Asymmetric X-ray Line Broadening of Plastically Deformed Crystals. I. Theory

BY I. GROMA AND T. UNGÁR

Institute for General Physics, Eötvös University, H-1445 Budapest, PO Box 323, Hungary

AND M. WILKENS

Max-Planck-Institut für Metallforschung, Institut für Physik, Heisenbergstrasse 1, D-7000 Stuttgart 80, Federal Republic of Germany

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Abstract

X-ray diffraction line profiles of plastically deformed Cu single crystals orientated for ideal multiple slip were recently found to be markedly asymmetric. A theory is developed to interpret this kind of asymmetric line broadening in terms of the average dislocation density, the dipole polarization of the dislocation structure and the mean square fluctuation of the dislocation density.

1. Introduction

The analysis of broadened X-ray diffraction lines is one of the most powerful methods of investigating the bulk dislocation structure in heavily deformed materials. After several attempts to interpret the X-ray line profiles in terms of a microscopic model of materials (Wilson, 1942; Eastabrook & Wilson, 1952; Warren & Averbach, 1952; Krivoglaz & Ryaboshapka, 1963), Wilkens (1970a, b) developed a theory for symmetrical X-ray diffraction lines broadened by dislocations. This theory was successfully verified by the experimental study of tensile deformed Cu single crystals oriented for single slip (Wilkens, Herz & Mughrabi, 1980; Ungár, Mughrabi & Wilkens, 1982).

In a recent study of X-ray line broadening of [001] Cu single crystals orientated for ideal multiple slip and deformed in a tensile test, a marked asymmetric broadening of the 200 Bragg reflections was observed (Ungár, Mughrabi, Rönnpagel & Wilkens, 1984). This asymmetry was interpreted on the basis of the quasi-composite model of heterogeneous dislocation distributions, first developed and applied for fatigued Cu crystals by Mughrabi (1983). The asymmetric line profiles could be resolved into two well behaved symmetrical subprofiles which were assigned in a straightforward manner to the cell walls and cell interiors of the dislocation cell structure. The symmetric subprofiles were analysed by the theory of Wilkens in terms of local dislocation densities (Ungár, Mughrabi, Rönnpagel & Wilkens, 1984) in good agreement with transmission electron microscopy (TEM) results (Göttler, 1973). The separation of the subprofiles was shown to be a direct indication and measure of long-range internal stresses prevailing in the dislocation cell structure (Mughrabi, 1983; Ungár, Mughrabi, Rönnpagel & Wilkens, 1984; Ungár, Mughrabi & Wilkens, 1984; Mughrabi, Ungár, Kienle & Wilkens, 1986).

The compatibility in the quasi-composite model requires the existence of geometrically necessary dislocations lying along the interface between cell walls and cell interiors. These dislocations are of the same nature as the geometrically necessary dislocations introduced by Ashby (1971) to describe the plastic behaviour of dispersion hardened materials. After tensile deformation of a crystal, these dislocations represent extra pushed-in lattice planes in the cell interiors which put these regions under an extra compressional stress in the unloaded state of the material. In the cell walls lying parallel to the tensile axis the same dislocations exert an extra tensile stress on the cell-wall material. Within the framework of Wilkens's theory these geometrically necessary dislocations are an ad hoc part of the dislocation structure which are only required by the quasi-composite model.

The earlier theories of Krivoglaz (1969) and Wilkens (1970a, b) are further developed in the present work in two ways. (i) It is shown that polarized dislocation dipoles cause asymmetric line broadening. The theory provides an analytical expression for the asymmetry of line profiles from which the polarization of the dislocation structure can be evaluated. (ii) The asymptotic form of the Fourier transform of the line profiles for small values of the Fourier parameter has been expanded up to a higher-order term than given by the theory of Wilkens (1970a, b) and Krivoglaz, Martynenko & Ryaboshapka (1983). The coefficient of this higher-order term is proportional to the mean square fluctuation of the dislocation density.
2. The theory of line broadening caused by dislocations

The present theory is based on the kinematical X-ray diffraction theory of crystals containing dislocations developed by Krivoglaz (1969) and Wilkens (1969, 1970a, b). Recent considerations on dislocation dipoles made by Wilkens (1984), Drews (1984) and Gaál (1984) were fruitful for the development of the present theory.

2.1. The description of dislocation distributions

We consider 2N dislocations with line vectors $l$ lying parallel to the $z$ axis of a Cartesian coordinate system. The numbers of dislocations with positive and negative Burgers vectors, $N_+$ and $N_-$, are equal and $N_+ + N_- = 2N$.

The probability distribution function of the dislocation system is denoted as

$$W(v_1, v_2, \ldots, v_{2N}) = W\{v_j\}. \quad (1)$$

This function gives the probability density that the 2N dislocations are located exactly at the positions determined by the $\{v_j\}$ vector system.

