2n_1n_2\sigma_{12}) \tag{84}$$

Γ^o depends on the reflecting plane used and is given in equation (49). The method to evaluate s_{ij}, T_{ij} and T_o due to Kröner was described in part 3.

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FIGURE CAPTIONS

Fig 1 Stereographic projection of the configuration where the reflecting plane normal $\underline{n}$ and the incident beam direction $\underline{i}$ lie in a plane perpendicular to the plane in which the specimen normal $\hat{x}_3$ is tilted an angle Ψ relative to $\underline{i}$.

Fig 2 Stereographic projection of the configuration where the reflecting plane normal $\underline{n}$, the incident beam direction $\underline{i}$ and the specimen normal $\hat{x}_3$ lie in the same plane.

Fig 3 Definition of angles Ψ, κ and $\frac{\pi}{2} - \theta$ for rotation of the coordinate system $x_1x_2x_3$ so that $\hat{x}_3$ is made to coincide with the reflecting plane normal $\underline{n}$.

Fig 4 Kröner average X-ray elastic constants. s_1 and $s_2/2$, equations (74), and (75), as a function of Γ^o, equation (49). Single crystal data are from ref [16].
Fe: $C_{11} = 22.9$, $C_{12} = 13.4$ and $C_{44} = 11.5$ (10^4 MPa).
UO_2: $C_{11} = 39.6$, $C_{12} = 12.1$ and $C_{44} = 6.41$ (10^4 MPa).
Notice the scales and the zero point suppression.

Fig 5 Strain as a function of angle of rotation around the reflecting plane normal $\underline{n}$. $\underline{n}^o = (310)$. $\sigma_{11} = 200$ MPa, all other stresses zero. Material Fe with single crystal data from ref [16].
Single crystal: $S_{11} = 0.764$, $S_{12} = -0.281$, $S_{44} = 0.218$ (10^{-5} $(\text{MPa})^{-1}$)
Kröner: $S_{11} = 0.579$, $S_{12} = -0.189$, $S_{44} = 0.257$ (10^{-5} $(\text{MPa})^{-1}$).

