the scattering angle $2\theta_B$ is non-zero. Nevertheless, these terms have proved satisfactory in many situations and thus constitute a good approximation. The greater parts of the corrections here come from scattering from the L shells, which belong to the atomic cores, and should not be greatly affected by pressure. As far as the Debye–Waller factors are concerned, a guess can be made for the effect of stress by comparing a fractional change in volume due to hydrostatic pressure with the same change due to temperature. A pressure of 0·1 GPa at room temperature is roughly equivalent to a reduction of 80 K from room temperature. This latter change would reduce B_1 and B_2 by 32%, corresponding to an increase in T_1 and T_2 of about 6%. All in all, the factors neglected might mean an uncertainty of ±5% in the values of S and I that are used to locate the end points (marked 0·25) of the theoretical lines in Fig. 2. The factors neglected are in no way large enough to account for the inconsistencies.

5. Conclusion

The theoretical basis for determining the internal strain in zinc-blende-structure materials has been presented and earlier work on gallium arsenide has been shown to have been inadequately analysed. Reanalysis in the manner of the present paper reveals strange inconsistencies.

I am grateful to Leif Gerward of the Technical University of Denmark for supplying the dispersion corrections.

References

CARDONA, M., KUNC, K. & MARTIN, R. M. (1982). *Solid State Commun.* **44**, 1205–1207.

COUSINS, C. S. G., GERWARD, L., NIELSEN, K., OLSEN, J. S., SELSMARK, B., SHELDON, B. J. & WEBSTER, G. E. (1982). *J. Phys. C*, **15**, L651–654.

COUSINS, C. S. G., GERWARD, L., OLSEN, J. S., SELSMARK, B. & SHELDON, B. J. (1982). *J. Appl. Cryst.* **15**, 154–159.

CROMER, D. T. & LIBERMAN, D. (1970). *Los Alamos Scientific Laboratory Report* LA-4403.

International Tables for X-ray Crystallography (1974). Vol. 4. Birmingham: Kynoch Press.

KOUMELIS, C. N. & ROZIS, E. K. (1975). *Acta Cryst.* A**31**, 84–87; erratum: *Acta Cryst.* (1976). A**32**, 170.

KOUMELIS, C. N., ZARDAS, G. E., LONDOS, C. A. & LEVENTOURI, D. K. (1976). *Acta Cryst.* A**32**, 306–311.

REID, J. S. (1983). *Acta Cryst.* A**39**, 1–13.

Acta Cryst. (1984). A**40**, 120–126

A Novel Approach to Dynamical Neutron Diffraction by a Deformed Crystal

BY J. KULDA

Nuclear Physics Institute, Czechoslovak Academy of Sciences, 250 68 Řež near Prague, Czechoslovakia

(*Received* 1 *June* 1983; *accepted* 13 *September* 1983)

Abstract

The propagation of neutron waves in a deformed crystal is considered from the point of view of quantum mechanics. Instead of solving the Takagi–Taupin equations the probability of transitions, induced by the variation of the interaction potential, between quantum states corresponding to the two sheets of the dispersion surface is calculated. In this way transmission and reflection coefficients for an incident plane wave are obtained after a simple analytical calculation for a wide class of crystal deformations. The predictions of this theory are found to be in agreement with direct solutions of the Takagi–Taupin equations as well as with the experimental results.

1. Introduction

A large number of papers have appeared in the last two decades confined to the theoretical treatment of dynamical diffraction phenomena in deformed crystals. Starting from the pioneering works of Penning & Polder (1961) and Kato (1964) the theory has developed considerably after the amplitude-coupling equations for the propagation of the transmitted and reflected beams were formulated by Takagi (1962, 1969) and Taupin (1964). These equations, however, can be solved analytically only in the case of crystals with a constant strain gradient – for a complete treatment including an exhaustive list of references one should consult the paper of Chukhovskii & Petrashen (1977). The solution is a degenerated hypergeometric function being rather complicated for practical integrated intensity evaluation. Although a simplified asymptotic expression for the wave amplitudes is available, little insight into the process of wave propagation is obtained from this solution.

The theory of neutron diffraction by deformed crystals has been simply adopted from the X-ray literature

0108-7673/84/020120-07$01.50

(*e.g.* Klar & Rustichelli, 1972; Michalec, Mikula & Vrána, 1975) without regard to some specific properties of neutron radiation. The nonzero rest mass and the low velocity of propagation makes it possible to treat the whole problem in terms of nonrelativistic quantum mechanics, which are more adequate to deal with diffraction of neutrons in crystals than classical optics. First results of such an approach leading to a simple calculation of the reflectivity of a bent crystal are reported in the present paper.

