Table 1. *List of crystal space groups with the enantiomorphous ambiguity*

Crystal system	Space groups
Monoclinic	$P2$, $B2$, $C2$, $P2_1$, Pm, Bm, Cm, Pb, Pc, Bb, Cc
Orthorhombic	$Pmm2$, $Amm2$, $Cmm2$, $Fmm2$, $Imm2$, $Pmc2_1$, $Cmc2_1$, $Pcc2$, $Ccc2$, $Pma2$, $Ama2$, $Ima2$, $Pca2_1$, $Pnc2$, $Pmn2_1$, $Pba2$, $Aba2$, $Pna2_1$, $Iba2$, $Pnn2$, $Abm2$, $Fdd2$
Tetragonal	$P4$, $I4$, $P4_1$, $I4_1$, $P4_2$, $P4_3$, $P4mm$, $I4mm$, $P4bm$, $P4_2cm$, $P4_2nm$, $P4cc$, $P4nc$, $P4_2mc$, $P4_2bc$, $I4cm$, $I4_1md$, $I4_1cd$
Hexagonal	$P6$, $P6_1$, $P6_2$, $P6_3$, $P6_4$, $P6_5$, $P6mm$, $P6cc$, $P6_3cm$, $P6_3mc$

Concluding remarks

For the practical application of the proposed method it is necessary to know at least one atomic position. This problem can be solved by the trial-and-error method

$$\mathbf{r}_t \rightarrow \mathbf{S}(\mathbf{r}_t) \rightarrow \mathbf{V}[\mathbf{S}(\mathbf{r}_t)]$$

and if $\mathbf{V}[\mathbf{S}(\mathbf{r}_t)] \subset \mathbf{V}(\mathbf{X})$, then $\mathbf{r}_t \in \mathbf{X}$. Note that the vector sets of the factor sets $\mathbf{S}(\mathbf{r})$ and $\mathbf{S}(\boldsymbol{\omega} - \mathbf{r})$, as we have already mentioned, are always homometric. Therefore the scanning area for the trial vectors $\mathbf{r}_t$ should cover, in general, only the $1/(LKM)$th part of the unit cell, where L is the number of symmetry operations, K is the number of centering translations, and M is the number of EO vectors.

The application of the S-filtration method is especially effective for crystals with heavy atoms and high-order symmetries. Serious problems arise for so-called difficult structures, when the crystal symmetry belongs to polar space groups (except for the trigonal system; see Table 1). In this case either Patterson or conventional direct methods would provide an ambiguous solution in which the true structure and its enantiomorph are superimposed. This obstructs the solution of the structures. Special methods have been proposed to overcome this obstacle. For a detailed discussion on this topic, the reader is referred to the paper by Fan Hai-fu (1984).

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X-ray Diffraction by a Low-Angle Twist Boundary Perpendicular to Crystal Surface. III. The Integral Characteristics

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Abstract

For X-ray diffraction by a pure low-angle twist boundary perpendicular to a crystal surface, within the framework of the kinematic and dynamical theories, the following integral characteristics are calculated: (a) the bicrystal reflectivity in the vicinity of the lth reflection; (b) the integrated intensity of the lth reflection; (c) the bicrystal total reflectivity, *i.e.* the sum of the integrated intensities over all reflections. The case for even $\mathbf{h}\,.\,\mathbf{b}$ ($\mathbf{h}$ is the diffraction vector, $\mathbf{b}$ is the Burgers vector of the boundary screw dislocations) is considered. In dynamical theory an increase of the total reflectivity of a bicrystal due to the boundary dislocation structure is obtained.