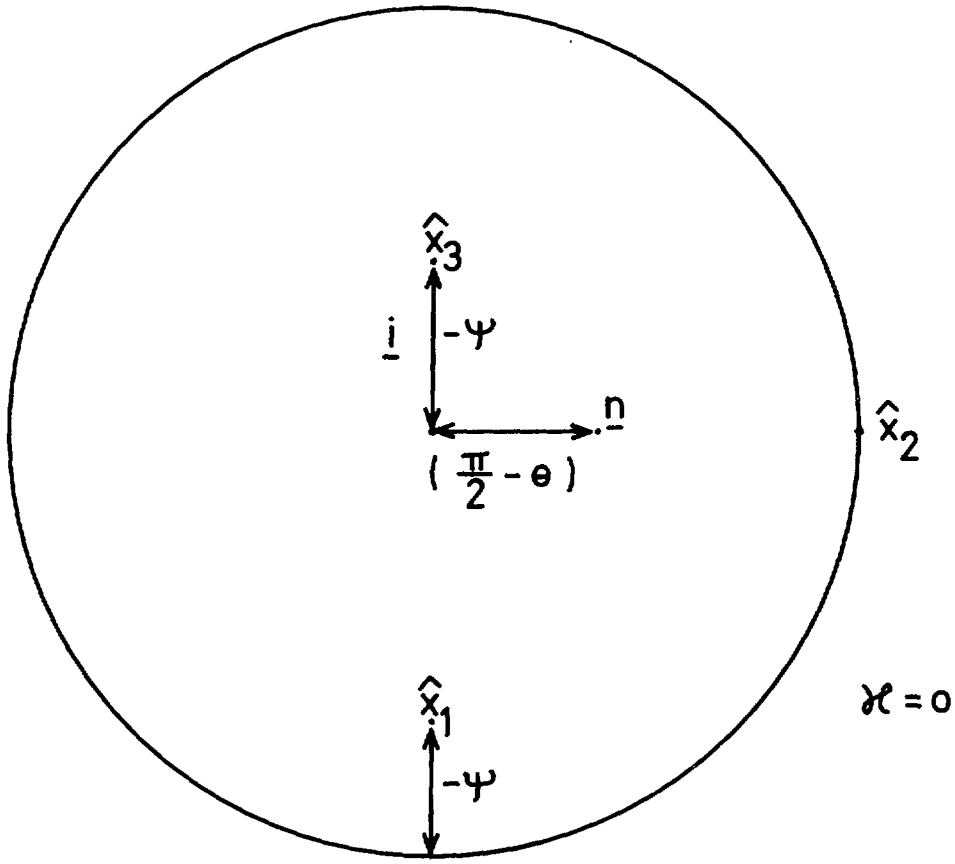

$\hat{x}_3$
$\underline{i}$
$-\psi$
$\underline{n}$
$\hat{x}_2$
$(\frac{\pi}{2} - \theta)$
$\hat{x}_1$
$\varkappa = 0$
$-\psi$