In the kinematical theory of X-ray diffraction the Fourier transform of the intensity distribution in the vicinity of a reciprocal-lattice point can be written as (Drews, 1984)

$$A(n) = \left(\frac{1}{F}\right) \int F \left\{ W\{v_j\} \right\}$$

$$\times \exp \left\{ 2\pi i g \sum_{j=1}^{2N} \left[ u(r - v_j - \frac{1}{2}ne) - u(r - v_j + \frac{1}{2}ne) \right] \right\} d^2r \int_1^{2N} d^2v_j, \quad (2)$$

where $n$ is the Fourier parameter, the $+$ ($-$) sign refers to positive (negative) Burgers vectors, and $g$ is the diffraction vector, $g = k - k_0$, where $k$ and $k_0$ are the wave vectors of the scattered and incident radiation, respectively. $u$ is the displacement field of the dislocations, $e$ is a vector parallel to the $(x, y)$ resolution of $g$, i.e. $e = \sin \psi (g_x, g_y, 0)/(g_x^2 + g_y^2)^{1/2}$, where $\psi$ is the angle between $g$ and $l$, and $F$ is the cross section of the crystal in the $(x, y)$ plane. We introduce the following notation in a similar way to Drews (1984):

$$a(r) = 2\pi gu(r), \quad (3)$$

$$B(r, n) = 1 - \exp \left\{ i[a(r - \frac{1}{2}ne) - a(r + \frac{1}{2}ne)] \right\}. \quad (4)$$

With this notation $A(n)$ can be written as

$$A(n) = \left(\frac{1}{F}\right) \int F \left\{ W\{v_j\} \right\}$$

$$\times \int_{j=1}^{2N} \left[ 1 - B(r - v_j, n) \right] d^2r \int_{j=1}^{2N} d^2v_j, \quad (5)$$

For small values of $n$ the absolute value of $B$ is small and so $A(n)$ can be developed into a power series of $B$ as follows:

$$A(n) = \left(\frac{1}{F}\right) \int d^2r \left\{ 1 - \int dv_1 \left[ Nw+(v_1)B(r - v_1, n) \right. \right.$$}

$$\left. + Nw-(v_1)B^*(r - v_1, n) \right\}$$

$$\int d^2v_2 \left[ \frac{N(N - 1)}{2} \right]$$

$$\times \left[ w_+(v_1, v_2)B(r - v_1, n)B(r - v_2, n) \right. \right.$$}

$$+ w_-(v_1, v_2)B^*(r - v_1, n)B^*(r - v_2, n) \right.$$}

$$+ w_-(v_1, v_2)B(r - v_1, n)B^*(r - v_2, n) \right.$$}

$$+ w_+(v_1, v_2)B^*(r - v_1, n)B(r - v_2, n) \right.$$}

$$+ \cdots + c^2 \right\}, \quad (6)$$

where

$$w_+(v_1, v_2) = \int \cdots \int W\{v_j\} \prod_{i=1}^{2N} d^2v_i, \quad (7)$$

and

$$w_-(v_1, v_2) = \int \cdots \int W\{v_j\} \prod_{i=1}^{2N} d^2v_i. \quad (8)$$

are the one- and two-particle distribution functions, respectively.

The $+$ and/or $-$ signs indicate that the $v_j$ and/or $v_k$ vectors point to dislocations with positive and/or negative Burgers vectors, respectively.

By trivial algebraic transformations (6) can be reformulated in the form

$$A(n) = \left(\frac{1}{F}\right) \int d^2r \exp \left\{ \ln(1 + q_1 + q_2 + \cdots) \right\}, \quad (9)$$

where

$$q_1 = - \int dv_1 \left\{ \cdots \right\} \quad (10)$$

and

$$q_2 = \int dv_1 dv_2 \left\{ \cdots \right\} \quad (11)$$

are the two integrals inside the braces in (6).

By means of the logarithmic series expansion

$$\ln(1 + q_1 + q_2 + \cdots) \approx q_1 + q_2 - \frac{1}{2}q_1^2 + \cdots, \quad (12)$$

$A(n)$ can be rearranged with terms up to second order taken into account:

$$A(n) = \left(\frac{1}{F}\right) \int d^2r \exp \left\{ L_1(r, n) + L_2(r, n) \right\}, \quad (13)$$

where

$$L_1(r, n) = - \int \left[ Nw+(v_1)B(r - v_1, n) \right. \right.$$}

$$\left. + Nw-(v_1)B^*(r - v_1, n) \right] dv_1 \quad (14)$$

$$L_2(r, n) = \int \left[ w_+(v_1, v_2)B(r - v_1, n)B(r - v_2, n) \right. \right.$$}

$$+ w_-(v_1, v_2)B^*(r - v_1, n)B^*(r - v_2, n) \right.$$}

$$+ w_-(v_1, v_2)B(r - v_1, n)B^*(r - v_2, n) \right.$$}

$$+ w_+(v_1, v_2)B^*(r - v_1, n)B(r - v_2, n) \right.$$}

$$+ \cdots + c^2 \right\}.$$
\[ L_2(r, n) = \frac{N_1^2}{2} \int \int [T_{+}(v_1, v_2)