2. The neutron states in the crystal interior

Proceeding in a way analogous to the conventional treatment of the dynamical theory, we shall start with a plane wave $\Psi_0 = u \exp(i\mathbf{kr})$ incident from vacuum upon the crystal surface. The vacuum wave generates in the crystal a coherent wave $\Psi(\mathbf{r})$ that has to satisfy the Schrödinger equation

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})\right]\Psi(\mathbf{r}) = E\Psi(\mathbf{r}). \tag{1}$$

The interaction potential is taken in the form of the Fermi pseudopotential

$$V(\mathbf{r}) = (2\pi\hbar^2/m)\sum_i \delta(\mathbf{r}-\mathbf{r}_i),$$

where m denotes the neutron rest mass and b_i the scattering length of the ith nucleus. Equation (1) is then solved using the Bloch waves $\Psi(\mathbf{r}) = u(\mathbf{r})\exp(i\mathbf{Kr})$ and passing by a Fourier transformation from (1) to a homogeneous set of linear equations in terms of the Fourier components V_0, V_G and u_0, u_G of $V(\mathbf{r})$ and $u(\mathbf{r})$, respectively. In the case of two strong crystal waves the system reads

$$\begin{aligned}(T_0 + V_0 - E)\cdot u_0 + V_{-G}u_G &= 0\\ V_G u_0 + (T_G + V_0 - E)u_G &= 0\end{aligned} \tag{2}$$

with $T_0 = \hbar^2K^2/(2m)$ and $T_G = \hbar^2(\mathbf{K}+\mathbf{G})^2/(2m)$, where $\mathbf{G}$ is the reciprocal-lattice vector representing the actual reflection. The two roots of the determinant of this system are the energy eigenvalues of the permitted neutron states in the crystal

$$E_{1,2} = T_0 + V_0 + \tfrac{1}{2}\{T_G - T_0 \pm [(T_G - T_0)^2 + 4V_G V_{-G}]^{1/2}\} \tag{3}$$

and define the wave vectors of the crystal waves. To determine their amplitudes the boundary conditions at the crystal surface have to be used in addition to (2). The complete description of this procedure including the derivation of some of the formulas used in this section is found in the book by Pinsker (1978) and in the papers on neutron dynamical diffraction by, for example, Sears (1978) or Rauch & Petrascheck (1978) – whose notation we use.

The deviation of the scattering angle θ from the precise Bragg angle θ_B for the incident vacuum wave will be represented by a parameter α,

$$\alpha = (G^2 + 2\mathbf{k}.\mathbf{G})/k^2 = 2\sin 2\theta_B(\theta_B - \theta) \tag{4}$$

or by the parameter y,

$$y = \frac{\alpha b - (1-b)\chi_0}{2|b|^{1/2}\chi_G} \tag{5}$$

with $\chi_{0,G} = V_{0,G}/E$ (assuming a centrosymmetrical crystal to ensure $\chi_G = \chi_{-G}$) and b being the ratio of the direction cosines of the incident and reflected wave vectors with respect to the inner surface normal, $b = \gamma_0/\gamma_G$. To be able to deal with angular deviations for the wavefields inside the crystal, we shall introduce a second pair of similar parameters

$$a = (G^2 + 2\mathbf{K}\cdot\mathbf{G})/K^2 \tag{6}$$

and

$$Y = a/(2\chi_G). \tag{7}$$

Clearly α and a differ from each other just by the angular shift caused by refraction at the crystal surface,

$$a = \alpha + \left(1 - \frac{1}{b}\right)\chi_0. \tag{8}$$

From (5) and (7) it then follows that

$$Y = y/|b|^{1/2}. \tag{9}$$

The factor $|b|$ is included in the definition (5) of y to ensure the particle-flux conservation at the crystal surface for an arbitrary case of asymmetric reflection. On the other hand, Y refers to the crystal interior, where the flux is related directly to the reflecting planes–a situation equivalent to $|b| = 1$.

The wavefields in the directions of the transmitted and reflected wave are superpositions of the contributions from both permitted states $\psi^{(1)}$ and $\psi^{(2)}$:

$$\begin{aligned}\psi_0 &= \psi_0^{(1)} + \psi_0^{(2)}\\ &= u_0^{(1)}\exp(i\mathbf{K}_1\mathbf{r}) + u_0^{(2)}\exp(i\mathbf{K}_2\mathbf{r}),\\ \psi_G &= \psi_G^{(1)} + \psi_G^{(2)}\\ &= u_G^{(1)}\exp[i(\mathbf{K}_1+\mathbf{G})\mathbf{r}] + u_G^{(2)}\exp[i(\mathbf{K}_2+\mathbf{G})\mathbf{r}].\end{aligned} \tag{10}$$