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1. Introduction

Diffraction methods have been successfully used in studies of the structure of grain boundaries. A detailed presentation of the results of such studies performed by the use of X-ray and electron diffraction was given in the review paper of Sass (1980). The use of X-radiation is greatly preferable, firstly because it lacks double diffraction, which complicates the diffraction pattern, and secondly because it enables the investigation of relatively thick samples. X-ray diffraction studies of bicrystal block boundaries were carried out for the case when the boundary plane is parallel to the crystal surface. Both the high-angle and low-angle twist boundaries were investigated by Guan & Sass

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(1973, 1979), Gaudig & Sass (1979) and Budai, Bristowe & Sass (1983). A method for the direct determination of screw dislocation core structure was suggested (Guan & Sass, 1973) and the boundary thickness was determined (Budai, Gaudig & Sass, 1979).

In these works the studies were carried out on artificial bicrystals of gold and silver. Bicrystals of lead chalcogenides were used by Michailov, Savitsky, Sipatov, Fedorenko & Shpakovskaya (1983). The work of Lamarre, Schmückle, Sickafus & Sass (1984) was devoted to the treatment of effects of block materials, bond types (ionic, metallic or covalent) therein, and solute segregation on the boundary structure of the blocks.

The electron diffraction technique has been developed to study the thickness of pure tilt grain boundaries perpendicular or inclined to the foil surface (Carter, Donald & Sass, 1979, 1980).

Unfortunately, the problem of X-ray diffraction by a bicrystal with a grain boundary parallel or perpendicular to the crystal surface has not so far been solved analytically, except for the case of a low-angle pure twist boundary perpendicular to the foil surface (Vardanyan & Petrosyan, 1987*a*; hereafter referred to as paper I). Such a theory would enable the intensities and half-widths of extra reflections to be estimated and compared with experimental data. In paper I the superstructure factor approximation is used, which is valid at $z_0 \ll \Lambda$ (z_0 is the dislocation superlattice period, Λ is the extinction length), *i.e.* when the diffraction in one cell of the superlattice (SL) is considered in the kinematic approximation (Vardanyan, Manoukyan & Petrosyan, 1985). The condition $z_0 \ll \Lambda$ means that the twist angle $\Delta\theta$ between the crystalline lattices of bicrystal blocks exceeds 10^{-4} rad. Since in the case of a low-angle boundary $\Delta\theta < 10^{-1}$ rad, the problem treated by us is restricted by the twist angles $10^{-4} < \Delta\theta < 10^{-1}$ rad.

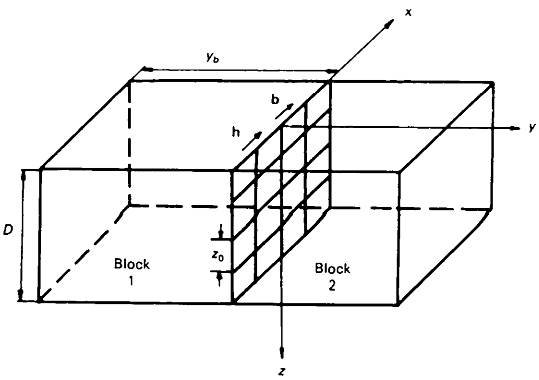

Fig. 1. Bicrystal with a twist boundary perpendicular to the foil surface. D is the block thickness, y_b is the block size in the y direction, z_0 is the period of a dislocational superlattice, **b** is the Burgers vector of the dislocation parallel to the crystal surface, **h** is the diffraction vector. For dislocations perpendicular to the foil surface (**hb**) = 0.

The expression for the dislocation SL superstructure factor $M_{l,n}$ (l is a reflection number; $n = \pm\mathbf{hb}$) is given in paper I. The analysis of that expression is carried out in paper II (Vardanyan & Petrosyan, 1987*b*), where the plane-wave image profiles of the boundary are also constructed. The image of the boundary is a narrow dark line (or several lines), so narrow that its width is less than the X-ray film resolution. Therefore, useful information about the boundary structure can be obtained using X-ray diffractometry. Since the entrance width of a counter is much larger than the effective size of the near-boundary region, the counter will detect the integrated intensity taken along the y axis perpendicular to the boundary plane (Fig. 1).