\times B(r - v_1, n) B(r - v_2, n)

+ T_{-}(v_1, v_2) B^*(r - v_1, n) B^*(r - v_2, n)

+ T_{+}(v_1, v_2) B(r - v_1, n) B(r - v_2, n)

+ T_{-}(v_1, v_2) B^*(r - v_1, n) B(r - v_2, n)]

\times B(r - v_1, n)] d v_1 d v_2 \]  

and

\[ T_{+}(v_1, v_2) = w_{+}(v_1, v_2) + w_{+}(v_1) w_{+}(v_2), \]  

where \( T \) is the so-called first-order correlation function of dislocations which vanishes in the case of randomly distributed dislocations.

2.2. The effect of higher-order correlation terms on the validity of equation (13)

The so-called three-particle distribution function, \( w_3(v_1, v_2, v_3) \) can be given in a form known as the Mayer cluster expansion (Gaál, 1973):

\[ w_3(v_1, v_2, v_3) = w_1(v_1) w_1(v_2) w_1(v_3) \]

\[ + w_1(v_1) T_2(v_2, v_3) \]

\[ + w_1(v_2) T_2(v_1, v_3) \]

\[ + w_1(v_3) T_2(v_1, v_2) \]

\[ + T_3(v_1, v_2, v_3), \]  

where the + and − signs were omitted for the sake of brevity, and \( T_3 \) is the so-called second-order correlation function.

The next term, \( L_3(r, n) \), which is not indicated in (13), would be proportional to \( T_3 \). It is assumed that \( T_3 \) and higher-order correlation terms can be neglected. In other words this means that \( w_3(v_1, v_2, v_3) \) and the higher-order distribution functions can be built up by appropriate algebraic combinations of the two- and one-particle distribution functions.

This assumption means that for the sake of obtaining \( n^3 \) and/or higher-order terms of \( A(n) \) it is enough to investigate the higher-order terms in \( L_1 \) and \( L_2 \).

2.3. Local parameters describing the density and the polarization of dislocations

We introduce a sign-independent dislocation density function,

\[ n(v) = \frac{1}{c^2} \int \int [v'(v + z) d^2 z, \]  

where

\[ v'(v) = N w_+(v) + N w_-(v). \]  

The integral is taken over an appropriately small region of height \( z \) in the \((x, y)\) plane. The above equation smears the distribution function of dislocations consisting of delta functions, \( v'(v) \), into a continuous dislocation density function, \( n(v) \).

The following notation is also introduced:

\[ k(v) = N w_+(v) - N w_-(v). \]  

After some simple algebraic transformations \( L_1(r, n) \) can be written as

\[ L_1(r, n) = -f(r, n) - ig(r, n), \]

where

\[ f(r, n) = \int f'(v) \Re [B(r - v, n)] d^2 v, \]

\[ g(r, n) = \int k(v) \Im [B(r - v, n)] d^2 v. \]  

Assuming that \( f'(v) \) and \( k(v) \) are functions such that \( f(r, n) \) and \( g(r, n) \) have finite values while \( F \to \infty \), we can extend the integration in (21) and (22) to infinity and so the variable \( r - v \) can be replaced by \( v \). As will be shown, this assumption is only temporarily necessary in order to continue with the calculations. Later it will turn out that this assumption can be dissolved retrospectively and therefore it does not influence the final results.

With the help of (4) \( f \) and \( g \) can be written in the form

\[ f(r, n) = \int f'(v) \Re [B(r - v, n)] d^2 v \]

\[ g(r, n) = \int k(v) \Im [B(r - v, n)] d^2 v. \]  

In order to evaluate \( g(r, n) \) we subdivide the \((x, y)\) plane into small squares with side \( c \) in such a way that each square includes at least one dislocation dipole. Then

\[ \int_{c \in \Omega} k(r) d^2 r \approx 0. \]  

This integral gives exactly zero when integrated over the entire \((x, y)\) plane and we assume that this still remains valid if \( c \) is a fine but not too fine mesh.

Within each cell of integration we introduce the position vector

\[ x = v - mc, \]  

where \( m \) is a plane vector with integer coordinates.