The ratio of the amplitudes is governed by the internal reflection coefficients $c_{1,2} = u_G^{(1,2)}/u_0^{(1,2)}$ that are easily obtained from (2) and (3) in the form

$$\begin{aligned}c_{1,2} &= \frac{E_{1,2} - (T_0 + V_0)}{V_G}\\ &= \frac{T_G - T_0 \pm [(T_G - T_0)^2 + 4V_G^2]^{1/2}}{2V_G}\end{aligned}$$

or, with the help of (6) and (7),

$$c_{1,2} = Y \pm (Y^2 + 1)^{1/2}. \tag{11}$$

The direction of the neutron flux in the crystal is parallel to the dispersion-surface normal, hence in the Bragg case at most one of the states $\psi^{(1)}$, $\psi^{(2)}$ has to be considered in the boundary conditions while in the Laue case both states always play a role. At large $|Y|$ values these differences become less important and it follows from (10) and (11) that in both cases for $Y \ll 0$ only $u_0^{(1)}$ may differ from zero appreciably, so that

$$\lim_{Y\to-\infty} \Psi = \psi_0^{(1)}. \qquad (12a)$$

Similarly, for large positive deviations, $Y \gg 0$, we have $u_0^{(2)} \doteq u$ and

$$\lim_{Y\to+\infty} \Psi = \psi_0^{(2)}. \qquad (12b)$$

An evaluation of the intensities of the partial waves $\psi_0^{(1)}$, $\psi_0^{(2)}$ and $\psi_G^{(1)}$, $\psi_G^{(2)}$ shows that already at $Y = -2$ the wave $\psi_0^{(1)}$ carries about 90% of the energy of the whole crystal wave Ψ (obviously the same holds for $\psi_0^{(2)}$ at $Y = 2$).

3. Calculation of the transmission and reflection coefficients

Let us consider a deformed crystal in which the angular deviation $\Delta\theta = \theta_B - \theta$ is a function of position. As coordinates we shall choose, similarly to the Takagi–Taupin theory, the flight paths s_0 and s_G in the directions of the transmitted and reflected beam, respectively. The internal deviation parameter a consists now of two parts: $a_S = a(0, 0)$ related by (8) to α being a measure of deviation from Bragg angle of the incident vacuum wave with respect to the entrance surface and $-a_v = -2\lambda\,(\partial/\partial s_G)\,(\mathbf{G}.\mathbf{u})$, a position-dependent contribution of the deformation in the crystal interior (*e.g.* Takagi, 1969), where λ is the neutron wavelength and $\mathbf{u}$ denotes the local deformation amplitude. Again, we can pass to the dimensionless parameter

$$Y = Y_s - Y_v(s_0, s_G) = \left[a(0,0) - 2\lambda \frac{\partial}{\partial s_G}(\mathbf{G}.\mathbf{u})\right]/(2x_G). \qquad (13)$$

In what follows we shall assume that Y_v has a derivative $\partial Y_v/\partial s_0$ which is continuous along s_0 and that Y_v varies on a mactoscopic scale only, *i.e.*

$$\lambda \frac{\partial}{\partial s_0} Y_v(s_0, s_G) \ll 1.$$

An incident vacuum wave Ψ_0 satisfying the Bragg condition somewhere inside the crystal but being far from it at the surface will excite only a strong refracted wave travelling into the crystal interior. Let us assume $Y_s \ll 0$, then, according to (12a), $\Psi \doteq \psi_0^{(1)}$ and the neutron is in the state $\psi^{(1)}$ with energy E_1 (the lower branch of the dispersion surface). According to the adiabatical theorem of quantum mechanics (*e.g.* Messiah, 1962) in the case of an infinitely slow variation of the parameter Y along the flight path the quantum state of the neutron would not change. Hence, along all the flight path $\Psi = \psi^{(1)}$ and only the internal reflection coefficient c_1 varies with Y according to (11). After passing into the range of $Y \gg 0$, we have $\Psi \doteq \psi_G$ and total reflection will occur (*i.e.* unit probability for transition from ψ_0 to ψ_G). This result is equivalent to that obtained for X-rays on the basis of the theory developed by Penning & Polder (1961).

The formal apparatus of quantum mechanics permits us to make one very important step more, to calculate the probability w_{12} of transition from the state $\psi^{(1)}$ into the state $\psi^{(2)}$ caused by a finite rate of variation of the parameter Y. We shall examine the transmission probability that the neutron being initially (time $\tau \to -\infty$, deviation $Y \to -\infty$) in the state $\psi_0^{(1)}$ will be found at $\tau \to +\infty$, $Y \to +\infty$ in the state $\psi_0^{(2)}$. According to the quasi-classical approach described by Landau & Lifshitz (1965) w_{12} in our case may be computed as

$$w_{12} = \exp\left(\frac{2}{\hbar}\,\mathrm{Im}\int_C E\,\mathrm{d}\tau\right), \qquad (14)$$

