4. Concluding remarks

The nature of the thermal diffuse scattering in barium fluoride and calcium fluoride, as observed in time-of-flight neutron diffraction, was described earlier by Carlile & Willis (1989). These observations were restricted to the scattering régime in which the neutron velocity v_n was within the range

$$c_s > v_n > c_s \cos\theta,$$

where c_s is the velocity of sound in the crystal. For this régime there are two TDS peaks for a given offset angle from the Bragg position: one peak corresponds to phonon emisson and the other to phonon absorption.

In the present paper the measurements on barium fluoride have been extended to neutron velocities in the range

$$v_n < c_s \cos\theta.$$

Theory indicates that for this régime (Willis, 1986) there is only one TDS peak for a given offset angle $(\theta - \theta_B)$. The peak is due to phonon emisson for $\theta < \theta_B$ and to phonon absorption for $\theta > \theta_B$. Our measurements have confirmed the existence of this single peak and we have derived from it an estimate of the velocity of sound in BaF_2. This estimate is in good agreement with the independent value derived earlier from observations in the first velocity régime.

APPENDIX

To calculate the difference in time of flight between the TDS peak and the Bragg peak, we refer to the diagram in Fig. 5. Here O is the origin of reciprocal space, **OB** is the wave vector $\mathbf{k}_0$ of the incident beam and **BC** the wave vector of the scattered beam. The line ON at an angle $\pi/2-\theta$ to OB is the 'elastic line', *i.e.* the locus of the endpoints of scattered neutron wave vectors that undergo no change of energy on being scattered through 2θ. The centre of the ellipsoid scattering surface is represented by C; P is the nearest reciprocal-lattice point. P is at the focus of the ellipsoid and the elastic line ON coincides with the directrix.

From elementary geometry we have

$$CP = ae,$$

$$CN = a/e,$$

$$PN = a(1/e - e) = 2k_B(\sin\theta)\Delta\theta,$$

where $\mathbf{k}_B$ is the wave vector for Bragg scattering, $2a$ is the length of the major axis of the ellipsoid and e is its eccentricity. Also, OD in Fig. 5 has the length k_B, OB has length k_0, so

$$DB = k_B - k_0 = -\Delta k_0.$$

For the SXD, the path length of the scattered beam is much shorter than for the direct beam, so we can write

$$\Delta t/t_B = -\Delta k_0/k_B.$$

Recalling that $1/e = \beta\cos\theta$ (Willis, 1986), we obtain finally

$$\Delta t/\Delta 2\theta = \tfrac{1}{2}t_B(\tan\theta)/(\beta^2\cos^2\theta - 1).$$

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A Note on the Darwin–Prins Rocking Curve for Perfect Crystals

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Abstract

For the purpose of calculating the reflectivity of perfect crystals in the Bragg case, taking into account both normal and Borrmann absorption, it is suggested that its original form is used expressed in terms of complex variables. Care is required regarding the phase angle for the algebraic expression of the square root. Two expressions which are directly usable for programming are presented. One of them is equivalent to the traditional one given by Zachariasen [*Theory of X-ray Diffraction in Crystals* (1945). New York: Wiley]. The other can be used without any problems of infinite values whatever values the

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Fourier coefficients of the polarizability takes. Some numerical examples of rocking curves are demonstrated for very special values of the Fourier coefficients.

1. Introduction

Bragg reflection in Bragg geometry is an old topic of dynamical diffraction and has been studied by many authors [Darwin, 1914; Ewald, 1917; Prins, 1930; Hirsch & Ramachandran, 1950; Cole & Stemple, 1962; Fingerland, 1971; Kato, Katagawa & Saka, 1971 (KKS)]. Also, other important literature and related subjects are described in many text books and review articles. In particular, the theoretical details are discussed by Zachariasen (1945) (ZT), James (1963), Batterman & Cole (1964) and Kato (1974) (KT).

The aim of this paper is principally to propose a simple method to calculate rocking curves numerically by dealing directly with complex functions. The method can be applied to most general cases: for non-centrosymmetric crystals and for a wide range of crystal parameters. Some numerical examples are presented for a set of parameters which are not usually dealt with. Some comments will be given with simple proofs on the characteristic features of rocking curves (RC).