With this the integral in (24) can be replaced by the sum

\[ g(r, n) = \sum_{m \in \Omega} \int_{c \in \Omega} k(r - mc - x) \sin [a(mc + x - \frac{1}{2} ne)] - a(mc + x + \frac{1}{2} ne)] d^2 x. \]  

(27)
This can be expanded and is approximately

\[ g(r, n) \approx \sum_m \left\{ \left[ \frac{\partial a}{\partial r} (mc - \frac{1}{2} ne) \right] \right. \\
- \left. \left[ \frac{\partial a}{\partial r} (mc + \frac{1}{2} ne) \right] \right\} \times \cos \left[ a(mc - \frac{1}{2} ne) - a(mc + \frac{1}{2} ne) \right] \\
\times \int_{\mathbb{C}} k(r - mc - x)x \, d^2x. \tag{28} \]

Let us define the local polarization vector \( \mathbf{P}(r) \) as

\[ \mathbf{P}(r) = \left( \frac{1}{c^2} \right) \int k(r + x)x \, d^2x. \tag{29} \]

If one substitutes this into (28) the sum can be approximated by the integral

\[ g(r, n) = \int \mathbf{P}(r - v) \left\{ \frac{\partial [a(v - \frac{1}{2} ne) - a(v + \frac{1}{2} ne)]}{\partial v} \right\} \\
\times \cos \left[ a(v - \frac{1}{2} ne) - a(v + \frac{1}{2} ne) \right] \, d^2v. \tag{30} \]

The multiplier of \( \mathbf{P} \) in the above integrand is the derivative of \( \sin \left[ a(v - \frac{1}{2} ne) - a(v + \frac{1}{2} ne) \right] \). Thus if \( \mathbf{P} \) is a constant over the crystal volume then \( g(r, n) = 0 \). At the same time this means that the average value of \( \mathbf{P} \) does not give any contribution to \( g(r, n) \).

In a similar way as in (27), with the procedure of subdividing the \( (x, y) \) plane into small areas of height \( z \), the \( \mathcal{V}(v) \) function in (21) and (23) can simply be replaced by the \( \mathcal{V}(v) \) function introduced in (18).

### 2.4. The evaluation of the real part of the Fourier coefficients

In order to analyse the expansion of the function \( f \) according to \( n \) we now investigate the first non-vanishing coefficient

\[ \left( \frac{\partial^2 f}{\partial n^2} \right)_{n=0} = \int_{-\infty}^{\infty} \mathcal{V}(v) \{ e(\partial \mathcal{V}/\partial v)(v) \}^2 \, d^2v. \tag{31} \]

The factor of \( \mathcal{V}(v) \) in the integrand is positive definite and of order \( 1/|v|^2 \). Therefore, if \( \mathcal{V}(v) \) is different from zero, the integrand will be divergent. The problem of divergence can be overcome by the introduction of the function

\[ D(r, n) = \int_{-\infty}^{\infty} \{ \mathcal{V}(v) - \mathcal{V}(v - 2v) \} \\
\times \{ 1 - \cos \left[ a(v - \frac{1}{2} ne) - a(v + \frac{1}{2} ne) \right] \} \, d^2v. \tag{32} \]

The second derivative of \( D(r, n) \) with respect to \( n \) is finite since \( \mathcal{V}(v - 2v) - \mathcal{V}(v - 2v) \) is at most of order \( |v| \) in the vicinity of \( v = 0 \).

It can be shown that \( D(r, n = 0) = 0 \) and that \( D \) is an even function of \( n \). Therefore, for small values of \( n \) one obtains

\[ D(r, n) \approx d(r)n^2. \tag{33} \]

If one separates the integral in (32) into two terms and makes the substitution \( v' = 2v \) in the second term, for small \( n \) one obtains

\[ D(r, n) = f(r, n) - \frac{1}{2} f(r, 2n) \approx d(r)n^2. \tag{34} \]

In the above equation the following property of the displacement field of dislocations (irrespective of edge or screw type) was used:

\[ a(v - ne) - a(v + ne) = a(\frac{1}{2}v - \frac{1}{2}ne) - a(\frac{1}{2}v + \frac{1}{2}ne). \tag{35} \]

The solution of (34) is

\[ f(r, n) = - \frac{[d(r)/(2n)]^2 \ln[R_0(r)/n]}{\rho^* (r)n^2 \ln[R_0(r)/n]}, \tag{36} \]

where \( R_0(r) \) is a parameter of dimension length.