In the present paper, within the framework of the kinematic and dynamical theories the following characteristics are calculated: (*a*) the bicrystal reflectivity in the vicinity of the lth reflection; (*b*) the integrated intensity of the lth reflection; (*c*) the bicrystal total reflectivity, *i.e.* the sum of the integrated intensities over all reflections.

The case of even **hb** only is treated. Absorption is not taken into account.

2. The bicrystal reflectivity

We denote by $R_{l,n}(p, Y)$ the reflectivity of the diffraction plane $y = \text{constant}$, where

$$Y = y/z_0 \tag{1}$$

is the dimensionless coordinate of the diffraction plane; $n = \mathbf{hb}$ at $y > 0$ (block 2) and $n = -\mathbf{hb}$ at $y < 0$ (block 1) and

$$\begin{aligned} p &= \Lambda(s - s_l) \\ &= (\sin 2\theta_B / C|\chi_h|)(\theta - \theta_l) \end{aligned} \tag{2}$$

is a parameter proportional to the deviation from the lth reflection direction $s_l = l/2z_0$; $\Lambda = \lambda \cos\theta_B/(C|\chi_h|)$ is the crystal extinction length; C is the polarization factor and χ_h is the Fourier component of the crystal susceptibility.

The approach developed by Vardanyan, Manoukyan & Petrosyan (1985) is that within the limits of the lth reflection one may consider the SL as an ideal crystal with the modified Fourier component of the crystal susceptibility

$$\chi_{hl} = M_{l,n}\chi_h \tag{3}$$

where $M_{l,n}$ is the superstructure factor.

Therefore the formula for the reflectivity of the diffraction plane $y = \text{constant}$ is identical to the corresponding formula for an ideal crystal, if in the latter $\chi_{h,l}$ is used instead of χ_h.

As is noted in paper I, the dislocation SL superstructure factor $M_{l,n}$ satisfies the following relations [see equations (I-9), (I-21) and (I-22)]:

$$M_{l,n} = M_{-l,-n} \quad (4a)$$

$$lM_{l,n} = nM_{n,l} \quad (4b)$$

$$\sum_{l=-\infty}^{\infty} M_{l,n}^2 = 1. \quad (4c)$$

The relations (4a) and (4b) enable us to restrict consideration only to the case of $|l| \geq |n|$. The l and n are of the same parity. The value $l = n$ corresponds to the principal reflections of blocks 1 and 2, and values $l \neq n$ correspond to extra ones. For even n the superstructure factor has the form

$$M_{l,n} = q^{|n|/4}, \quad \text{at } l = 0 \quad (5a)$$

$$M_{l,n} = (1-q)q^{(|l|-|n|)/4} \times P_{(|n|/2)-1}^{((|l|-|n|)/2,1)}(1-2q), \quad \text{at } ln > 0 \quad (5b)$$

$$M_{l,n} = 0, \quad \text{at } ln < 0, \quad (5c)$$

where

$$q = \exp(-4\pi|Y|) \quad (6)$$

and $P_n^{(\alpha,\beta)}(x)$ are Jacobi polynomials.

The bicrystal reflectivity is defined as

$$R_{l,n}(p) = (2y_b)^{-1} \int_{-y_b}^{y_b} R_{l,n}(p, Y)\,\mathrm{d}y \quad (7)$$

where y_b is the block size in the direction perpendicular to the boundary plane.

