J. Appl. Cryst. (1988). **21**, 59–66

X-ray Diffraction Line Broadening Due to Dislocations in Non-Cubic Materials. I. General Considerations and the Case of Elastic Isotropy Applied to Hexagonal Crystals

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(*Received 5 January* 1987; *accepted* 28 *September* 1987)

Abstract

Use is made of the theory of dislocation-induced X-ray diffraction line broadening in the form presented by Krivoglaz, Martynenko & Ryaboshapka [*Fiz. Metall. Metalloved.* (1983), **55**, 5–17] to express the so-called orientation factors occurring in the relations of diffraction profile parameters (*e.g.* Fourier coefficients, line widths) in a form which systematically takes into account both the lattice geometry and the elastic behaviour of the scattering crystals. The formalism can be used, in principle, for any materials and types of dislocations. In the case of elastically isotropic media the orientation factors can be described by analytical expressions. The application of the formalism is demonstrated in some detail for various slip systems in hexagonal polycrystals with random orientation of grains.

1. Introduction

Dislocations in crystals are the so-called lattice defects of the second kind which destroy the long-range order of the crystal structure and cause significant X-ray diffraction line broadening. Appropriate theories leading to very similar predictions of dislocation-induced diffraction effects were elaborated by Krivoglaz *et al.* (Krivoglaz & Ryaboshapka, 1963; Ryaboshapka, 1965; Krivoglaz, Martynenko & Ryaboshapka, 1983; Krivoglaz, 1967) and by Wilkens (1970*a*, *b*, 1984). The results of the theoretical work have been verified and used successfully by several authors in investigations of the dislocation content of both plastically deformed single crystals (*e.g.* Dubrovskiy & Locko, 1968; Wilkens & Bargouth, 1968; Matucha, Franzbecker & Wilkens, 1969; Wilkens, 1976; Wilkens, Herz & Mughrabi, 1980; Karasevskaya & Ryaboshapka, 1980; Ungar, Mughrabi & Wilkens, 1982; Ungar, Mughrabi, Rönnpagel & Wilkens, 1984) and polycrystalline materials (*e.g.* Oettel, 1971, 1973; Dao Van Tan, 1972; Yamada, Tanaka & Furusawa, 1974; Klimanek, Grosse & Hensger, 1982; Klimanek, Scherke & Bergner, 1982; Wang Yuming, Lee Shanshan & Lee Yenchin, 1982; Wang Yuming & Zhang Zigung, 1984; Ungar, Toth, Illy & Kovacs, 1986; Tung, Zwui & Wang, 1986). Most of the experimental investigations were performed with cubic materials, of course. Although the influence of the elastic anisotropy was treated by Ryaboshapka (1965), Novominskiy & Ryaboshapka (1966) and more recently by Wilkens, Herz & Mughrabi (1980) (*cf.* also Ungar *et al.*, 1982, 1984), the evaluation of diffraction data was frequently based on the assumption that the scattering object is elastically isotropic. Particularly in X-ray profile analysis of technologically interesting polycrystalline objects with a cubic lattice such a treatment is possible since only one type of slip system, $\langle uvw\rangle\{hkl\}$, has to be taken into account; separation of different types of diffraction line broadening (*e.g.* particle size effect, stacking-fault broadening *etc.*) can be done by means of different reflection orders as, for instance, 110–220 for b.c.c. lattices or 111–222 in f.c.c. structures; and the influence of the elastic anisotropy can be neglected if a constant error in the absolute values of dislocation densities has no significant importance.

In investigations of plastically deformed non-cubic materials different types of slip systems $\langle uvw\rangle\{hkl\}$, must usually be taken into consideration, and the measurement of several corresponding reflection orders is often very difficult because of diffraction-peak overlapping. Moreover, as must be concluded from the work of Raychenko & Martynova (1970) the influence of the elastic anisotropy on the diffraction line broadening cannot in general be expected to be low. Therefore, with regard to the practical application of X-ray diffraction in the analysis of the dislocation content of non-cubic materials a more systematic treatment of the effects of the elastic anisotropy seems to be necessary. If the theory of Krivo-

0021-8898/88/010059-08$03.00

glaz (1967) is used for this purpose, the so-called orientation factors occurring in the expressions of the parameters (Fourier coefficients, line widths) of a diffraction line profile have to be calculated in a form which takes into account both the lattice geometry and the elastic behaviour of the scattering crystal. The present paper reports the results of such calculations which, in principle, can be used for any materials and dislocations (slip systems). After general considerations the scattering by elastically isotropic materials is discussed in some detail. In this case, which may be important in practice as an approximation, the orientation factors can be described by analytical expressions. Application of the formalism is demonstrated by explicit representation of the orientation factors for various slip systems in hexagonal polycrystals with random orientation of grains. The effect of the elastic anisotropy, which must be treated by numerical computation, will form the subject of part II of this work.