In the following the function \( \rho^*(r) \) will be analysed in more detail. If one takes the second derivative with respect to \( n \) of the function \( D(r, n) \) at \( n = 0 \) and uses the relation in (34) it follows from (36) that

\[ \rho^*(r) = \lim_{n \to 0} \left( \frac{1}{2 \ln 2} \int_{-\infty}^{\infty} \mathcal{V}(v) - \mathcal{V}(v - 2v) \right) \times e(\partial \mathcal{V}/\partial v)(v) \, d^2v. \tag{37} \]

The correlation between \( \rho^* \) and the dislocation density \( v \) can be obtained by the following renormalization procedure. In \( (\phi, v) \) polar coordinates instead of \( (v_x, v_y) \) coordinates, (37) can be written in the form

\[ \rho^*(r) = - \lim_{n \to 0} \left( \frac{1}{2 \ln 2} \int_{-\infty}^{\infty} \mathcal{V}(v) - \mathcal{V}(v - 2v) \right) K(\phi)/v, \tag{38} \]

where \( K(\phi) \) is a trigonometric polynomial which can be derived from the expression in braces in (37). In this evaluation the explicit form of the displacement fields of screw and/or edge dislocations have to be used.

Equation (38) can be transformed as follows:

\[ \rho^*(r) = \lim_{n \to 0} \left( \frac{1}{2 \ln 2} \int_{0}^{2\pi} d\phi K(\phi) \right) \times \frac{\mathcal{V}(v - v) - \mathcal{V}(v - 2v)}{v} \, d\phi. \tag{39} \]

The evaluation of the above expression yields for \( \rho^*(r) \)

\[ \rho^*(r) = v(r)^2 \int_{0}^{2\pi} d\phi K(\phi). \tag{40} \]

The integral in (40) has been evaluated for screw and edge dislocations. In the notation of Wilkens (1970a) the relation between the local dislocation
density \( \nu(\mathbf{r}) \) and the so-called formal value of the local dislocation density, \( \rho^*(\mathbf{r}) \), has the form

\[
\nu(\mathbf{r}) = \frac{2\pi}{N} \rho^*(\mathbf{r})/(gb)^2 C,
\]
where

\[
C = C' \sin^2 \psi
\]

with

\[
C' = \cos^2 \psi
\]
for screw dislocations and

\[
C' = \sin^2 \psi F(\gamma)
\]
for edge dislocations, where

\[
F(\gamma) = \left[1/8(1 - \nu)^2 \right] \left[1 - 4\nu + 8\nu^2 + 4(1 - 2\nu) \cos^2 \gamma \right].
\]

Here \( \nu \) is the Poisson ratio, \( \gamma \) is the angle between \( \mathbf{b} \) and the projection of \( \mathbf{g} \) on the \((x, y)\) plane and \( \psi \) is the angle between \( \mathbf{g} \) and \( \mathbf{I} \).

From (21) it follows that if the average dislocation density in the whole crystal is not zero then the parameter \( R_0 \) diverges in proportion to the crystal dimensions. This type of divergence first appeared in the line-broadening calculation of Krivoglaz & Ryaboshapka (1963). Wilkens (1969) and Gaál (1976) have shown that this divergence is of the same kind as that appearing in the expression for the elastic stored energy of dislocations:

\[
E = VApGb^2 \ln (R_0/r_0),
\]
where \( V \) is the volume and \( R_0 \) the linear dimension of the crystal. \( A \) is a constant, \( G \) is the shear modulus, \( \rho \) is the average dislocation density and \( r_0 \) is the so-called inner cut-off radius of dislocations, \( r_0 \approx b \). As is well known, in the above expression of the stored energy \( R_0 \) is always replaced by the so-called effective outer cut-off radius, \( R_e \) (Nabarro, 1967). This procedure is based on the fact that the long-range components of the strain field of dislocations are screened by the neighbouring dislocations.

In the present case \( R_0 \) is renormalized by taking into account the second-order correlations in the dislocation distribution. As in the calculations of Gaál (1976) this can be done by investigating the structure of the correlation term \( L_2 \) in (15). Since we are only dealing with the divergence of the real part of \( L_1 \), only the real part of \( L_2 \) will be investigated. Without going into details we state that

\[
\text{Re} (L_2)_{n=0} = 0
\]
and

\[
\frac{\partial [\text{Re} (L_2)]}{\partial n}|_{n=0} = 0.
\]

In the second derivative of \( L_2 \) with respect to \( n \) there is no divergence in the vicinity of \( v = 0 \) for \( n = 0 \). This means that for small \( n \) values the real part of \( L_2 \) can be approximated by

\[
\text{Re} [L_2(n)] \approx -\alpha(n^2)
\]
where \( \alpha(\mathbf{r}) \) is a space-dependent function.

The divergence of the real part of \( L_1 \) due to \( R_0 \) can be removed by defining an effective outer cut-off radius \( R_e(\mathbf{r}) \) via

\[
\alpha(\mathbf{r}) = \rho^*(\mathbf{r}) \ln [R_e(\mathbf{r})/R_0(\mathbf{r})],
\]
and substituting \( L_1 + L_2 \) in (13) by

\[
-\left[ f(\mathbf{r}, n) + \alpha(\mathbf{r})n^2 \right] = -\rho^*(\mathbf{r})n^2 \ln [R_e(\mathbf{r})/n].
\]

A similar procedure to eliminate this type of divergence was applied recently by Krivoglaz, Martynenko & Ryaboshapka (1983).