Fig 1

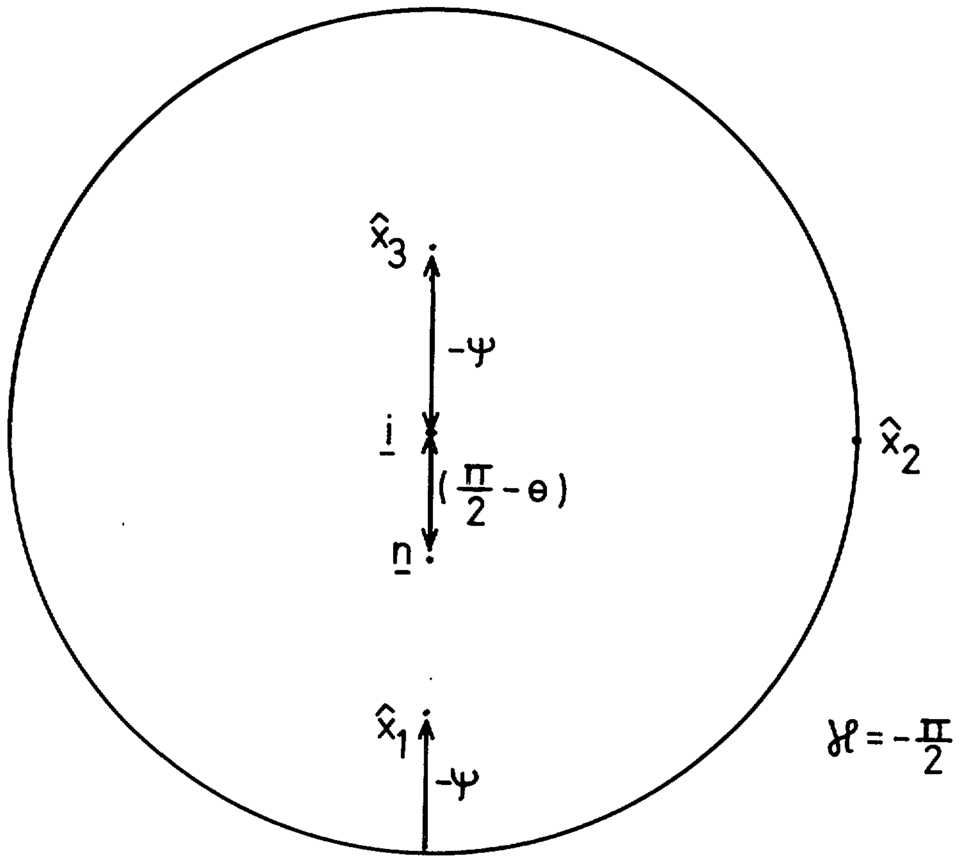