where the label Im indicates that only the imaginary part is taken of the action integral $S = \int_C E(\tau)d\tau$. The integration path C in the complex plane includes one of the roots τ_i of $E(\tau)$ representing the classically inaccessible transition points between the states $\psi^{(1)}$ and $\psi^{(2)}$, where $E_1(\tau_j) = E_2(\tau_j)$. As the energy E is always real for real values of the time variable τ, the imaginary part of S is formed only along that part of the path C where $d\tau$ has a nonzero imaginary component, while E still remains real. As a consequence, any shift of the coordinate system in the direction of the real axis leaves Im S unaffected and we may always choose the origin in such a way to ensure $\tau_j = i\,\xi_j$ with ξ_j real so that

$$\mathrm{Im}\,S = \mathrm{Im}\left(\int_0^{i\xi_j} E_j\,\mathrm{d}\tau + \int_{i\xi_j}^{0} E_k\,\mathrm{d}\tau\right), \qquad j,k = 1,2. \qquad (15)$$

One has to bear in mind that the positive sense of integration along C corresponds to a counter-clockwise passage in the complex plane and on the left-hand and right-hand sides with respect to the imaginary axis the energy attains different eigenvalues E_j. From a pair of possible integration paths $C_{1,2}$ (including different transition points τ_j), that one has to be chosen that yields a negative value of Im S to satisfy in (13) the natural requirement $0 \le w_{jk} \le 1$. Once more benefitting from the fact that $E_{1,2}$ are real along the integration path, we can use the substitution $\tau = \pm i\tau'$ to express Im S by integrals of real functions

of a real variable (which will be denoted by τ again):

$$\mathrm{Im}\, S = \int_0^{\xi_j} E_j(i\tau)\mathrm{d}\tau - \int_{-\xi_j}^{0} E_k(i\tau)\mathrm{d}\tau. \qquad (16)$$

The different signs $\pm$ in the substitution have to be applied to keep the integration paths on the proper side of the origin corresponding to the different quantum states.

In our case the interaction energy depends on time only indirectly through the deviation parameter Y. After some straight-forward manipulations the energy eigenvalues $E_{1,2}$ (equation 3) are expressed with the help of the quantity Y as

$$E_{1,2} = \tfrac{1}{2}(T_0 + T_G + 2V_0) \pm V_G(Y^2+1)^{1/2}. \qquad (17)$$

The part of the right-hand side of (17) contained in the round brackets remains always real and can be omitted in the following calculations. The rest has two purely imaginary roots $Y_{1,2} = \pm i$ representing the transition points between the two permitted states, obviously $Y_{1,2} = Y(\tau_{1,2})$. Analogously to $\tau_{1,2}$ in (15), we shall write them as $Y_{1,2} = i\eta_{1,2}$ and, setting $\pm iY$ instead of Y in (17) [leading to $E_{1,2} = \pm V_G(1-Y^2)^{1/2}$], we return to the real axis. Recalling that $s_0 = v_n\tau$ and assuming a monotonic dependence of Y on s_0 [to guarantee the existence of the inverse function to $Y(\tau)$] we can use the inverse of the substitution $Y = Y(\tau)$ leading to $\mathrm{d}\tau = (Y')^{-1}\mathrm{d}Y$ with $Y' = v_n\partial Y/\partial s_0$, where v_n is the neutron velocity, to arrive at an expression analogous to (16):

$$\mathrm{Im}\, S = V_G\left[\int_0^{\eta_j} \mathrm{sgn}(j)(1-Y^2)^{1/2}(Y')^{-1}\mathrm{d}Y - \int_{-\eta_j}^{0} \mathrm{sgn}(k)(1-Y^2)^{1/2}(Y')^{-1}\,\mathrm{d}Y\right].$$

According to (17) the signs of the energy eigenvalues are opposite, $\mathrm{sgn}(j) = -\mathrm{sgn}(k)$, so that we may write

$$w_{jk} = \exp\left[2\frac{V_G}{\hbar}\mathrm{sgn}(j)\int_{-\eta_j}^{+\eta_j}(1-Y^2)^{1/2}(Y')^{-1}\mathrm{d}Y\right]. \qquad (18)$$

The choice of the proper value η_j is seen at best with the help of Fig. 1 which displays the asymptotic behaviour of the neutron wave functions $\psi^{(1)}$ and $\psi^{(2)}$ together with the integration paths C_1 and C_2. In accordance with (12*a*, *b*), the sign + in the left-hand part of the integration paths and the sign − in the right-hand part should be taken in (15) and (16) for $E = E_1$ and $E = E_2$, respectively. When w_{12} is calculated, $Y' > 0$ and $\mathrm{sgn}(1) = +1$ holds: to achieve a negative value of the integral ξ_1 has to be negative. The transition points on both the τ and Y scale lie in the same half of the complex plane with respect to the real axis and the integration is performed along the path C_1 including the point $Y = -i$ in Fig. 1. Similarly w_{21} corresponds to C_2 and $Y = +i$.