2. A summary of basic formulae

It is well known that the reflectivity (the power ratio of the Bragg reflected beam and the incident beam) is given as a function of the glancing angle θ with respect to the net plane in the form (*e.g.* KT)

$$R(\theta)=|\chi_g/\chi_{-g}|\,|[u-(u^2-U^2)^{1/2}]/U|^2, \quad (1)$$

where

$$u=|b|(\theta-\theta_B)\sin 2\theta_B+\tfrac{1}{2}(1+|b|)\chi_0, \quad (2a)^*$$

which is identical to Zachariasen's parameter z, and

$$U=|b|^{1/2}P(\chi_g\chi_{-g})^{1/2}, \quad (2b)^*$$

the square of which is Zachariasen's q. Here, b is also Zachariasen's parameter which specifies obliqueness of the net plane to the entrance surface (negative for the Bragg case), P is the polarization factor of the X-rays, θ_B is the value of θ which satisfies the exact Bragg condition and χ_0 and χ_g are Fourier coefficients of 4π times the complex polarizability of the crystal, $\chi=\chi^r+i\chi^i$.

Equation (1) can be derived by the standard dynamical theory either assuming a half-infinite crystal from the start (as in KT) or assuming first a parallel-sided crystal with a finite absorption (as in ZT). In the second method, (1) is obtained as an asymptotic form for an infinitely thick crystal. A single discrepancy between the two approaches appears in the case of absolutely non-absorbing crystals. The physical reason is fully discussed in KKS and KT. Often, (1) is called Darwin's curve and that derived by the second approach is called Ewald's curve (ZT). In practice, however, we need not bother with the discrepancy and it is safe to use (1). Ewald's curve is valid only when the crystal thickness is extremely thin, the crystal surfaces are very flat and parallel and the plane-wave front is sufficiently wide that all multiply reflected waves on the entrance and exit surfaces contribute coherently to the final result.

Since the Fourier coefficients of χ are crucially important in the following arguments, some relevant formulae are summarized.

$$\chi_0=\chi_0^r+i\chi_0^i \quad (3)$$

$$\chi_g^r=|\chi_g^r|\exp i\varphi_1, \quad \chi_g^i=|\chi_g^i|\exp i\varphi_2 \quad (4a,b)$$

$$|\chi_g|^2=|\chi_g^r|^2+|\chi_g^i|^2+2|\chi_g^r||\chi_g^i|\sin(\varphi_1-\varphi_2) \quad (5a)$$

$$|\chi_{-g}|^2=|\chi_g^r|^2+|\chi_g^i|^2-2|\chi_g^r||\chi_g^i|\sin(\varphi_1-\varphi_2) \quad (5b)$$

$$\chi_g\chi_{-g}=|\chi_g^r|^2-|\chi_g^i|^2+2i|\chi_g^r||\chi_g^i|\cos(\varphi_1-\varphi_2). \quad (5c)$$

According to the theorem of Fourier integrals, the following relations hold in general:

$$|\chi_0^r|\geq|\chi_g^r|, \quad |\chi_0^i|\geq|\chi_g^i|. \quad (6a,b)$$

In centrosymmetric (non-polar) crystals, one can make φ_1 and φ_2 zero, so that

$$|\chi_g|=|\chi_{-g}|. \quad (7)$$

Zachariasen dealt with this case under an additional limitation that the absolute value of

$$\kappa=\chi_g^i/\chi_g^r \quad (8)$$

(real in non-polar crystals) is much smaller than unity. The parameter κ indicates the magnitude of Borrmann absorption.

Following Zachariasen's theory, Hirsch & Ramachandran (1950) extended the theory to large $|\kappa|$. Cole & Stemple (1962) and Fingerland (1971) extended the theory to polar crystals, introducing the parameter of polarity

$$s=|\kappa|\sin(\varphi_1-\varphi_2) \quad (9)$$

in the present notation. All authors, following Zachariasen, use two further important parameters:

$$y^r=\{|b|(\theta-\theta_B)\sin 2\theta_B+\tfrac{1}{2}(1+|b|)\chi_0^r\}/|b|^{1/2}P|\chi_g^r| \quad (10)$$

$$g=\tfrac{1}{2}(1+|b|)\chi_0^i/|b|^{1/2}P|\chi_g^r|, \quad (11)$$

which specify the deviation from the Bragg condition and the magnitude of normal absorption, respectively.