2. Formal interpretation of the dislocation-induced broadening of X-ray diffraction lines

2.1. *One slip system*

According to Krivoglaz (1967), Krivoglaz, Martynenko & Ryaboshapka (1983) and Wilkens (1970*a*, *b*) the intensity distribution of an X-ray diffraction peak due to a large crystal containing dislocations can be described (in electron units) by the expression

$$I_H(\mathbf{q}) = F_H^2 \sum_{\mathbf{R}} e^{i\mathbf{qR}} \exp[-T(\mathbf{R}, \mathbf{Q}\mathbf{u}_R, c_{ij})], \qquad (1)$$

where $\mathbf{H}$ is the reciprocal-lattice vector associated with the reflecting lattice planes (hkl) with interplanar spacing d_{hkl}; $\mathbf{Q} = (4\pi/\lambda)\mathbf{m}$ is the diffraction vector ($\mathbf{m}$ is a unit vector); $\mathbf{q} = \mathbf{Q} - \mathbf{H}$ is the distance from the point $\mathbf{H}$ of reciprocal space; F_H^2 is the structure factor of the lattice planes (hkl); $\mathbf{R} = \mathbf{n}R$ are distance vectors of the lattice-cell pairs in the perfect crystal structure; $\mathbf{u}_R$ is the dislocation-induced displacement vector of the cell pairs at distance R; and c_{ij} are elastic constants of the scattering crystal. The factor T in (1) depends on both the single-defect characteristics [Burgers vector $\mathbf{b}$, line vector $\boldsymbol{\tau}$, displacement field $\mathbf{u}(\mathbf{r})$] and the spatial distribution of the dislocations present in the scattering object. But if the influence of the defect arrangement is taken into account by means of correlation functions (Krivoglaz, Martynenko & Ryaboshapka, 1983, for instance) they are essentially determined by the quantities ($\mathbf{r} = \mathbf{n}'r$, where r is the distance from the dislocation line; see Fig. 1)

$$(\mathbf{Q}\mathbf{u}_{\mathbf{R},\alpha}) \simeq \mathbf{R}\partial(\mathbf{Q}\mathbf{u}_{\mathbf{r},\alpha})/\partial r = Qb_\alpha R\psi_\alpha(\mathbf{b}_\alpha, \boldsymbol{\tau}_\alpha, \mathbf{m}, \mathbf{n}, \mathbf{n}', c_{ij})/2\pi r \qquad (2)$$

associated with the long-range part ($R \ll r$) of the displacement fields $\mathbf{u}_{\mathbf{r},\alpha}$ of isolated dislocations on different slip systems α. An example for the calculation of $(\mathbf{Q}\mathbf{u}_{\mathbf{R}})$ and ψ is given in the Appendix.

Provided that only one active slip system must be taken into consideration (the index α can then be omitted), the function $T(R)$ is given by the equation

$$T(R) = [(Qb)^2/8\pi]\chi(\mathbf{m})\rho R^2 \ln(\eta R_c/R). \qquad (3)$$

ρ is the dislocation density, R_c denotes the outer cutoff radius of the dislocation strain field (Wilkens, 1970*a*, *b*) and η is a factor which depends weakly on the orientation distribution of the dislocations with respect to the diffraction vector $\mathbf{Q}$. The influence of the factor η increases with decreasing values of the ratio R_c/R, but if there is no strong defect correlation, $\ln \eta$ can be neglected in comparison with $\ln R_c/R$ in many cases. The effect of the diffraction vector orientation ($\mathbf{m}$) on the line broadening of the X-ray reflections is essentially determined by the so-called orientation factor $\chi(\mathbf{m})$ which is obtained by integration of the function ψ^2 over a polar coordinate φ associated with the slip plane of the dislocation:

$$\chi(\mathbf{m}) = (1/\pi) \int_0^{2\pi} \psi^2 \, \mathrm{d}\varphi. \qquad (4)$$

The procedure for the calculation of the quantity $\chi(\mathbf{m})$ will be described in § 3. In experimental investigations the intensity distribution of an X-ray reflection is usually measured by means of θ–2θ scanning (*i.e.* along the direction of the diffraction vector). Therefore, in order to obtain the diffraction-line profile parameters it is necessary to take $\mathbf{R} \parallel \mathbf{Q}$ in the calculations of the quantities T and χ, which leads to the following equations for the profile parameters.