It is important to note that the procedure described above is only valid if \( n \) is considerably smaller than \( R_e \).

Wilkens (1969) has shown that the divergence caused by \( R_0 \) in the real part of \( L_1 \) can be dissolved by introducing the so-called restrictedly random dislocation distribution. According to this, \( R_0 \) can be replaced by the outer effective cut-off radius of dislocation, \( R_e \). In its effect the procedure of the present work described in (44)–(48) for \( n \ll R_e \) is the same as that of the restrictedly random dislocation distribution of Wilkens.

2.5. The evaluation of the imaginary part of the Fourier coefficients

In this section the function \( g(\mathbf{r}, n) \) in (30) will be investigated. As was mentioned before, if \( P \) is a constant then \( g(\mathbf{r}, n) = 0 \). In the case of a space-dependent dislocation polarization \( P(\mathbf{r}) \), \( g(\mathbf{r}, n) \) can be expanded into a power series of \( n \). From (30) it can be seen that \( g(\mathbf{r}, 0) = 0 \). Therefore we investigate the derivative

\[
\left( \partial g/\partial n \right)_{n=0} = \int_{-\infty}^{\infty} P(\mathbf{r} - \nu) \{ e(\mathbf{v}^2/dv/dv) \} d^2v.
\]

Since the second derivative in the braces is of the order of \( 1/|v|^2 \) the expression in (50) to be investigated for singularity. It can be shown that the displacement fields of straight dislocations have such a structure that the integral in (50) is not singular. This means that the first derivative of \( g \) with respect to \( n \) is finite and so \( g(\mathbf{r}, n) \) can be expanded as follows:

\[
g(\mathbf{r}, n) \approx (\partial g/\partial n)_{n=0} n.
\]

Below we use the notation

\[
S(\mathbf{r}) = [\partial g(\mathbf{r}, n)/\partial n]_{n=0}.
\]

From the construction of \( S(\mathbf{r}) \) and (22) and (25) it
follows that
\[ \int_{-\infty}^{\infty} S(r) \, d^2r = 0. \quad (53) \]

3. The structure of the Fourier coefficients

From (13), (20), (36), (48), (51) and (52) the Fourier coefficients have the following form:

\[ A(n) = \left( \frac{1}{F} \right) \int_{-\infty}^{\infty} \exp \left\{ -\rho^*(r)n^2 \ln \left[ R_e(r)/n \right] ight\} \]
\[ - iS(r)n \, d^2r \quad (54) \]

for small values of \( n \).

At this point it is important to note that the procedure described in (32)-(36) can be extended to terms proportional to \( n^4 \) in the real part and to \( n^3 \) and \( n^5 \) in the imaginary part of the Fourier coefficients. These higher-order terms are obtained from the evolution of \( L_1 \) and \( L_2 \) according to the method of (32)-(36). It has been shown that the contribution of the higher-order terms has no effect on the structure of the series expansion of \( A(n) \) as given in (55) and (57). The only effects of the higher-order terms in \( L_1 \) are some minor modifications in the physical interpretation of the expansion coefficients in (55) and (57). The details of these calculations will be published elsewhere but are available as a typescript on request from the authors.

The series expansion of the exponential function up to fifth-order terms yields the result

\[ A(n) \simeq \left( \frac{1}{F} \right) \int_{-\infty}^{\infty} \left\{ 1 - \rho^*(r)n^2 \ln \left( a_0/n \right) \right\} \]
\[ - \left[ \rho^*(r) \ln \left( R_e/a_0 \right) + S(r)^2/2 \right] n^2 \]
\[ + \frac{1}{2} \rho^*(r)^2n^4 \ln^2 \left( a_0/n \right) \]
\[ + \tau_1 n^4 \ln \left( a_0/n \right) + \tau_2 n^4 \]
\[ + i\rho^*(r)S(r)n^3 \ln \left( a_0/n \right) \]
\[ + i\tau_3 n^3 \]
\[ - i\frac{1}{2} S(r)\rho^*(r)^2n^5 \ln^2 \left( a_0/n \right) \]
\[ + i\tau_4 n^5 \ln \left( a_0/n \right) + i\tau_5 n^5 \right\} \, d^2r, \quad (55) \]

where \( a_0 \) is an arbitrary constant of dimension length and \( \tau_1...5 \) are formal parameters which in principle can be derived from the distribution functions \( v \) and \( P \).