* Slight modifications are made to the previous formulae (KT) in order to fit in with Zachariasen's notation. For example, K $(=2\pi/\lambda)$ is dropped in $(2a)$, $(2b)$. However, the physical meaning is not changed.

For the general case, KKS and Fingerland discussed the functional structure of (1). The details are also described by KT and can be summarized as follows.

(a) The physically allowable condition is represented by

$$|\mathrm{Im}\,[U]| \leq \mathrm{Im}\,[u]. \tag{12a}$$

(b) Under the above condition,

$$R(\theta) \leq 1 \tag{12b}$$

always, as it should be.

(c) The maximum of $R(\theta)$ occurs only once at

$$\mathrm{Re}\,[\bar{u}] \equiv \bar{w} = \mathrm{Re}\,[U]\,\mathrm{Im}\,[U]/\mathrm{Im}\,[u]. \tag{12c}$$

(d) As a corollary of (c), from the condition (12a),

$$|\bar{w}| \leq |\mathrm{Re}\,[U]|. \tag{12d}$$

(e) To meet the physical condition, the expression $-(u^2-U^2)^{1/2}$ must belong to the negative Riemann surface of Z in the algebraic equation, $Z^2=(u^2-U^2)$.

3. Suggestions for the numerical calculation of RCs

Although the original expression (1) is very simple, if one wishes to represent it in terms of real variables, the expression becomes very complex, particularly for polar crystals. Such a task had to be carried out for the numerical calculation of RCs and for some theoretical treatments. Nowadays, however, it is popular to carry out numerical calculation in terms of complex variables even on personal computers. For this reason, it is much simpler to calculate $R(\theta)$ directly from (1) as it is.

Care is required only for calculating $-(u^2-U^2)^{1/2}$. In order to fit the statement (e) above, it is suggested that the relation

$$(u^2-U^2)^{1/2} = (u+U)^{1/2}(u-U)^{1/2} \tag{13}$$

is used with the usual convention that the angular phase of $(\zeta)^{1/2}$ lies between $\pm(\pi/2)$ for any complex number ζ. Because of (12a), $\mathrm{Im}\,[u \pm U] \geq 0$. Therefore, the angular phase of $(u^2-U^2)^{1/2}$ always lies between π and 0 in our problem; *i.e.* $-(u^2-U^2)^{1/2}$ belongs to the negative Riemann surface.

Often, for reducing the number of parameters involved, $R(\theta)$ is expressed in terms of normalized parameters. This gives rise to another complication or confusion, as pointed out by Fingerland. As seen in the definitions listed in (8) to (11), the traditional parameters have been normalized essentially with $|\chi_g^r|$ for the divisor. In general, this must be a real positive quantity. Also, it is desirable for the divisor to be defined easily from the Fourier coefficients, χ_g^r, χ_g^i and $(\varphi_1-\varphi_2)$. Certainly, the traditional normalization meets these requirements but, as a result, the expressions for $R(\theta)$ so far obtained were rather complicated. Moreover, if $|\chi_g^r|$ is close to zero, one may encounter the problem of infinity.

In order to find a suitable normalization, we shall consider the following quantities:

$$A = \mathrm{abs}\,[\chi_g\chi_{-g}] \geq 0, \quad \Phi = \arg\,[\chi_g\chi_{-g}], \tag{14a,b}$$

where abs [. . .] and arg [. . .] are operators (or computer commands) to obtain, respectively, the absolute value and the phase angle between $\pm\pi$ of any complex number. A and Φ are calculable easily from (5c) provided that the right-hand side is given. Then, we have

$$(\chi_g\chi_{-g})^{1/2} = A^{1/2}\exp(i\Phi/2). \tag{15}$$

Now, we introduce the following parameters:

$$N = \mathrm{Re}\,[(\chi_g\chi_{-g})^{1/2}] = A^{1/2}\cos(\Phi/2) \geq 0 \tag{16a}$$

$$k = \mathrm{Im}\,[(\chi_g\chi_{-g})^{1/2}]/\mathrm{Re}\,[(\chi_g\chi_{-g})^{1/2}] = \tan(\Phi/2). \tag{16b}$$