The *Fourier coefficients* are defined by the simple relation

$$\ln A_n = -T(nd_{hkl}\mathbf{m}) = -T(L\mathbf{m}), \quad L = nd_{hkl} \qquad (5)$$

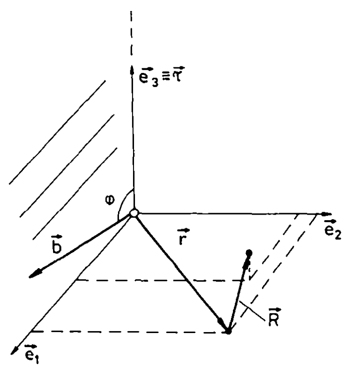

Fig. 1. Slip coordinate system is given by unit vectors $\mathbf{e}_1$, $\mathbf{e}_2$, $\mathbf{e}_3$, where $\mathbf{e}_3$ is parallel to the dislocation line and $\mathbf{e}_2$ is perpendicular to the slip plane; φ is the dislocation character.

and

$$A_n = \exp[-B(\mathbf{m})(nd_{hkl})^2 \ln(r_c/nd_{hkl})] \quad (6)$$
$$A_L = \exp[-B(\mathbf{m})L^2 \ln(r_c/L)]$$

respectively, with

$$B(\mathbf{m}) = [(Qb)^2/8\pi]\rho\chi, \quad r_c = \eta R_c.$$

The *integral breadth* of the reflection can be obtained in units of Q by the well known formula

$$\beta^{-1} = \int_0^\infty A(L)\,\mathrm{d}L \quad (7)$$

where the upper limit must, however, be taken as finite (r_c). Otherwise the approximation (Krivoglaz *et al.*, 1983)

$$\beta = [4B(\mathbf{m}) \ln P]^{1/2}\left[1 - \frac{\ln(\ln P)}{4\ln P}\right]^{-1}, \quad (8)$$
$$P = \eta R_c[B(\mathbf{m})]^{1/2},$$

can be used for $\ln P \gtrsim 2$. The parameter P is related to the quantity M of the theory of Wilkens (1970*b*) by $P \simeq 3M$.

It should be noted here that (3) is sufficiently accurate for $P \gtrsim 3$, when there is no strong defect correlation (dislocation dipoles, dislocation walls, loops *etc.*).

2.2. *Several slip systems*

In the plastic deformation of crystalline materials the following types of slip processes are possible: (i) single slip in single crystals (§ 2.1); (ii) multiple slip in single crystals; (iii) selection of slip systems by texture (grain orientation) or the deformation conditions in polycrystals; and (iv) multiple slip in polycrystalline materials with (nearly) random orientation of the grains. A systematic treatment of cases (ii) and (iii) is obviously difficult because of the diversity of possible situations. For this reason only case (iv) is considered in the present paper. In this connection two situations have to be taken into account. (i) Provided there is only one type of slip system, $\langle uvw\rangle\{hkl\}$, it is sufficient to replace the factor $B(\mathbf{m})$ in (6) and (8) by the average

$$B_p = [(Qb)^2/8\pi]\chi_p, \quad \chi_p = \langle\chi\rangle = \sum_{\alpha}^{N} (\rho_\alpha/\rho)\chi_\alpha \quad (9)$$

where N is the number of crystallographically equivalent Burgers vectors $\mathbf{b}$ and ρ is the total dislocation density. (ii) Provided there are different types of slip systems, the quantity B_p has to be replaced by the average

$$\langle B_p\rangle = \sum_{j}^{v} (\rho_j/\rho)B_{pj}(\mathbf{m}), \quad B_{pj} = [(Qb)^2/8\pi]\chi_{pj} \quad (10)$$

where v is the number of all slip-system types.

Strictly speaking the values of η and R_c should also be averaged (Krivoglaz *et al.*, 1983), but in connection with the determination of dislocation densities (which is the main purpose of X-ray profile analysis in investigations of polycrystals) their effect is of second order and the influence of the averaging can be neglected in a first approximation. A suitable average value of $\ln P$ can be estimated from the shape of an experimentally measured diffraction line profile according to Wilkens (1970*b*), if the dislocation content of different grains is similar.

3. Calculation of orientation factors

3.1. *The general procedure of calculation for polycrystals*

If one uses the classical formulae for the displacement fields around dislocation lines in elastically isotropic media as well as in elastically anisotropic materials (*e.g.* Steeds, 1973; Teodosiu, 1982) it is always possible to obtain relations of the type (2) with an explicit form of the function ψ. For this reason it is not difficult to show that the orientation factor χ_p of a polycrystalline material with randomly oriented grains can be conveniently written in the general form

$$\chi_p = \sum_{K,L} \langle G_{KL}\rangle E_{KL} \quad (K, L = 1, 2, \ldots, 6). \quad (11)$$

$\mathbf{G}$ and $\mathbf{E}$ are symmetrical matrices. The former describes the so-called geometrical, the latter the elastic part of the orientation factor.