2.1. *Kinematic theory*

Under the condition $D \ll \Lambda_l$, where D is the block thickness and $\Lambda_l = \Lambda/M_{l,n}$ the extinction length for the lth reflection, the multifold reflections between SL cells can be neglected. In this approximation the reflectivity of the diffraction plane $y = \text{constant}$ has the form

$$R_{l,n}(p, Y) = M_{l,n}^2 R_{\mathrm{id}}(p) \quad (8)$$

where

$$R_{\mathrm{id}}(p) = \sin^2(\pi A p)/p^2 \quad (9)$$

is an ideal crystal reflectivity in the kinematic approximation (James, 1950), and

$$A = D/\Lambda. \quad (10)$$

Substitution of (8) into (7) gives

$$R_{l,n}(p) = R_{\mathrm{id}}(p)(2y_b)^{-1} \int_{-y_b}^{y_b} M_{l,n}^2\,\mathrm{d}y. \quad (11)$$

The evaluation of the integral in (11) is performed in Appendix A. The result is:

(a) for the extra reflections ($l \neq n$)

$$R_{l,n}(p) = R_{\mathrm{id}}(p)\frac{z_0}{2\pi y_b} \times \begin{cases} \dfrac{|n|}{n^2 - l^2}, & \text{at } |l| < |n| \quad (12a) \\ \dfrac{n^2}{|l|(l^2 - n^2)}, & \text{at } |l| > |n|; \quad (12b) \end{cases}$$

(b) for the principal reflections ($l = n$)

$$R_{n,n}(p) = R_{\mathrm{id}}(p)\left(\frac{1}{2} - \frac{z_0}{4\pi y_b}\sum_{i=1}^{(|n|/2)-1}\frac{1}{i} - \frac{3z_0}{8\pi|n|y_b}\right). \quad (13)$$

In Fig. 2 the values of the bicrystal reflectivity at $\mathbf{hb} = 2$ and $\mathbf{hb} = 4$ are shown. Since $z_0 \ll y_b$, the intensities of the principal reflections $l = \pm 2$ and $l = \pm 4$ greatly exceed those of the extra one. That is why in Fig. 2 the intensities of the principal reflections are not shown. The half-widths of all the reflections are the same and depend upon the block thickness.

As noted in paper II, the superstructure factor $M_{l,n}$ at $l \neq n$ is significant in a narrow near-boundary region only. Both the centre and the effective size of that region depend on l and n (see Table 1 in paper II). Therefore the radiation scattered just in that narrow region essentially contributes to the magnitude of $R_{l,n}(p)$. For example, the superstructure factor of the extra reflection $l = 0$ has a sharp maximum $|M_{0,n}|_{\max} = 1$ at $y = 0$. The half-width of the maximum decreases as $|n|$ increases. Therefore, by increasing $|n|$ we decrease the effective size of the region essentially contributing to the magnitude of $R_{0,n}$, the form of which is determined from (12a) as

$$R_{0,n}(p) = R_{\mathrm{id}}(p) z_0 / 2\pi|n|y_b. \quad (14)$$

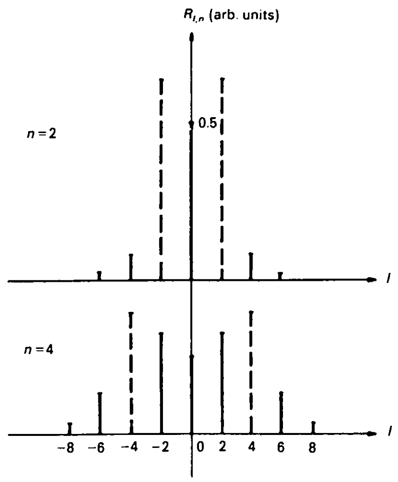

Fig. 2. Bicrystal reflectivity in the kinematic approximation ($A \ll 1$). l is a reflection number; $l = \pm n$ are the principal reflections of the blocks. Half-widths of all the reflections are identical.

From (4*b*) and (11) it follows that in the kinematic approximation

$$n^2 R_{n,l}(p) = l^2 R_{l,n}(p). \quad (15)$$

Note that in (15) the fact that χ_h changes with changing $|n|$ is not taken into account.