Recalling the remark concerning (13), one can write RCs in the form suitable for computer programming:

$$\begin{aligned} R(\theta) = {} & |\chi_g/\chi_{-g}|(1+k^2)^{-1} \\ & \times |(x+ia)-[(x+ia)+(1+ik)]^{1/2} \\ & \times [(x+ia)-(1+ik)]^{1/2}|^2, \end{aligned} \tag{17}$$

where

$$(x+ia) = u/|b|^{1/2}PN. \tag{18}$$

In summary, (17) can be used under the physical condition (12a). The normalized parameters are x, a (equation 18) and k (equation 16b). The first two differ from Zachariasen's y^r and g only in the divisor so their physical implications are identical. The parameter k is a generalization of κ (equation 8), including the effect of polarity. All three parameters can be determined uniquely from the Fourier coefficients.

Equation (17), however, is not very satisfactory for numerical calculation. Similar to traditional normalization, it gives rise to infinite values when Φ tends to $\pm\pi$, *i.e.* N is close to zero. Nevertheless, (17) is useful for theoretical arguments. A few examples are given below.

When $k=\pm a$ and if $x=\pm 1$, respectively, one of the factors $[\ldots]^{1/2}$ will be zero. Then,

$$R(\theta) = |\chi_g/\chi_{-g}|(1+k^2)^{-1}|1+ik|^2 = |\chi_g/\chi_{-g}|. \tag{19}$$

One remark is worth making. Equation (19) appears contradictory to (12b) when $|\chi_g/\chi_{-g}|$ is larger than unity in polar crystals. However, this is not so. Equation (19) was derived under the constraint $|k| = a$, which holds only when the crystal is non-polar ($s=0$) and other diffraction conditions are satisfied (see Appendix). In fact, a is the maximum value of $|k|$. Otherwise, the physically allowable condition (PAC), *i.e.* (12a), will be violated. Henceforth, when

the equality holds the case will be called the extreme PAC.

Next, we shall compare the cases of $+\Phi$ and $-\Phi$ in (17). In the latter case, taking the complex conjugate and replacing x by $-x$ inside $|\ldots|$, we shall have the same expression as in the former case multiplied by $-$ inside the $|\ldots|$, which gives the same $R(\theta)$. Therefore, in any case, RCs for $\pm\Phi$ are mirror symmetric with respect to $x=0$.

Returning to the problem of numerical calculation, in order to avoid the difficulty of infinite values for normalized parameters, we may use a divisor

$$N' = A^{1/2} \tag{20}$$

instead of N. Then, RCs have the form

$$\begin{aligned} R(\theta) = |\chi_g/\chi_{-g}|\,|&(x'+ia') \\ &-[(x'+ia')+\exp(i\Phi/2)]^{1/2} \\ &\times[(x'+ia')-\exp(i\Phi/2)]^{1/2}|^2, \end{aligned} \tag{21}$$

where

$$x'+ia' = u/|b|^{1/2}PN'. \tag{22}$$

This method is better than the previous one because N' does not become zero. If it does, no reflection occurs. As mentioned before, the divisor N' and the phase Φ are obtainable directly from (5c) if $\chi_g\chi_{-g}$ is given.

One can develop similar arguments described in connection with (17). Corresponding to the extreme PAC ($a=|k|$) in the previous case, the equivalent condition is $a'=|\sin\Phi/2|$. If a' is less than unity, it should be noted that the limit of $|\Phi/2|$ is fixed by $\sin^{-1}(a')$.

The traditional approach is also simplified along the line of similar considerations. Then, the RC can be written in the form

$$\begin{aligned} R(\theta) = |\chi_g/\chi_{-g}|B^{-2} \\ \times|(y^r+ig)-[(y^r+ig)+B\exp(iF/2)]^{1/2} \\ \times[(y^r+ig)-B\exp(iF/2)]^{1/2}|^2 \end{aligned} \tag{23}$$

with the auxiliary relations

$$B = \mathrm{abs}\,[Q], \quad F = \arg[Q], \tag{24a,b}$$

and

$$Q = (1-|\kappa|^2) \pm 2i(|\kappa|^2-s^2)^{1/2}, \tag{24c}$$

where the alternative sign is selected in accordance with the sign of $\cos(\varphi_1-\varphi_2)$.