In order to obtain the *elastic part* E_{KL} of the factor χ_p the following procedures are necessary: determination of the displacement field $u_i(x_1, x_2)$ around an isolated dislocation line in the structure considered; calculation of the derivatives

$$D_{ij} = (2\pi r/b)\partial u_i(\varphi)/\partial x_j \quad (12)$$

including transformation into polar coordinates r, φ ($r^2 = x_1^2 + x_2^2$); and calculation of the integrals

$$\hat{E}_{ijkl} = (1/\pi)\int_0^{2\pi} D_{ij}D_{kl}\,\mathrm{d}\varphi. \quad (13)$$

The matrix $\hat{\mathbf{E}}$ can be rewritten as $\mathbf{E}$ according to the rule ($i, k = 1, 2, 3$; $j, l = 1, 2$; $K = i$ for $j = 1$, $K = i + 3$ for $j = 2$; $L = k$ for $l = 1$, $L = k + 3$ for $l = 2$).

The *geometric part* G_{KL} of the orientation factor χ_p is obtained from a matrix $\hat{\mathbf{G}}$,

$$\hat{G}_{ijkl} = A_{ij}A_{kl}, \quad A_{ij} = \gamma_i\gamma_j \quad (14)$$

following the same rule as in the calculations of E_{KL}. The factors γ_i are the directional cosines of the angles between the axis i of the coordinate system associated with the slip plane (*cf.* Fig. 1 for the slip coordinate system) and the direction $\mathbf{m}$ of the diffraction vector $\mathbf{Q}$. Of course, in the case of a polycrystal the matrix G_{KL} related to a given diffraction vector must be calculated for all N equivalent Burgers vectors $\mathbf{b}$ and averaged as follows:

$$\langle G_{KL}\rangle = \sum_{\alpha}^{N} G_{KL}^{\alpha}/N.$$

This can always be done by means of a computer.

It should be noted here, that the unit vector $\mathbf{m}$ is approximately taken as parallel to the vector $\mathbf{H}$, *i.e.* as a constant for a given Bragg reflection.

3.2. *Elastically isotropic materials*

If the scattering crystal is assumed to be elastically isotropic and only pure edge or screw dislocations are taken into consideration, the integrals (13) can be solved analytically in a simple manner. The results may be summarized as follows.

For pure edge dislocations the non-zero components of the matrix E_{KL} are (ν = Poisson number)

$$\begin{aligned}
E_{11} &= \hat{E}_{1111} = \mu(5/2 - 6\nu + 4\nu^2)\\
E_{22} &= \hat{E}_{2121} = \mu(13/2 - 10\nu + 4\nu^2)\\
E_{44} &= \hat{E}_{1212} = E_{11} \qquad\qquad \mu = [4(1-\nu)^2]^{-1}\\
E_{55} &= \hat{E}_{2222} = \mu(1/2 - 2\nu + 4\nu^2)\\
E_{15} &= \hat{E}_{2112} = \mu(1/2 - 4\nu + 4\nu^2)\\
E_{24} &= \hat{E}_{1122} = \mu(7/2 - 8\nu + 4\nu^2).
\end{aligned}$$

In the case of a pure screw dislocation the only non-zero terms of E_{KL} are $E_{33} = E_{66} = 1$.

Because of the restrictions concerning the dislocation character the calculation of the matrix G_{KL} can be simplified and one obtains the following equations for the factor χ associated with a special slip system [$\gamma_i = (\mathbf{me}_i)$, e = edge dislocation, s = screw dislocation]:

$$\begin{aligned}
\chi^e &= E_{11}\gamma_1^4 + E_{55}\gamma_2^4 + a\gamma_1^2\gamma_2^2 \qquad (15)\\
\chi^s &= \gamma_3^2(\gamma_1^2 + \gamma_2^2) = \gamma_3^2(1-\gamma_3^2)\\
a &= (3 - 8\nu + 8\nu^2)\mu.
\end{aligned}$$

In order to find χ_p the quantities (15) must be averaged over all N equivalent slip systems of a given type, $\langle uvw\rangle\{hkl\}$. Since the direction cosines γ_i for each slip system can be expressed in terms of the Miller indices of the reflecting lattice planes and the geometry of the lattice cell, the averaging leads to relatively simple relations.

For dislocations with screw and edge components (mixed dislocations) the derivation of analytical expressions is more laborious and the orientation factors χ_p can be obtained numerically with less effort.

4. Orientation factors for hexagonal crystals

4.1. *Analytical expressions*

Orientation factors for the evaluation of dislocation-induced X-ray line broadening in cubic crystals have repeatedly been published (*e.g.* Ryaboshapka & Tikhonov, 1961; Krivoglaz, 1967; Krivoglaz *et al.*, 1983; Wilkens 1970*a*, *b*). For non-cubic materials no systematic work concerning this subject is known. The present paper deals with the case of hexagonal polycrystals, investigations of which are of interest in many branches of materials science and technology.