For the spatial average of a function we shall use the notation

\[ \left( \frac{1}{F} \right) \int_{-\infty}^{\infty} \cdots d^2r = \left\langle \cdots \right\rangle. \quad (56) \]

In this notation (55) can be written in the form

\[ A(n) \simeq 1 - \left\langle \rho^* \right\rangle n^2 \ln \left( R_{eff}/n \right) \]
\[ - i\left\langle S\rho^* \right\rangle n^3 \ln \left( R_1/n \right) \]
\[ + \frac{1}{2} \left\langle \rho^* \right\rangle^2 n^4 \ln \left( R_2/n \right) \ln \left( R_3/n \right) \]
\[ - \left( i/2 \right) \left\langle S\rho^* \right\rangle^2 n^5 \ln \left( R_4/n \right) \ln \left( R_5/n \right), \quad (57) \]

where

\[ R_{eff} = \exp \left\{ \frac{\left\langle \rho^* \right\rangle \ln R_e + \left\langle S^2 \right\rangle /2}{\left\langle \rho^* \right\rangle} \right\} \quad (58) \]

and

\[ R_1 = \exp \left\{ \frac{\left\langle S\rho^* \right\rangle \ln R_e - \left\langle S^3 \right\rangle /6}{\left\langle \rho\rho^* \right\rangle} \right\} \quad (59) \]

Here we note that \( \left\langle S(r) \right\rangle \) vanishes according to (53).

The explicit expressions for \( R_2, R_3, R_4 \) and \( R_5 \) are somewhat lengthy and are not given here since no use of them will be made in the following.

One may use the logarithmic equality in (12) to transform (57) to the form

\[ \ln A(n) = - \left\langle \rho^* \right\rangle n^2 \ln \left( R_{eff}/n \right) \]
\[ + \frac{1}{2} \left\langle \rho^* \right\rangle^2 - \left\langle \rho^* \right\rangle^2 \]
\[ \times n^4 \ln \left( R_2/n \right) \ln \left( R_3/n \right) \]
\[ - i\left\langle S\rho^* \right\rangle n^3 \ln \left( R_1/n \right) \]
\[ - \left( i/2 \right) \left\langle S\rho^* \right\rangle^2 - 2\left\langle \rho^* \right\rangle \left\langle S\rho^* \right\rangle \]
\[ \times n^5 \ln \left( R_4/n \right) \ln \left( R_5/n \right), \quad (60) \]

where the sixth- and higher-order terms are neglected.

The terms \( R_2, R_3, R_4 \) and \( R_5 \) can be derived from a quadratic expression of the terms \( R_2, R_3, R_4, R_5, R_{eff} \) and \( \left\langle \rho^* \right\rangle \). This correlation is not given in an explicit form, however, since \( R_2, R_3, R_4 \) and \( R_5 \) are not interpreted physically in the present case.

4. Discussion

The theory developed in the present work describes the asymmetric broadening of X-ray diffraction lines on the basis of the kinematical diffraction theory by taking into account the displacement fields of dislocations. Theoretical considerations have given an expression for the Fourier transform of X-ray line profiles, equation (60), in which a quite general dislocation structure can be characterized by four distinct parameters. These parameters are as follows:

(i) The formal dislocation density, \( \rho^* \), defined by (37). This equation gives the connection between an arbitrary dislocation distribution function, \( v(r) \), and \( \rho^* \). Equation (37) can be reduced to a simpler correlation between \( v(r) \) and \( \rho^* \) as in (41). In the simplest case \( \rho^*(r) \) can be replaced by the average dislocation density \( \left\langle \rho^* \right\rangle \) as in (60).

(ii) The weighted polarization of the dislocation distribution, \( S(r) \), defined by (50) and (52). These equations give the connection between \( S(r) \) and a given dislocation polarization distribution function, \( P(r) \).

(iii) The effective outer cut-off radius of dislocations, \( R_{eff} \). This has a similar physical meaning to \( R_e \) in the theory of Wilkens (1970b), and is proportional to \( R_e \) as it appears in the elastically stored energy of dislocations (Nabarro, 1967).

(iv) The fluctuation of the dislocation structure \( \left\langle \rho^* \right\rangle^2 - \left\langle \rho^* \right\rangle^2 \).
Since the present theory was born as a further development of the theory of Wilkens (1970a, b), the parameters involved in the two theories will now be discussed. In the theory of Wilkens the dislocation structure is characterized by two parameters which are the average dislocation density, \( \rho \), and the so-called stress parameter, \( M \). The latter characterizes the effectiveness of screening of the strain fields of neighbouring dislocations. In this respect it is in strong correlation with the effective outer cut-off radius of dislocations, \( R_e \), as it appears in the expression of the elastically stored energy (Nabarro, 1967).