2.2. *Dynamical theory*

If the condition $D \ll \Lambda_l$ is not fulfilled, then the multifold reflections between SL cells cannot be neglected. According to the dynamical theory, the ideal crystal reflectivity is (Pinsker, 1978)

$$R_{\rm id}(p) = \frac{\sin^2[\pi A(p^2+1)^{1/2}]}{p^2+1}. \quad (16)$$

In accordance with the general approach, replacing χ_h by χ_{hl} in (16), for the reflectivity of the diffraction plane y = constant, one can write

$$R_{l,n}(p, Y) = M_{l,n}^2 \frac{\sin^2[\pi A(p^2+M_{l,n}^2)^{1/2}]}{p^2+M_{l,n}^2}. \quad (17)$$

Substituting (17) into (7), for the bicrystal reflectivity we have

$$R_{l,n}(p) = \frac{1}{2y_b} \int_{-y_b}^{y_b} M_{l,n}^2 \frac{\sin^2[\pi A(p^2+M_{l,n}^2)^{1/2}]}{p^2+M_{l,n}^2}\, {\rm d}y. \quad (18)$$

For the extra reflection $l=0$, substituting (5*a*) and (6) into (18) and using the approximation $A \ll \exp(4\pi y_b/z_0)$ we can write

$$R_{0,n}(p) = \frac{z_0}{4\pi y_b} \int_0^1 \frac{\sin^2[\pi A(p^2+q^{|n|/2})^{1/2}]}{p^2+q^{|n|/2}} q^{(|n|/2)-1}\, {\rm d}q,$$

which after a simple transformation is reduced to the tabulated integral (Proudnikov, Brychkov & Marichev, 1981)

$$R_{0,n}(p) = \frac{z_0}{\pi|n|y_b} \int_{\pi A|p|}^{\pi A(p^2+1)^{1/2}} \frac{\sin^2(x)}{x}\, {\rm d}x$$
$$= \frac{z_0}{2\pi|n|y_b} \{f[2\pi A(p^2+1)^{1/2}] - f(2\pi A|p|)\} \quad (19)$$

where $f(x) = \gamma + \ln x - {\rm ci}(x)$; ${\rm ci}(x)$ is the cosine-integral function and $\gamma = 0{\cdot}5772$ is the Euler constant. The $f(x)$ values are tabulated by Abramowitz & Stegun (1965).

Fig. 3 shows the p dependence of $R_{0,n}$ for three values of bicrystal thickness. With increasing thickness the reflection curve narrows around the $p=0$ direction. At the reflection centre $p=0$ we have

$$R_{0,n}(0) = (z_0/2\pi|n|y_b) f(2\pi A). \quad (20)$$

According to the kinematic theory, from (14) we obtain

$$R_{0,n}^{\rm kin}(0) = (z_0/2\pi|n|y_b)(\pi A)^2. \quad (21)$$

Fig. 4 shows the thickness dependence of $R_{0,n}(0)$ in the kinematic and dynamical theories.

As seen from (16) in the dynamical theory the ideal crystal reflectivity $R_{\rm id}(0) = \sin^2(\pi A)$ has an oscillatory behaviour, which is due to the X-ray multiple reflections inside the crystal (extinction). In the bicrystal case, for the $l=0$ extra reflection, the

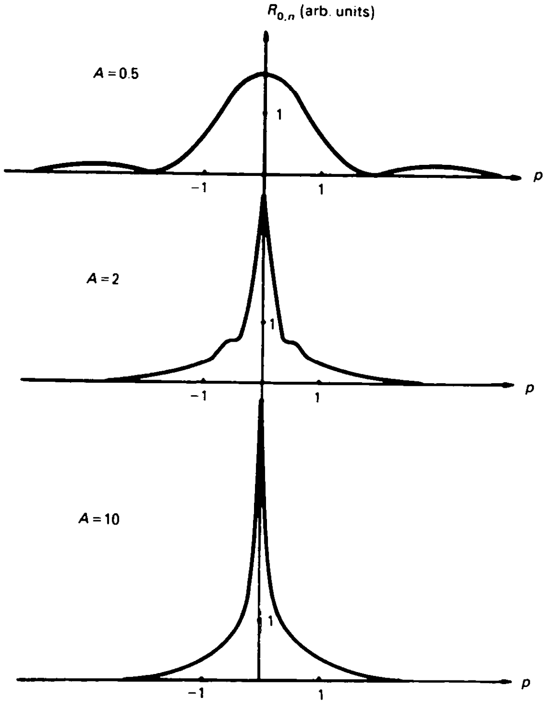

Fig. 3. Rocking curve of the $l=0$ reflection according to dynamical theory.