With respect to an easy derivation of equivalent lattice directions of the hexagonal structure it is useful to treat the orientation factors χ_p in terms of Bravais indices. The direction cosines γ_j of (15) are then given by

$$\gamma_j = \frac{hu_j + kv_j + iw_j + lz_j}{(h^2 + k^2 + i^2 + Zl^2)^{1/2}(u_j^2 + v_j^2 + w_j^2 + z_j^2/Z)^{1/2}} \qquad (16)$$

with $Q = Q(h, k, i, l)$, $e_j = e_j(u_j, v_j, w_j, z_j)$, $Z = 1{\cdot}5a_0^2/c_0^2$ (a_0, c_0 are lattice parameters).

If one uses (16) it is not difficult to determine the factors χ_p for various dislocation types and slip systems as functions of the Bravais indices, Poisson number and the ratio a_0/c_0.

The calculations were performed for the well known slip systems in hexagonal crystals (*e.g.* Predvoditelev & Troickiy, 1973) which are illustrated in Fig. 2. There are three basic kinds of Burgers vectors in a hexagonal structure: Burgers vector with a zero c_0 component, $a_0/3\langle 2\bar{1}\bar{1}0\rangle$; Burgers vector $\langle 11\bar{2}3\rangle a_0/3$; Burgers vector with a zero basal component $\langle 0001\rangle$. The final formulae for the orientation factors χ_p are presented in Table 1 and can be used directly.

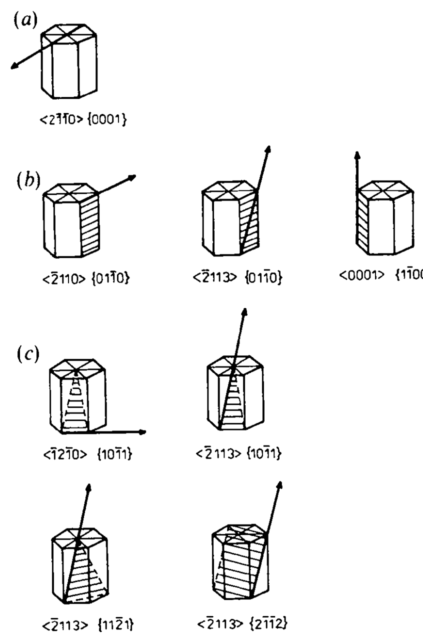

Fig. 2. The slip systems considered in hexagonal materials with slip planes and directions of Burgers vectors illustrated. (*a*) Basal slip, (*b*) prismatic slip, (*c*) pyramidal slip.

Table 1. *Orientation factors χ_p for various slip systems in hexagonal materials*

$H = h^2 + hk + k^2$ $\quad$ $A = 5/2 - 6\nu + 4\nu^2$ $\quad$ $\mu = 0{\cdot}25(1-\nu)^{-2}$

$\Sigma = h^2 + k^2 + i^2 + Zl^2$ $\quad$ $Z = 1{\cdot}5a_0/c_0$ $\quad$ $B = 3 - 8\nu + 8\nu^2$

$i = -(h+k)$ $\quad$ a_0, c_0 = lattice parameters $\quad$ $C = 0{\cdot}5 - \nu + \nu^2$ $\quad$ ν = Poisson number