As the only term in the integrand representing the crystal deformation

$$Y' = v_n\frac{\partial Y}{\partial s_0} = -\frac{\lambda v_n}{\pi}\frac{\partial^2(\mathbf{G}.\mathbf{u})}{\partial s_0 \partial s_G}$$

is symmetric in s_0, s_G, the interchange of the incident and reflected beams brings about just the opposite case with $Y_s \gg 0$ and transition from $\psi^{(2)}$ to $\psi^{(1)}$. Invariance with respect to the inversion of the beam directions is obtained in this way similarly to the optical treatment and there is no necessity to distinguish between w_{12} and w_{21} in the rest of this section.

Using the concept of the reduced flight path

$$A_{0,G} = \frac{\pi}{\lambda}\chi_G s_{0,G} = \frac{V_G}{\hbar}\frac{1}{v_n}s_{0,G},$$

we arrive at the final expression for the probability of reflection in a non-absorbing crystal

$$r(Y_s) = 1 - w(Y_s) = 1 - \exp\left[-2\int_{-1}^{1}(1-Y^2)^{1/2}\left|\frac{\partial Y}{\partial A_0}\right|^{-1}\mathrm{d}Y\right], \qquad (19)$$

which follows immediately from the particle conservation law $r(Y_S) + w(Y_S) = 1$.

To obtain the integrated reflectivity ρ_y we have to sum the contributions from all the incident plane waves (represented by angular deviation parameter y) satisfying the Bragg condition in the crystal interior

$$\rho_y = \int r(Y_s)\mathrm{d}y.$$

With the help of (9) and recalling from (13) that $Y = 0$ implies $Y_s = Y_v$, we arrive at an approximate result;

$$\rho_y = b^{1/2}\left|\int_{Y_v} r(Y_s)\,\mathrm{d}Y_s\right|, \qquad (20)$$

not taking into account the intensity scattered at the

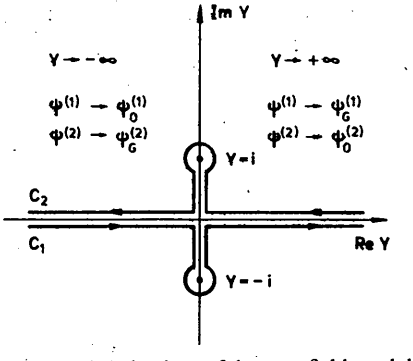

Fig. 1. The asymptotic behaviour of the wavefields and the integration paths in the complex Y plane.

crystal surface. On the angular scale we have then

$$\rho_\theta = \frac{\chi_G}{\sin 2\theta_B}\frac{1}{b^{1/2}}\rho_y$$

$$= \frac{\chi_G}{\sin 2\theta_B}\left|\int_{Y_v} r(Y_s)\,\mathrm{d}Y_s\right|, \qquad (21)$$

a value independent of the asymmetry factor $1/b^{1/2}$ similar to the result of the kinematical theory for an ideally imperfect crystal.

4. The reflecting power of a bent crystal

As an example of application of these results we shall calculate in this section the probability of reflection of a neutron by a homogeneously bent crystal in the symmetric Bragg case. Klar & Rustichelli (1972) have performed a similar calculation by numerical integration of the Takagi equations; their paper can be also referred to for a more detailed derivation of the following expressions.

The internal deviation field is introduced in the form

$$Y_v(A) = cA, \qquad (22)$$

where A is a reduced depth parameter related to the reduced flight paths by

$$A = -(\gamma_0 A_0 + \gamma_G A_G)/(\gamma_0|\gamma_G|)^{1/2}. \qquad (23)$$

For practical purposes it is more convenient to connect A to the depth t in the crystal plate directly by

$$A = (2F_{hkl}d_{hkl}/\Omega)t, \qquad (24)$$

where F_{hkl} and d_{hkl} are the structure factor and the interplanar spacing, respectively, and Ω is the unit-cell volume. The angular deviation $\Delta\theta$ caused by the deformation is related to the Y parameter by

$$\Delta\theta = 2Y\frac{F_{hkl}d_{hkl}^2}{\pi\Omega}\tan\theta_B. \qquad (25)$$

From simple geometrical considerations it follows that the angular misorientation along the neutron flight path over a crystal plate of thickness Δt bent with radius R is given by

$$\delta\theta = \frac{\Delta t}{R}\cot\theta_B. \qquad (26)$$

Combining the last four equations, we arrive at an expression for the constant c,

$$c = \frac{\Delta Y_v}{\Delta A} = \frac{\pi\Omega^2\cot^2\theta_B}{4F_{hkl}^2 d_{hkl}^3}\frac{1}{R}. \qquad (27)$$