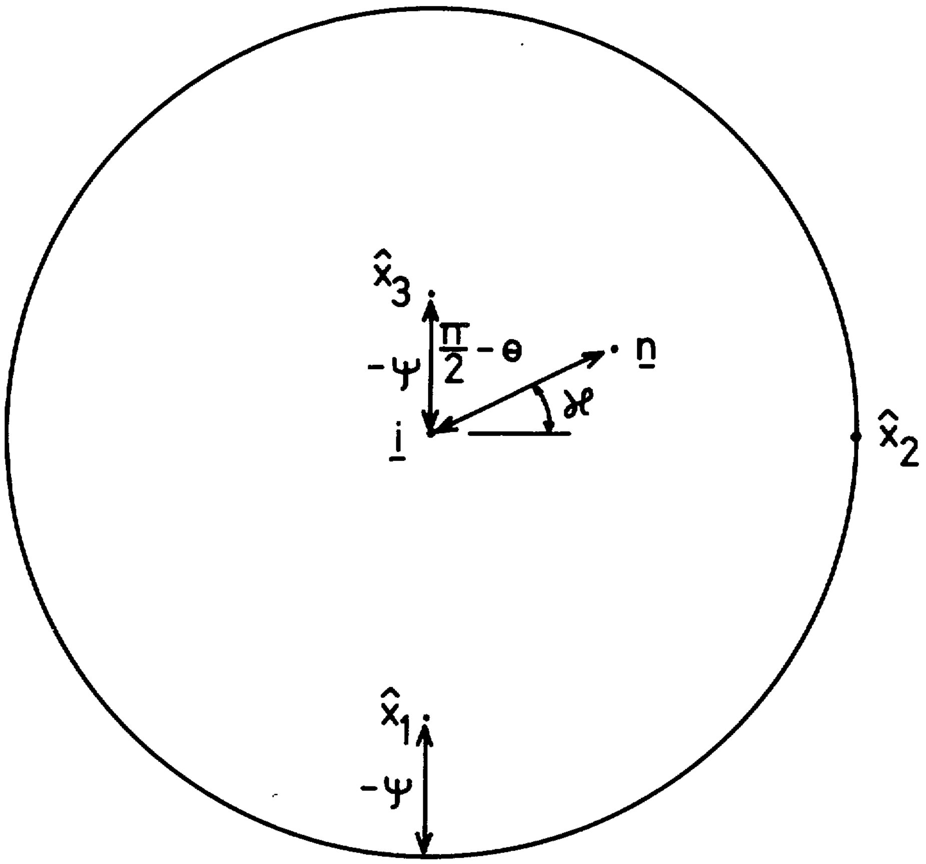
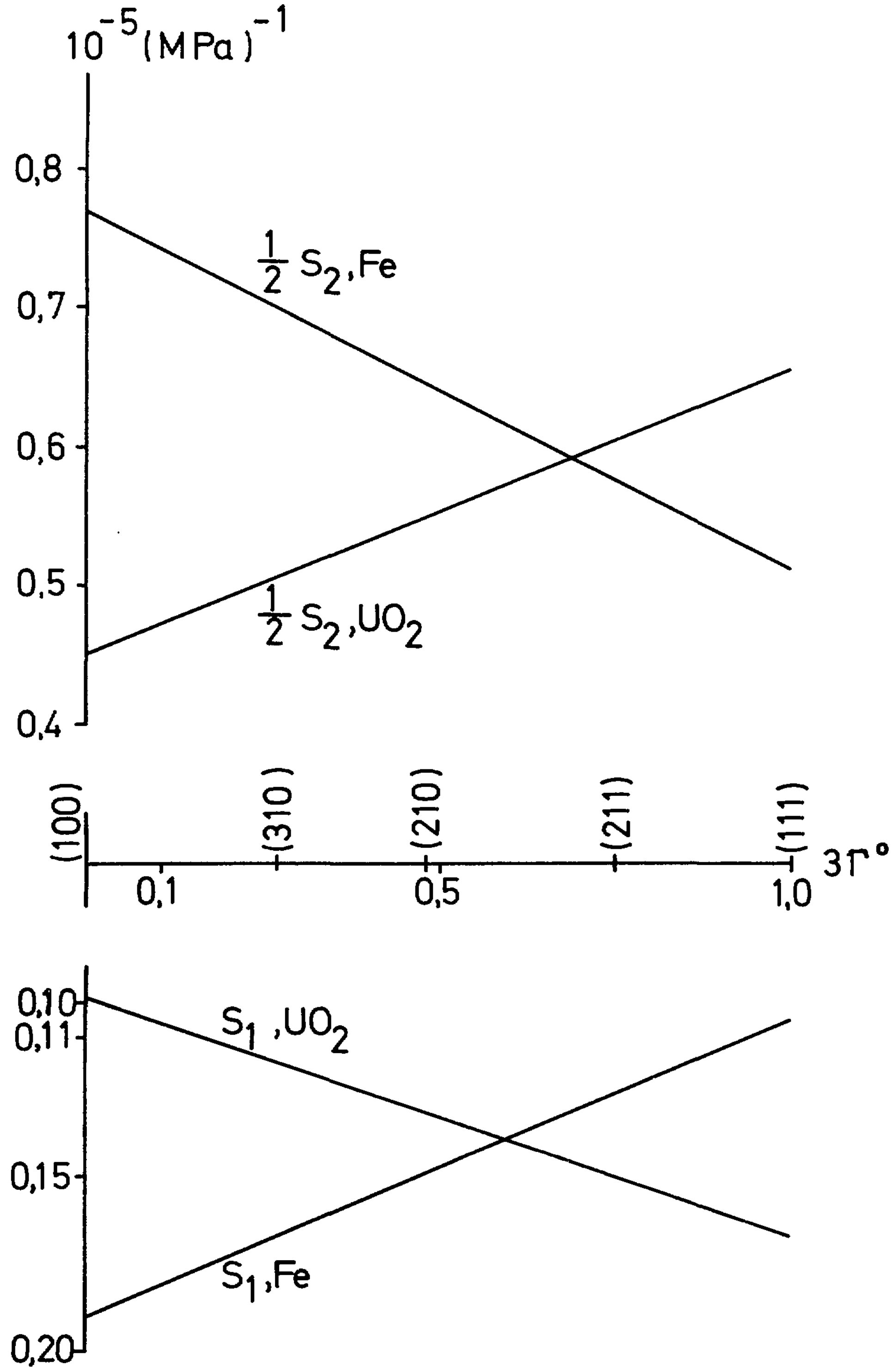