Screw dislocations	$\chi_p\Sigma^2$
$\langle 11\bar{2}0\rangle$	$H(H/2 + Zl^2)$
$\langle 0001\rangle$	$2Zl^2H$
$\langle 11\bar{2}3\rangle$	$0{\cdot}5\left[\dfrac{H^2(6+Z) + H(9l^2 - 9l^2Z + 2l^2Z^2) + 3l^4Z^2}{(2+3/Z)(3+2Z)}\right]$
Edge dislocations	$\chi_p\mu\Sigma^2$
$\langle 11\bar{2}0\rangle\{0001\}$	$1{\cdot}5AH^2 + BZl^2H + CZ^2l^4$
$\langle 11\bar{2}0\rangle\{1\bar{1}00\}$	$H^2(7 - 15\nu + 10\nu^2)$
$\langle 0001\rangle\{10\bar{1}0\}$	$AZ^2l^4 + BZl^2H + 1{\cdot}5CH^2$
$\langle 11\bar{2}0\rangle\{0\bar{1}11\}$	$1{\cdot}5AH^2 + \dfrac{B}{2+Z}(H^2 + l^2Z^2H) + \dfrac{C}{(2+Z)^2}(6H^2 + l^4Z^4 + 12l^2Z^2H)$
$\langle 11\bar{2}3\rangle\{10\bar{1}0\}$	$\dfrac{Aa_1}{(2+3/Z)^2} + \dfrac{B}{(2+3/Z)}(H^2 + 3l^2H) + 1{\cdot}5CH^2$; $a_1 = 18H^2 + 27l^4 + 108l^2H$
$\langle 11\bar{2}3\rangle\{0\bar{1}11\}$	$\dfrac{Aa_1}{(2+3/Z)^2} + \dfrac{Ba_2}{(2+3/Z)(2+Z)} + \dfrac{C}{(2+Z)^2}(6H^2 + l^4Z^4 + 12l^2Z^2H)$; $a_2 = 5H^2 + 3l^4Z^2 + 6l^2H + l^2Z^2H - 12l^2ZH$
$\langle 11\bar{2}3\rangle\{2\bar{1}\bar{1}2\}$	$\dfrac{Aa_1}{(2+3/Z)^2} + \dfrac{Ba_3}{(2+3/Z)(3+2Z)} + \dfrac{C}{(3+2Z)^2}(27H^2 + 8l^4Z^4 + 72l^2Z^2H)$; $a_3 = 6l^4Z^2 + 4l^2Z^2H - 24l^2ZH + 9l^2H + 3H^2$
$\langle 11\bar{2}3\rangle\{11\bar{2}1\}$	$\dfrac{Aa_1}{(2+3/Z)^2} + \dfrac{Ba_4}{(2+3/Z)(6+Z)} + \dfrac{C}{(6+Z)^2}(54H^2 + l^4Z^4 + 18l^2Z^2H)$; $a_4 = 9H^2 + 3l^4Z^2 + 2l^2Z^2H - 12l^2ZH + 18l^2H$

4.2. *Numerical calculations*

In addition to the analytical treatment the orientation factors of some selected hexagonal materials with different ratios a_0/c_0 and Poisson numbers were calculated numerically. A typical result of the calculations is plotted in the form $\chi_p = f(\delta)$ in Fig. 3. Here δ is the angle between the vector **H** and the c axis of the hexagonal lattice. In the diagrams the reflections hkl corresponding to special values of the angle δ are indicated. The aim of the graphs is to demonstrate the influence of the lattice geometry on the dislocation-induced diffraction line broadening. Therefore the functions $\chi_p(\delta)$ are presented for various dislocation types and slip systems regardless of the probability of their presence in the material considered. The influence of the dislocation character φ on the orientation factors is illustrated in Fig. 4.

The calculations have been performed for magnesium, but the results are similar for other hexagonal materials, too.

4.3. *Discussion of the results*

From the above treatment the following conclusions concerning the orientation factors χ_p can be drawn. There are, in general, great differences in the shapes of the functions $\chi_p = \chi_p(\delta)$ associated with different slip systems and/or dislocation types. The influence of the Poisson number and a_0/c_0 ratio on the shapes of the functions $\chi_p(\delta)$ is often small. By contrast the absolute values χ_p can be different, especially for dislocations with the Burgers vector of the second kind and for basal edge dislocations. The functions χ_p for mixed dislocations, calculated in the approximation of elastic isotropy, can often be estimated with sufficient accuracy by appropriate averaging of the values χ_p^e and χ_p^s for pure edge and screw dislocations.

In comparison with cubic crystals, the orientation factors χ_p of which cannot be zero because of the lattice symmetry, two features of the dislocation-induced diffraction line broadening in hexagonal crystals are striking: Provided a crystal contains dislocations with Burgers vectors $a_0/3\langle 2\bar{1}\bar{1}0\rangle$ which are very frequently present in hexagonal structures (Predvoditelev & Troickiy, 1973, for example), the broadening of 0001 reflections becomes very small in comparison with that of the other diffraction peaks. In the case of pure screw dislocations or pure prismatic slip it would even be exactly zero. This means that reduced X-ray line broadening of 0001 reflections indicates a high density of dislocations with the Burgers vector of the first kind. The effect of somewhat lower broadening of these reflections can be found in the literature (De & Sen, 1968; Lele & Anantharaman, 1967, for instance). On the other hand, if the crystal contains dislocations with Burgers vectors $a_0/3\langle 11\bar{2}3\rangle$ the line broadening of the 0001 peaks is significantly higher than that of the other peaks. Unlike the preceding case, however, there are no lines with zero broadening. The dependence of the orientation factors on the angle is strong for dislocations with Burgers vectors $\langle 0001\rangle$, but because their presence is not very probable in most hexagonal materials, this phenomenon is not discussed here.