All parameters are the same as those of Zachariasen defined above and s is defined by (9). If handling complex functions is allowed, the numerical calculation of $R(\theta)$ is straightforward. In this case, the extreme PAC is

$$g = B|\sin(F/2)|. \tag{25}$$

When $|g/B|<1$, a similar limitation to Φ has to be posed on F.

4. Numerical examples

In all the drawings, the ordinate represents $R(\theta)$ of (1), but the factor $|\chi_g/\chi_{-g}|$ is deliberately omitted. This does not mean the exclusion of polar crystals. However, it is worth noting that the curves having a singular peak refer to non-polar crystals with the conditions $|b|=1$, $P=1$ and $|\chi_0^i|=|\chi_g^i|$. The abscissa scale depends upon which method is employed.

Fig. 1(a) illustrates a set of examples calculated by (23). The unit of the abscissa scale is the traditional one, namely $|b|^{1/2}P|\chi_g^r|$. Here, we take up the case that $|\chi_g^r|=|\chi_g^i|$ so that $|\kappa|=1$ and $F=\pm\pi/2$ depending upon the sign of $\cos(\varphi_1-\varphi_2)$. As proved above, however, the opposite sign gives the mirror image. The crystal is assumed to be non-polar with $F=-\pi/2$ in the illustration. When $g=-\kappa=1$, the RC is singular and is unity at $y^r=-1$. For increasing g, the peak value decreases and shifts towards $y^r=0$. All features are similar to those reported by Hirsch & Ramachandran (1950) who, however, show results only for $|\kappa|\leq 0.2$.

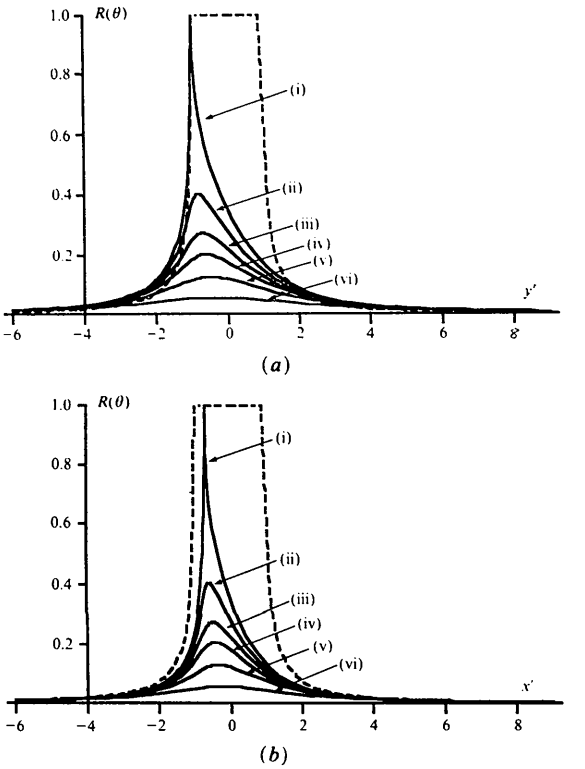

Fig. 1. (a) The rocking curves for $\kappa=-1$, *i.e.* $|\chi_g^r|=|\chi_g^i|$, calculated by the traditional method using (23). g values of (i) 1.0, (ii) 1.2, (iii) 1.4, (iv) 1.6, (v) 2.0, (vi) 3.0. Broken line: non-absorbing case ($g=0$ and $\kappa=0$). (b) The rocking curves for the same parameters as (a), calculated by the second method using (21). The ratio of the scale units of x' and y^r is $2^{1/2}$ and $a'/g=1/2^{1/2}$.