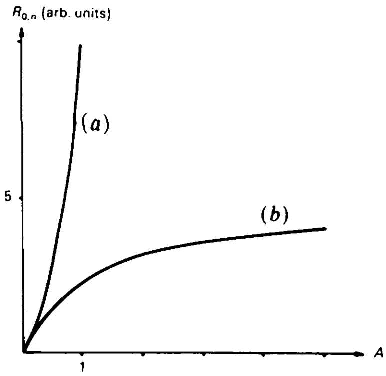

Fig. 4. Thickness dependence of the $l=0$ reflectivity at $p=0$ according to (*a*) kinematic and (*b*) dynamical theories.

dynamical features of the scattering occur in the near-boundary region only, since the extinction length of this reflection $\Lambda_{0,n}=\Lambda \exp(\pi|nY|)$ shows a minimum at $y=0$ and increases exponentially on both sides of the boundary plane. Therefore, under the condition $A \ll \exp(4\pi y_b/z_0)$, which is in fact always valid, $R_{0,n}(0)$ monotonically increases with A. For the other extra reflections one fails to obtain a simple analytical expression. However, from the above considerations one may state that the conclusions concerning $R_{0,n}$ are qualitatively also valid for $R_{l,n}$.

3. The integrated intensity of a bicrystal

As is well known, the integrated intensity is defined as a quantity proportional to the area under a reflection curve (Pinsker, 1978)

$$R^i_{l,n}=\alpha \int_{-\infty}^{\infty} R_{l,n}(p)\,\mathrm{d}p \tag{22}$$

where

$$\alpha = C|\chi_h|/\sin 2\theta_B.$$

3.1. *Kinematic theory*

Substituting (12*a*), (12*b*) and (13) into (22) and taking into account the relation valid in the kinematic approximation,

$$\int_{-\infty}^{\infty} R_{\mathrm{id}}(p)\,\mathrm{d}p=\pi^2 A,$$

we obtain:

(*a*) for the extra reflections ($l\neq n$)

$$R^i_{l,n}=\alpha\frac{\pi A z_0}{2y_b}\times\begin{cases}\dfrac{|n|}{n^2-l^2}, & \text{at } |l|<|n| \quad (23a)\\[2ex] \dfrac{n^2}{|l|(l^2-n^2)}, & \text{at } |l|>|n|; \quad (23b)\end{cases}$$

(*b*) for the principal reflections ($l=n$)

$$R^i_{n,n}=\alpha\pi^2 A\left(\tfrac{1}{2}-\frac{z_0}{4\pi y_b}\sum_{i=1}^{(|n|/2)-1}\frac{1}{i}-\frac{3z_0}{8\pi|n|y_b}\right). \tag{24}$$

Thus, in the kinematic approximation $R^i_{l,n}\sim A$. For the $l=0$ reflection from (23*a*) we have

$$R^i_{0,n}=\alpha\pi A z_0/2|n|y_b. \tag{25}$$

3.2. *Dynamical theory*

Substituting (18) into (22) and taking into account the tabulated integral

$$\int_{-\infty}^{\infty}\frac{\sin^2[\pi A(p^2+1)^{1/2}]}{p^2+1}\,\mathrm{d}p=\frac{\pi}{2}\bar{J}_0(2\pi A)$$

where $J_n(x)$ is the Bessel function of the nth order and

$$\bar{J}_0(x)=\int_0^x J_0(t)\,\mathrm{d}t$$

we obtain

$$R^i_{l,n}=\frac{\alpha\pi}{4y_b}\int_{-y_b}^{y_b} M_{l,n}\bar{J}_0(2\pi A M_{l,n})\,\mathrm{d}y. \tag{26}$$

The integral in (26) is evaluated in Appendix *B*.