The differences between orientation factors of various reflections decrease rapidly with the presence of more slip-system types. Therefore different contents of various dislocation types have also been considered. The simulation was performed for magnesium under the following presumptions: (*a*) the concentration of edge and screw dislocations with Burgers vectors of the same kind is equal; and (*b*) there are edge dislocations with Burgers vectors of the first kind in the basal, prismatic and pyramidal slip systems with the same concentration, and dislocations with the second kind of Burgers vector of the two pyramidal slip systems $\{0\bar{1}11\}$, $\{\bar{2}112\}$, again with equal density.

The quantity χ_p responsible for the X-ray line-broadening anisotropy has then been calculated as follows [see also (10)]:

$$\langle \chi_p \rangle = c_1 b_1^2 \chi_{p1} + (1 - c_1) b_2^2 \chi_{p2}. \qquad (17)$$

In the above formula 1, 2 denote the kinds of the Burgers vector and c_i are the fractions of the appropriate dislocations. The results of the calculations are shown in Fig. 5, by means of the $\langle \chi \rangle_p^{1/2}$ *vs* δ plots for different fractions of both dislocation types. The thick lines correspond to the pure cases, *i.e.* they show limits for the orientation factors in magnesium, and the dashed line was calculated for dislocations with Burgers vectors of the first kind but without the basal edge dislocations.

Some conclusions can be drawn from Fig. 5: the influence of the dislocations with Burgers vector $a_0/3\langle 11\bar{2}3\rangle$ is emphasized by the greater size of the vector **b**; the diffraction line broadening of 0001 peaks is very sensitive to the actual content of dislocations

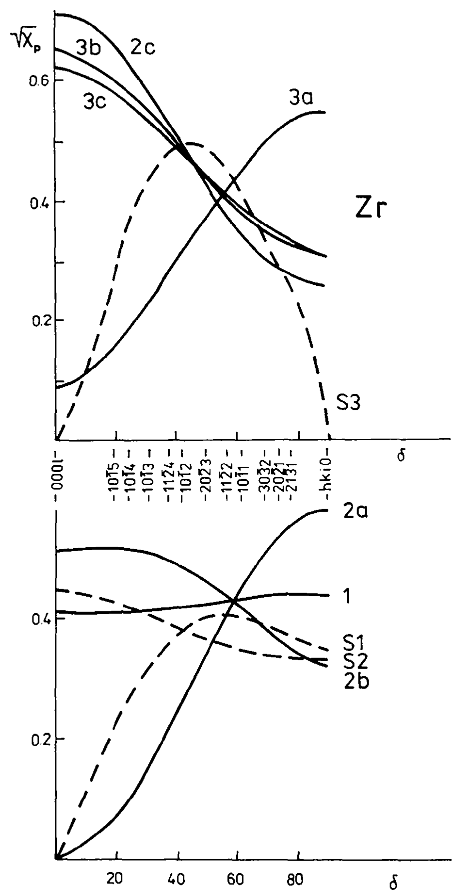

Fig. 3. Dependence of the orientation factors $\chi_p^{1/2}$ on the angle between the c axis and the diffraction vector for zirconium and the following dislocations: screw: *S*1 $\langle 2\bar{1}\bar{1}0\rangle$, *S*2 $\langle 11\bar{2}3\rangle$, *S*3 $\langle 0001\rangle$; edge: 1 basal, 2*a* prismatic $\langle 2\bar{1}\bar{1}0\rangle$, 2*b* prismatic $\langle 11\bar{2}3\rangle$, 2*c* prismatic $\langle 0001\rangle$, 3*a* pyramidal $\langle 2\bar{1}\bar{1}0\rangle\{0\bar{1}11\}$, 3*b* pyramidal $\langle \bar{2}113\rangle$ $\{2\bar{1}\bar{1}2\}$, 3*c* pyramidal $\langle \bar{2}113\rangle$ $\{10\bar{1}1\}$.

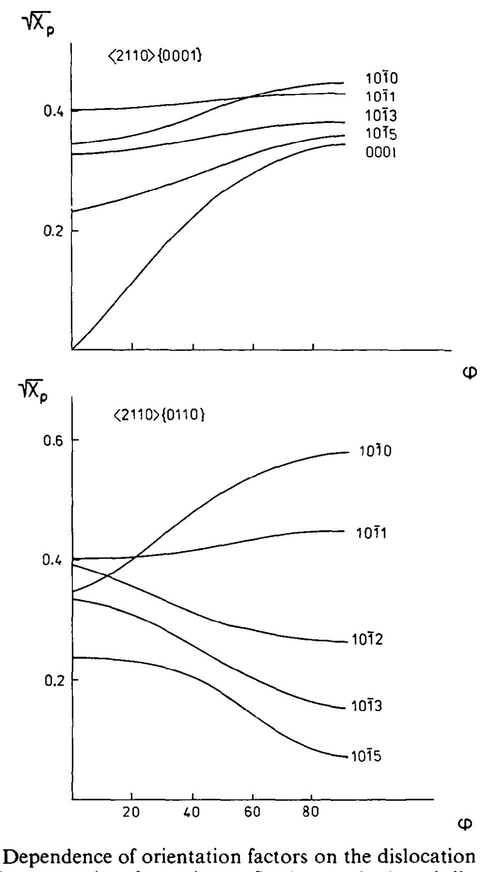

Fig. 4 Dependence of orientation factors on the dislocation character for magnesium for various reflections and selected slip systems $\langle 2\bar{1}\bar{1}0\rangle\{0001\}$, $\langle 2\bar{1}\bar{1}0\rangle\{01\bar{1}0\}$.