The constancy of c implies that the reflectivity for any incident plane wave satisfying at some depth A in the crystal interior the Bragg condition $Y_s - Y_v(A) = 0$ (13) does not depend on Y_s:

$$r = 1 - \exp\left[-\frac{2}{c}\int_{-1}^{1}(1-Y^2)^{1/2}\mathrm{d}Y\right]$$

$$= 1 - \exp(-\pi/c). \qquad (28)$$

To obtain the integrated reflectivity we shall use (20) with $b = -1$ yielding an approximate result

$$\rho_y = |\Delta Y_v|[1 - \exp(-\pi/c)]. \qquad (29)$$

On the angular scale there follows from (26), (27) and (29)

$$\rho_\theta = \frac{\Delta t}{R}\cot\theta_B \times\left[1 - \exp\left(-\frac{4F_{hkl}^2 d_{hkl}^3}{\Omega^2\cot^2\theta_B}R\right)\right]. \qquad (30)$$

The pre-exponential factor in (30) is nothing else than the integrated reflectivity ρ^{lam} predicted by the simple lamellar models (White, 1950; Egert & Dachs, 1970). The exponent may be rearranged as

$$Q\frac{\Delta t}{\sin\theta_B}\frac{R}{\Delta t\cot\theta_B}$$

denoting by $Q = \lambda^3 F_{hkl}^2/(\Omega^2\cot^2\theta_B)$ the kinematical reflectivity per unit beam path. Expression (30) acquires then a simpler form

$$\rho = \rho^{\mathrm{lam}}[1 - \exp(-\rho^{\mathrm{kin}}/\rho^{\mathrm{lam}})]. \qquad (31)$$

Obviously, at small deformations when $\rho^{\mathrm{lam}} \ll \rho^{\mathrm{kin}}$ the exponent in (31) becomes very small so that $\rho \doteq \rho^{\mathrm{lam}}$ and the integrated intensity is proportional to the deformation. At large deformations the reflectivity predicted by the lamellar model diverges, $\rho^{\mathrm{lam}} \gg \rho^{\mathrm{kin}}$, but the exponential approaches unity and the expansion

$$\exp\left(-\frac{\rho^{\mathrm{kin}}}{\rho^{\mathrm{lam}}}\right) \doteq 1 - \frac{\rho^{\mathrm{kin}}}{\rho^{\mathrm{lam}}}$$

can be used to obtain the proper physical limit $\rho = \rho^{\mathrm{kin}}$.

5. Comparison with experimental results

A sufficient test of the results obtained in the preceeding sections would be the comparison with the results of the exact solution of the Takagi equations for a homogeneously bent crystal. In the existing literature dealing with experimental studies of neutron diffraction by bent crystals, *e.g.* Egert & Dachs (1970), Albertini, Boeuf, Klar, Lagomarsini, Mazkedian, Melone, Puliti & Rustichelli (1977), Albertini, Boeuf, Mazkedian, Melone, Rozzi & Rustichelli (1977), considerable discrepancies can be found between observed intensities and theoretical predictions that cannot be

explained by the approximations contained in the simplified models. We are thus justified to include in this paper a comparison of our calculations with the results of a simple experiment.

In a nondispersive parallel double-crystal arrangement, symmetric 220 Bragg reflections from two silicon single-crystal plates of dimensions $200 \times 35 \times 5$ mm were used at a Bragg angle $\theta_B = 13.67°$ corresponding to the neutron wavelength $\lambda = 0{\cdot}091$ nm. The second crystal was mounted in a special bending holder with provision for a direct measurement of the deformation by a contact micrometer (for more details see Kulda & Mikula, 1983). The rocking curves for a number of the bending radius values R were then recorded, two of them are displayed in Fig. 2. They retain the box-like shape characteristic of the rocking curve of a perfect crystal, the peak reflectivity drops, however, at greater deformations.

The FWHM of the rocking curves in Fig. 3 increases proportionately to the reciprocal value of the bending radius as expected from (26). Instead of the crystal thickness, a modified value including the total width of the incident beam has to be employed. As it was not possible to fix it directly by the experimental arrangement with sufficient precision, we have determined it by fitting a straight line to the experimental points in Fig. 3. The resulting effective value is $\Delta t = 11{\cdot}4$ mm, hence the line in Fig. 3 corresponds to the dependence $\delta\theta = (0{\cdot}0114/R)$ cot $13{\cdot}67°$.

In Fig. 4 the experimental values of the peak count (a) and integrated intensity (b) are displayed together with the results of calculations for the actual values of the experimental parameters. The dashed lines represent the predictions of the simple lamellar model while the solid curves were computed from (28) and (30). A good quantitative agreement is found in the latter case for the whole range of bending radii, only the integrated intensities calculated from the rocking curves are, at higher deformations, systematically lower by 2–3% than the theoretical values. This is most probably an effect of the limited angular scanning range that made it impossible to measure the tails of the wider curves far enough from the peak position.