Fig. 1(b) shows the results calculated by (21). To compare the two methods, the same values of the relevant Fourier coefficients are employed. Therefore, the ratio of the scale units of x' and y^r is $N'/|\chi_g^r| = 2^{1/2}$ and $a'/g = 1/2^{1/2}$ in the present case. Taking into account these ratios, we see that the results of Figs. 1(a) and (b) are identical.

Next, we take up another special case, $|\chi_g^r| = 0$, to which the traditional approach using (23) is not applicable. Fig. 2 shows the results calculated by (21). In this case, $N' = |\chi_g^i|$ and $\Phi = \pm\pi$. When $a' = 1$, the peak is extremely sharp and symmetric, the height being unity. These properties are ideal for making optical devices with crystals. To obtain such a peculiar curve in practice, the condition $|\chi_g^r| = 0$ is not necessarily very exact, but the condition $a' = 1$ is very stringent as anticipated in the illustration. Numerically, if $a' = 1.01$, the peak height goes down to 0.75. For this reason, the case is merely of theoretical interest. A more important feature is that one can expect a weak reflection for a finite $|\chi_g^i|$ even when $|\chi_g^r| = 0$. In general, we have to take into account $|\chi_g^i|$ properly for weak reflections, *i.e.* $|\chi_g^r| \simeq 0$.

5. Concluding remarks

The mathematical structure of the RC [(1)] has been well investigated as summarized in § 2. With the recent progress of computer calculations, the present author suggests that the basic equation should be manipulated as a complex function. The second method [(21)] can be applied to all conceivable cases. A computer program can be written on the basis of an unconditional equation. No problem occurs through numerical divergence. Here, as a demonstration, we have taken two special cases, *i.e.* $|\chi_g^r| = |\chi_g^i|$ and $|\chi_g^r| = 0$ but $|\chi_g^i|$ finite. Because the tuning of X-ray wavelength has become feasible with synchrotron radiation, such special cases occur in practical experiments.

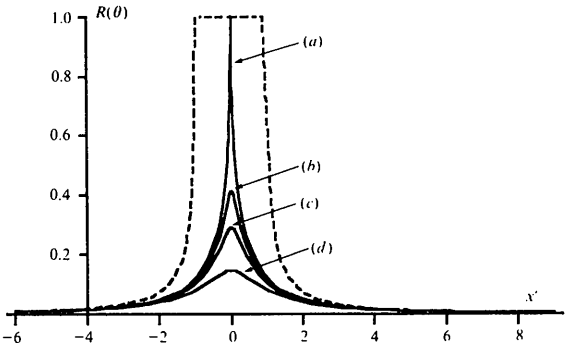

Fig. 2. The rocking curves for $|\chi_g^r| = 0$ calculated by (21). The a' values are (a) 1.0, (b) 1.1, (c) 1.2, (d) 1.4. $\Phi = -\pi/2$ for all curves.

The program used by the present author consists of only three command lines, corresponding to the functional definition of $R(\theta)$, the numerical calculation and the figure plotting, respectively. The time required to draw one curve in the above illustrations was of the order of 10 s with a commercial personal computer.

Finally, (17), (21) and (23) are also useful for understanding general features of RCs in a simple manner.

APPENDIX

The condition $a = |k|$ can be written explicitly in the form

$$(1/2P)[|b|^{1/2} + 1/|b|^{1/2}]\chi_0^i = \mathrm{Im}\,[(\chi_g\chi_{-g})^{1/2}]. \quad (A1)$$

However, we can prove that

$$(1/2P)[|b|^{1/2} + 1/|b|^{1/2}] \geq 1 \quad (A2a)$$

$$\chi_0^i \geq |\chi_g^i| \geq \mathrm{Im}\,[(\chi_g\chi_{-g})^{1/2}] \quad (A2b)$$

so that ($A1$) is satisfied only when (i) $P = 1$, (ii) $b = 1$, (iii) $\chi_0^i = |\chi_g^i|$ and (iv) $|\chi_g^i| = \mathrm{Im}\,[(\chi_g\chi_{-g})^{1/2}]$.