(*a*) For the extra reflection $l=0$

$$R^i_{0,n}=\frac{\alpha z_0}{2|n|y_b}[\bar{J}_0(2\pi A)-J_1(2\pi A)]. \tag{27}$$

(*b*) For other reflections we restrict ourselves to consideration of the case $\mathbf{hb}=2$. Then, from (5*b*) for the superstructure factor we have

$$M_{l,2}=q^{(|l|-2)/4}(1-q). \tag{28}$$

For the $|l|>2$ extra reflections we have

$$R^i_{l,2}=\frac{\alpha z_0}{4y_b(|l|+2)}\times\sum_{m=0}^{\infty}\frac{(-1)^m\Gamma(2m+1)\Gamma[\frac{1}{2}(|l|-2)(m+1)]}{2^{2m}\Gamma(m+1)\Gamma[\frac{1}{2}(|l|+2)(m+1)]}\times(2\pi A)^{2m+1} \tag{29}$$

where $\Gamma(x)$ is the gamma function.

From (29) we obtain

$$R_{4,2}=\frac{\alpha z_0}{4y_b}\frac{\pi\eta_4}{3}\times[J_{1/3}(\eta_4)J_{-1/3}(\eta_4)-J_{2/3}(\eta_4)J_{-2/3}(\eta_4)] \tag{30}$$

where

$$\eta_4=[(\surd 3)/9]2\pi A$$

and

$$R_{6,2}=\frac{\alpha z_0}{4y_b}\frac{\pi\surd 2}{16}\eta_6\times[J_{1/4}(\eta_6)J_{-1/4}(\eta_6)-J_{3/4}(\eta_6)J_{-3/4}(\eta_6)] \tag{31}$$

where

$$\eta_6=\tfrac{1}{8}2\pi A.$$

(*c*) For the principal reflection

$$\Delta R^i_{2,2}=R^i_{2,2}-R^i_{\mathrm{id}}=-\frac{\alpha z_0}{16y_b}\sum_{m=0}^{\infty}\frac{(-1)^m(2\pi A)^{2m+1}}{2^{2m}(m!)^2(2m+1)}\sum_{i=1}^{2m+2}\frac{1}{i} \tag{32}$$

where

$$R^i_{\mathrm{id}}=(\alpha\pi/4)\bar{J}_0(2\pi A) \tag{33}$$

is the integrated intensity of an ideal block. Note that $\Delta R^i_{2,2}<0$.

In Fig. 5 the thickness-dependent quantities $R^i_{l,2}$ for the $l=0$, $l=4$ and $l=6$ extra reflections are presented. At small A a linear increase of the integrated intensity is observed, which agrees well with the kinematic theory. With a further increase of A a deviation from the kinematic law $R^i \sim A$ is revealed (extinction).

At $A \gg 1$ from (26) we obtain

$$R^i_{l,2} = \frac{\alpha z_0}{4y_b} \times \begin{cases} 1, & \text{at } l=0 \quad (34a) \\ 4/(l^2-4), & \text{at } |l|>2 \quad (34b) \end{cases}$$

and

$$\Delta R^i_{2,2} = -(\alpha z_0/4y_b) \times \tfrac{1}{4}. \quad (34c)$$

4. The total reflectivity of a bicrystal

If the bicrystal and the counter are rotated in the vicinity of the lth reflection direction s_l, then the integrated intensity of the lth reflection is involved. However, if the rotation involves a much wider angular region, then the sum of the integrated intensities of all reflections is involved.