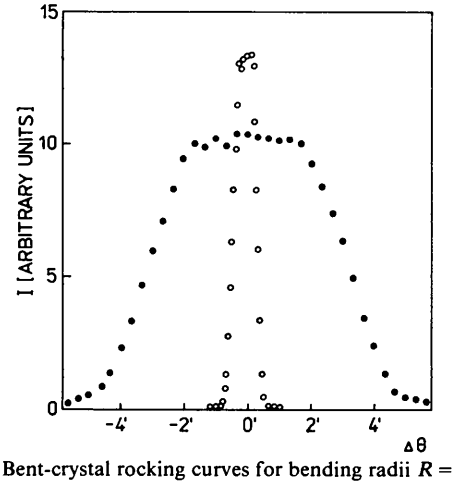

Fig. 2. Bent-crystal rocking curves for bending radii $R = 20$ m (●) and $R = 200$ m (○).

6. Discussion

The presented calculation of the reflecting power is based on a formula giving the transition probability between states $\psi^{(1)}$ and $\psi^{(2)}$ that only asymptotically coincide with the observable states ψ_0 and ψ_G. As a consequence, our treatment is valid only if the wave under consideration passes the whole range of reflection from negative to positive Y values or *vice versa*. Fortunately, this requirement represents no major restriction as already at $Y = \pm 2$ the waves $\psi_0^{(1,2)}$ carry 90% of the whole crystal wavefield intensity. For the

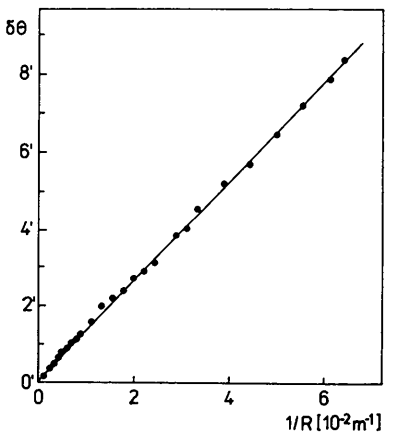

Fig. 3. FWHM of the bent-crystal rocking curves plotted against the reciprocal value of the bending radius.

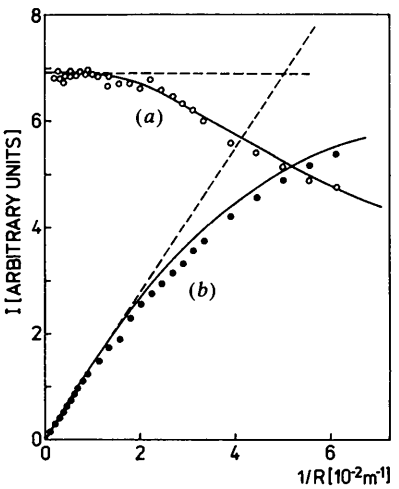

Fig. 4. Dependence of (a) peak intensities and (b) integrals of the bent-crystal rocking curves on the reciprocal value of the bending radius. The solid curves indicate the values calculated from (28) and (30).

same reason it is necessary that the wave enters and leaves the crystal at a Y_s value far enough from zero so that $\Psi = \psi_0^{(1)}$ or $\psi_0^{(2)}$ at the crystal surface. The reflection of waves satisfying the Bragg condition at the crystal surface is not included in this simple treatment. This means that only the central part of the rocking curve corresponding to incident plane waves satisfying the Bragg condition in the crystal interior can be calculated, not its tails.

Whenever the conditions for the validity of our approach are fulfilled, (28) and (29) give equally precise results as the solution of the Takagi–Taupin equations. The reflectivity expression (28) is indentical with the 'static factor' obtained by Chukhovskii & Petrashen (1977) from the asymptotic expansion of the analytical solution of the Takagi equations for a homogeneously bent crystal. Our derivation is, however, more general, not being limited to a special deformation case. Furthermore, we have compared the reflectivity values given by (28) with the results of numerical solution of the Takagi equations for a bent crystal reported by Klar & Rustichelli (1972) and by Albertini, Boeuf, Klar, Lagomarsino, Mazkedian, Melone, Puliti & Rustichelli (1977). Our formula yields precisely the top values of the computed rocking curves when the intensity oscillations of the exact solution are averaged.