A fundamental idea in Wilkens’s theory is the restrictedly random distribution of dislocations, which is, in a way, a renormalization procedure of the infinite crystal dimension into finite regions characterized by a length proportional to \( R_e \) (Wilkens, 1969). The theory can well be applied for relatively simple dislocation distributions (Wilkens, Herz & Mughrabi, 1980; Ungár, Mughrabi & Wilkens, 1982; Wilkens, 1984). However, asymmetric line profiles corresponding to more complicated dislocation structures, such as the dislocation cell structure after tensile deformation in Cu single crystals orientated for ideal multiple slip, cannot be described by Wilkens’s theory without making a number of auxiliary assumptions (Ungár, Mughrabi, Rönnpagel & Wilkens, 1984).

In the present theory the renormalization of the crystal dimensions is done via the appropriate manipulation of the higher-order correlation terms in \( L_2 \) [cf. (45)–(48)]. In its end effect the two parameters \( R_e \) and \( R_{eff} \) produced by the concept of restrictedly random dislocation distribution and by the procedure carried out with \( L_2 \), respectively, have the same physical meaning and are proportional to each other. Both \( R_e \) and \( R_{eff} \) give a qualitative measure of the screening of the stress or strain fields of neighbouring dislocations.

In the case of symmetric profiles the present and Wilkens’s theory give exactly the same values for the average dislocation density. One of the strengths of the present theory is that it yields the proper average dislocation density in a straightforward manner, even in the case of asymmetric profiles. More details of this will be discussed in the second paper of this series (Ungár, Groma & Wilkens, 1988).

The polarization and the fluctuation of the dislocation structure will also be discussed in the second paper of this series in an application of the present theory to the line broadening of [001] Cu single crystals after tensile deformation.

It is worth noting that in a recent paper Gaál (1984) investigated the line profiles corresponding to a crystal containing polarized screw dipoles. In this work the imaginary part of the Fourier transform was calculated [cf. equation (4) of Gaál (1984)]. It can be shown that by appropriate coordinate transform-

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References


Mirror and Bragg Reflections of Neutrons at a Nuclear Resonance

BY C. M. BATIGUN* AND R. M. BRUGGER
University of Missouri, Columbia, Missouri 65211, USA

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Abstract
A set of experiments has observed the mirror reflection and Bragg diffraction of neutrons at the energy of a low-lying nuclear resonance of $^{115}$In. The reflector was a mirror of In metal with the resonance at 1.457 eV. The mirror reflection for different angles of incidence was measured and sets of data showing the relative reflectivities were obtained. For the Bragg diffraction experiment the crystal was a wafer of InP and several examples of Bragg reflections near 1.456 eV were measured.

Introduction
Because of the wave nature of neutrons, materials have an index of refraction for neutrons trying to pass through them. As with light, if the conditions are right, neutrons can be totally reflected from an interface (Fermi & Zinn, 1946; Fermi & Marshall, 1947). For materials with a positive scattering amplitude, the index of refraction is smaller than unity and neutrons will be totally reflected when they try to pass from a vacuum into the material if the angle of incidence is small enough. The index of refraction is energy dependent and departs from unity as a function of the wavelength of the neutrons. For neutrons, the index of refraction is close to unity and the angle at which reflections can be observed is small. To have large enough angles to work with, most total-reflection experiments have been with thermal or cold neutrons for which the wavelength is larger. Total reflection of cold and thermal neutrons has led to measurements of scattering lengths of isotopes and to the construction of neutron guides (Carlile, Johnson & Williams, 1979).

Near the thermal region the scattering for most elements is constant, but at higher energies near a nuclear resonance the scattering cross sections $\sigma_s$ are constant, but at higher energies near a nuclear resonance the $\sigma_s$'s are not constant but increase markedly at the peaks of the resonances. Unfortunately, for the low-energy resonances the absorption cross sections are large and absorb neutrons that would otherwise be scattered. However, at some of these resonances the scattering is as large as a few percent of the absorption cross sections and it seemed that it might be worthwhile to examine Bragg scattering of neutrons from a crystal when the energy of the neutrons corresponded to the energy of the resonance (Carlile, Ward & Willis, 1985). A crystal of InP, again with the resonance of 1.457 eV, was used as an example.

The mirror experiment
The experiment was performed at the University of Missouri Research Reactor (MURR). A collimated beam of neutrons was extracted from the $F$ port of MURR and reflected from a mirror towards a set of neutron counters. Fig. 1 indicates the experimental arrangement. The detectors were scanned perpendicular to the beam to search out the peaks from straight-through and reflected beams and to determine the relative intensities of each beam. Cadmium filters were used to limit the measurements to epithermal neutrons, and an In filter with a filter difference calculation served to distinguish the resonance energy neutrons from other epicadmium neutrons.

A collimator was inserted into the $F$ port of the MURR to produce the well collimated beam needed for this experiment. The iron collimator was 1.948 m long with a slit 0.38 mm wide by 19 mm high at each end. Originally the slit was cut 1.27 mm wide, but as this did not give fine enough angular resolution,