The last inequality of ($A2b$) is proved as follows. For any complex number $\chi_g\chi_{-g} = \alpha + i\beta$ (α and β real),

$$B = \mathrm{Im}\,[(\alpha + i\beta)^{1/2}]$$
$$= (1/2^{1/2})\{(\alpha^2 + \beta^2)^{1/2} - \alpha\}^{1/2}. \quad (A3)$$

With the use of the explicit expressions for α and β given in ($5c$),

$$(\alpha^2 + \beta^2) = |\chi_g^r|^4 + |\chi_g^i|^4 + 2|\chi_g^r|^2|\chi_g^i|^2 \cos 2(\varphi_1 - \varphi_2). \quad (A4)$$

Therefore, max.$[(\alpha^2 + \beta^2)^{1/2}]$ is given by $|\chi_g^r|^2 + |\chi_g^i|^2$ under the condition (v) $(\varphi_1 - \varphi_2) = 0$ or π. Consequently, max.$[B^2]$ is given by $|\chi_g^i|^2$ so that the inequality is proved. Also, the necessary condition (iv) can be replaced by (v).

After all, the initial constraint $|k| = a$ implies that the polarity parameter s [(9)] is zero. Simultaneously, conditions (i), (ii) and (iii) must also be satisfied. Consequently, it turns out that the value of $|k|$ does not exceed a. A similar argument can be applied also to the other forms of the extreme PAC.

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The Darwin–Prins Rocking Curve for Distorted Crystals

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Abstract

Rocking curves (RC) of Darwin-Prins type of distorted crystals have been systematically studied with respect to various parameters which characterize the crystal and its deformation. The basic formula is given in an earlier paper [Kato (1990). *Acta Cryst.* A**46**, 672-681]. Through numerical analysis, characteristic features of RCs were deduced. In order to understand them, a simplified theory was developed based on a WKB approximation. Most of the features, in particular the oscillatory behaviour of RCs, could be interpreted by the geometrical configuration of the entrance surface and the bending *C* band, which was defined as a region where the local wave number is practically pure imaginary. The concept of the *C* band is analogous to the forbidden energy band of electrons popular in solid-state physics.

1. Introduction

Rocking curves (RC) in Bragg geometry are sensitive to lattice distortion near the crystal surface. Taupin (1964) proposed a fundamental (differential) equation to calculate the intensity of the Bragg reflection for distorted crystals. Since then, the theory has been widely used in many investigations. For example, Burgeat & Taupin (1968) and Fukuhara & Takano (1977) studied experimental RCs of impurity-doped crystals and showed a reasonable agreement with the theoretical curve based on the erfc-function model for the lattice distortion. More recently, Bensoussan, Malgrange & Sauvage-Simkin (1987) presented a similar work for a III-IV* heterojunction system. Many relevant articles are cited in that paper. They also obtained a good agreement between Taupin's theory and their experimental results. It seems, therefore, that there remains no serious problem in this research field from the practical point of view.

All authors, however, solve Taupin's differential equation numerically assuming some plausible model for the lattice distortion depending on their own samples. For this reason, it seems desirable to make a systematic analysis of RCs based on an exact and analytical solution of the wave field, which has been obtained recently by the present author (Kato, 1990). This is the primary subject of the present paper.

Here, the lattice spacing is assumed to have the form $D_o \tanh(\alpha x)$, where x is the coordinate normal to the net plane concerned. The model is similar to that of Bensoussan *et al.* (1987). By changing D_o, α and the position of the entrance surface x_e, one can represent various monotonic forms of the lattice expansion effective for diffraction. These forms give rise to different shapes of RC. There are parameters of another type characterizing the crystal concerned, which also change the shape of the RC. They are the structure factor and the normal and Borrmann absorption. With this complex situation in mind, results will be presented in terms of suitably normalized parameters (§ 3).

One interesting phenomenon is the oscillatory behaviour of a RC which appears under specific conditions. The phenomenon itself was recognized in both numerical simulations and real experiments by the authors mentioned above. Here, characteristic properties are interpreted by a simple theory to elucidate the physical significance (§ 4).

2. Glossary of formulae and parameters

(*a*) *Perfect crystals*

In order to give an idea of the present scheme of notation, RCs of perfect crystals are first dealt with. We are concerned only with the symmetrical case. The theoretical details are described in standard texts

* Groups 13-14 in IUPAC (1988) nomenclature.

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