Our approach provides an interesting link between the dynamical theory and the 'lamellar' models frequently used for interpretation of neutron diffraction effects in deformed crystals. In these models the crystal is divided into subregions mutually misoriented by the width of the total reflection range of the Darwin curve of a perfect crystal, *i.e.* by $\Delta y = 2$. For slight deformations, when the thickness of individual lamellae largely exceeds the extinction length and total reflection may be assumed, the model gives proper results. At strong deformations these assumptions become invalid and unphysical results are obtained, *e.g.* integrated intensity exceeding the value given by the kinematical formula. Efforts have been made either to include a phenomenological saturation factor (White, 1950) or to treat individual lamellae as perfect-crystal wafers (Albertini, Boeuf, Cesini, Mazkedian, Melone & Rustichelli, 1976; Albertini, Boeuf, Klar, Lagomarsino, Mazkedian, Melone, Puliti & Rustichelli, 1977; Albertini, Boeuf, Mazkedian, Melone, Rozzi & Rustichelli, 1977). No really satisfying results have been obtained in either case both from the view of labour content and of real physical insight into the problem. Our formula (19) relates the probability of reflection to the deformation in the crystal region where $-1 \leq Y \leq 1$, *i.e.* just inside one lamella. In this way the model is completed in the most natural way to provide correct description of diffraction effects in deformed crystals. In this context the presented treatment provides a derivation of an improved 'lamellar' model based on the dynamical theory of neutron diffraction and free of phenomenological arguments.

7. Conclusion

A new quantum-mechanical treatment of neutron diffraction by deformed crystals, leading to a simple analytical calculation of the reflecting power, has been reported. The results possess a physically proper asymptotical behaviour and explain correctly the observed variation of the diffracted intensity with the degree of deformation. The final expression for the reflectivity is a more general form of the 'static factor' obtained from the asymptotic expansion of the exact solution of the Takagi–Taupin equations for a homogeneous quadratic deformation. This coincidence suggests that the application range of the method presented here should be extended to the X-ray case despite the fact that it cannot be directly derived from the existing theory of X-ray dynamical scattering.

It is a pleasure to acknowledge the hospitality and interest of Dr R. T. Michalec and Dr L. N. Sedláková at the Laboratory of Neutron Physics, JINR Dubna, where a part of this work was performed. Also, I wish to express my sincere thanks to Dr M. Polcarová from the Institute of Physics and to Dr P. Mikula for fruitful discussions and to Mr A. Dvořák for his help with the preparation of the manuscript.

References

ALBERTINI, G., BOEUF, A., CESINI, G., MAZKEDIAN, S., MELONE, S. & RUSTICHELLI, F. (1976). *Acta Cryst.* A**32**, 863–872.

ALBERTINI, G., BOEUF, A., KLAR, B., LAGOMARSINO, S., MAZKEDIAN, S., MELONE, S., PULITI, P. & RUSTICHELLI, F. (1977). *Phys. Status Solidi a*, **44**, 127–136.

ALBERTINI, G., BOEUF, A., MAZKEDIAN, S., MELONE, S., ROZZI, V. & RUSTICHELLI, F. (1977). *J. Appl. Cryst.* **10**, 118–122.

CHUKHOVSKII, F. N. & PETRASHEN, P. V. (1977). *Acta Cryst.* A**33**, 311–319.

EGERT, G. & DACHS, H. (1970). *J. Appl. Cryst.* **3**, 214–220.

KATO, N. (1964). *J. Phys. Soc. Jpn.* **19**, 971–985.

KLAR, B. & RUSTICHELLI, F. (1972). *Nuovo Cimento B*, **13**, 249–271.

KULDA, J. & MIKULA, P. (1983). *J. Appl. Cryst.* **16**, 498–504.

LANDAU, L. D. & LIFSHITZ, E. M. (1965). *Quantum Mechanics*, ch. 7. Oxford: Pergamon Press.

MESSIAH, A. (1962). *Quantum Mechanics*, Vol. 2, ch. 17. Amsterdam: North-Holland.

MICHALEC, R., MIKULA, P. & VRÁNA, M. (1975). *The Kinematical and the Dynamical Theory of Neutron Diffraction by Vibrating Single Crystals* Internal report ÚJF/ONF/003, Nuclear Physics Institute, Řež (in Czech).

PENNING, P. & POLDER, D. (1961). *Philips Res. Rep.* **16**, 419–440.

PINSKER, Z. G. (1978). *Dynamical Scattering of X-rays in Crystals.* Berlin: Springer.

RAUCH, H. & PETRASCHECK, D. (1978). *Neutron Diffraction*, edited by H. DACHS, pp. 303–351. Berlin: Springer.

SEARS, V. F. (1978). *Can. J. Phys.* **56**, 1261–1288.

TAKAGI, S. (1962). *Acta Cryst.* **15**, 1311–1312.

TAKAGI, S. (1969). *J. Phys. Soc. Jpn*, **26**, 1239–1253.

TAUPIN, D. (1964). *Bull. Soc. Fr. Minéral. Crystallogr.* **87**, 469–486.

WHITE, J. E. (1950). *J. Appl. Phys.* **21**, 855–862.