$\hat{x}_3$
$-\psi$
$\underline{i}$
$(\frac{\pi}{2}-\theta)$
$\underline{n}$
$\hat{x}_2$
$\hat{x}_1$
$-\psi$
$\mathcal{H}=-\frac{\pi}{2}$

Fig 2



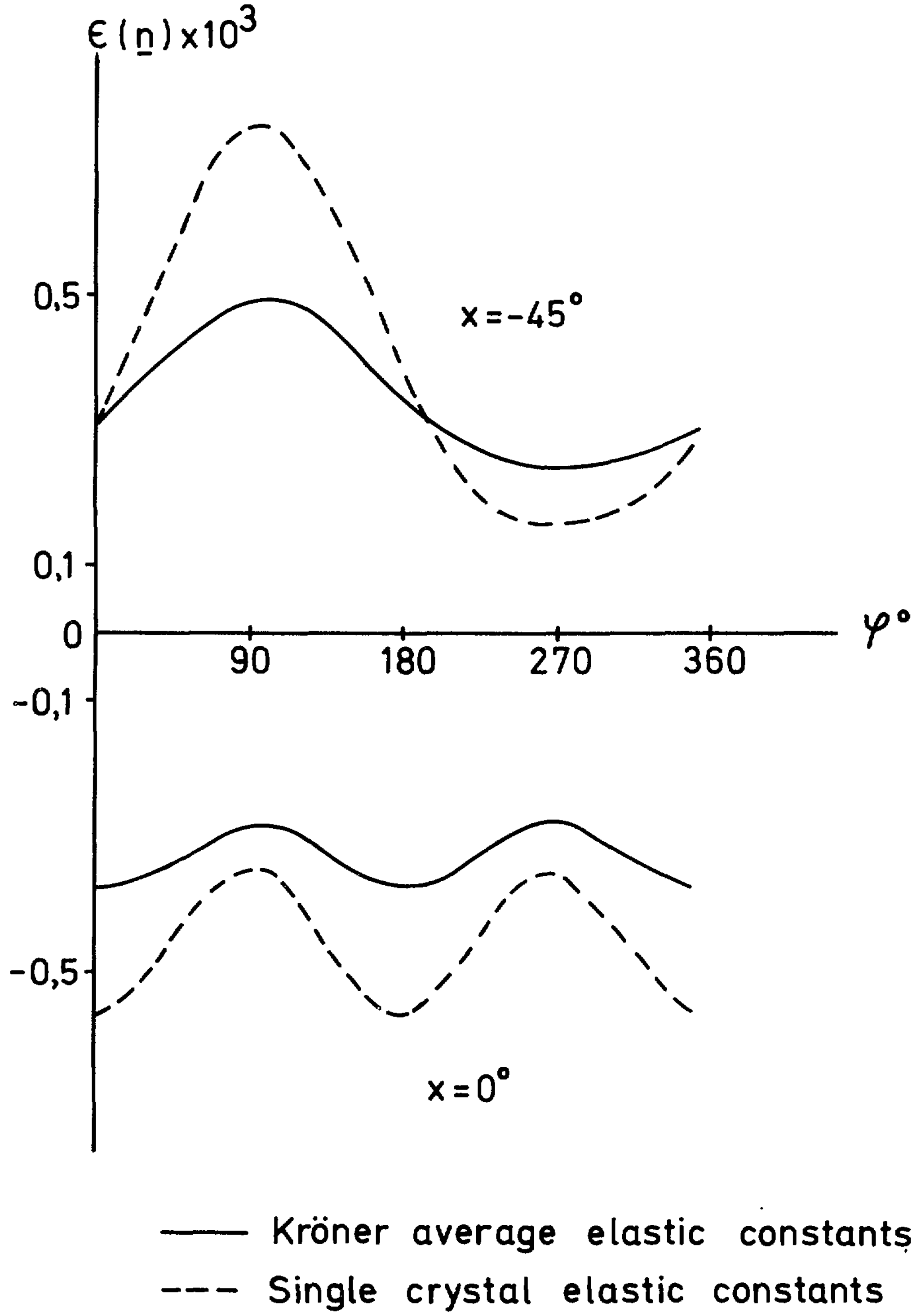
$\hat{x}_3$
$\frac{\pi}{2} - \theta$
$-\psi$
$\underline{n}$
$\varkappa$
$\underline{i}$
$\hat{x}_2$
$\hat{x}_1$
$-\psi$

Fig 3



10⁻⁵ (MPa)⁻¹
0,8
0,7
0,6
0,5
0,4
1/2 S2, Fe
1/2 S2, UO2
(100)
(310)
(210)
(211)
(111)
0,1
0,5
1,0
3Γ°
0,10
0,11
0,15
0,20
S1, UO2
S1, Fe

Fig 4



ϵ(n)x10^3
0,5
0,1
0
-0,1
-0,5
90
180
270
360
φ°
x=-45°
x=0°
Kröner average elastic constants
Single crystal elastic constants

Fig 5

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