with different kinds of Burgers vectors; and most of the other reflections are not very sensitive to this content.

Therefore, it is possible to use the reflections 0001 (sometimes also $10\bar{1}5$, $10\bar{1}4$, $10\bar{1}3$, $11\bar{2}4$), in comparison with others, for a rough estimation of the distribution of the Burgers vectors in hexagonal materials. On the other hand, reflections with similar values of the orientation factors can always be found (*e.g.* *hki*0, $21\bar{3}1$, $20\bar{2}1$, $30\bar{3}2$, $h0\bar{h}h$, ...). They may be used in X-ray line-profile analysis like different reflection orders.

APPENDIX

Relation (2) can be rewritten as

$$\mathbf{Qu}_{\mathbf{R},\alpha} = (\mathbf{Re}_1)\left[(\mathbf{Qe}_1)\frac{\partial u_1}{\partial x_1} + (\mathbf{Qe}_2)\frac{\partial u_2}{\partial x_1} + (\mathbf{Qe}_3)\frac{\partial u_3}{\partial x_1}\right]$$

$$+ (\mathbf{Re}_2)\left[(\mathbf{Qe}_1)\frac{\partial u_1}{\partial x_2} + (\mathbf{Qe}_2)\frac{\partial u_2}{\partial x_2} + (\mathbf{Qe}_3)\frac{\partial u_3}{\partial x_2}\right]$$

$$= QR\sum_{j=1}^{2}(\mathbf{ne}_j)\sum_{i=1}^{3}(\mathbf{me}_i)\frac{\partial u_i}{\partial x_j}.$$

In the case of polycrystalline material only the dependence along the diffraction vector, *i.e.* $\mathbf{n}\|\mathbf{m}$, is interesting. This means (the index α is omitted in the right-hand sides of equations)

$$\mathbf{Qu}_{\mathbf{R},\alpha} = QR\sum_{i=1}^{3}\sum_{j=1}^{2}(\mathbf{me}_i)(\mathbf{me}_j)\frac{\partial u_i}{\partial x_j}.$$

Introducing the quantities $D_{ij}(\varphi)$ [equation (12)] and

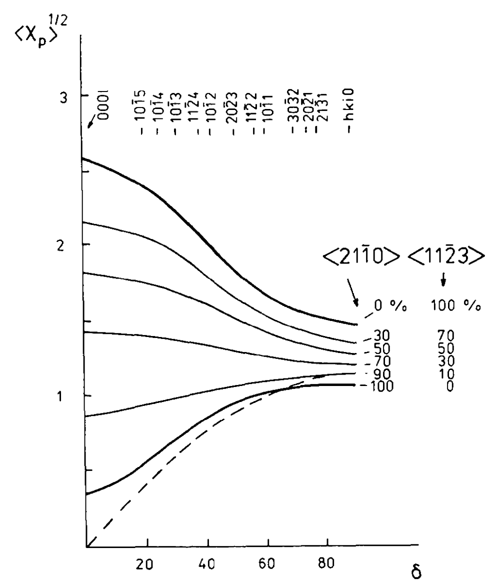

Fig. 5. Square roots of average orientation factors in the dependences on the angle δ for various fractions (in %) of dislocations with Burgers vectors $a_0/3\langle 2\bar{1}\bar{1}0\rangle$ and $a_0/3\langle 11\bar{2}3\rangle$.

γ_i [see equation (15)], we obtain the relation

$$\mathbf{Qu}_{\mathbf{R},\alpha} = (Qb/2\pi)(R/r)\psi_\alpha$$

where

$$\psi_\alpha = \sum_{i=1}^{3}\sum_{j=1}^{2}\gamma_i^{(\alpha)}\gamma_j^{(\alpha)}D_{ij}(\varphi).$$

This modification can be performed both for the elastic isotropy and the elastic anisotropy cases. It is now clear how to arrive at the relations (11)–(14), because an explicit form of the ψ function is available and expressions (4) and (9) can be used for polycrystalline material under the assumption that all dislocation densities in equivalent slip systems are the same.

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