Thus, the total reflectivity of a bicrystal will be determined as

$$R^i_n = \sum_{l=-\infty}^{\infty} R^i_{l,n}. \quad (35)$$

If a bicrystal is represented as a set of two ideal blocks and the dislocational structure of the boundary of the blocks is not taken into account, the total reflectivity of the bicrystal is equal to $2R^i_{\rm id}$, where $R^i_{\rm id}$ is given by (33). The relative change of the total reflectivity of the bicrystal due to the boundary structure is defined as

$$\varepsilon_n = (R^i_n - 2R^i_{\rm id})/2R^i_{\rm id}. \quad (36)$$

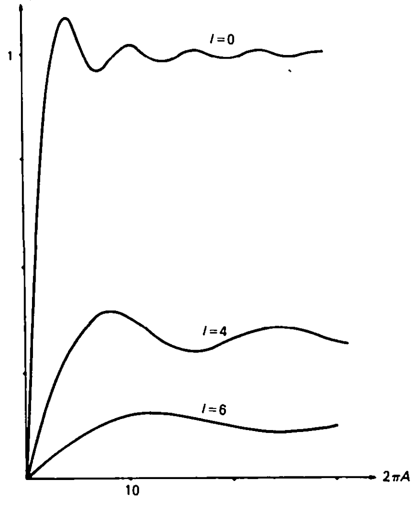

Fig. 5. Thickness dependence for the integrated intensity of a bicrystal at $n=2$ and $l=0$, 4 and 6.

Table 1. *Values of C_m for $m=1$ to 10*

m	1	2	3	4	5
C_m	32·9333	−107·6791	159·8271	−137·5375	77·5102
m	6	7	8	9	10
C_m	−30·8395	9·0948	−2·0275	0·3257	−0·0292

4.1. *Kinematic theory*

According to the kinematic theory, $R^i_{l,n} \sim M^2_{l,n}$, so using (4*b*) one can show that

$$\varepsilon_n = 0, \quad (37)$$

which means that in the kinematic approximation the dislocational structure of the boundary of the blocks does not change the total reflectivity of the bicrystal.

4.2. *Dynamical theory*

For $\mathbf{hb}=2$ we have

$$\varepsilon_2 = \frac{R^i_{0,2} + 2\sum_{k=2}^{\infty} R^i_{2k,2} + 2\Delta R^i_{2,2}}{2R^i_{\rm id}} \quad (38)$$

where the relation $R^i_{l,n} = R^i_{-l,-n}$ is used.

Substituting (27), (29) and (32) into (38), we obtain

$$\varepsilon_2 = (z_0/2\pi y_b) Q(2\pi A). \quad (39)$$

The $Q(x)$ function has a complicated form, but at $x \le 8$ it may be approximated by polynomials

$$Q(x) = \sum_{m=1}^{10} C_m (x/8)^{2m+1} / \bar{J}_0(x). \quad (40)$$

The C_m values are given in Table 1.

In the kinematic approximation $Q \simeq 0$ in accordance with (37).

At $x \gg 1$ from (34) we obtain

$$\lim_{x\to\infty} Q(x) = 2. \quad (41)$$

Fig. 6 shows the x dependence of Q computed from (40) at $x \le 8$. As seen from the figure the curve has maximum $Q_m \simeq 3{\cdot}15$ at $x \simeq 5{\cdot}4$, which coincides

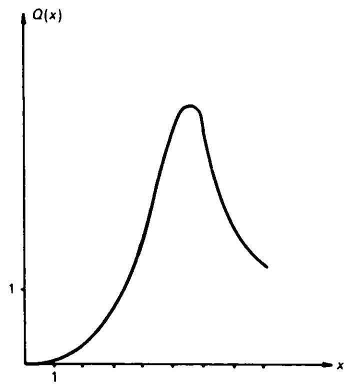

Fig. 6. The $Q(x)$ function at $x \le 8$.

with the minimum of $\Delta R^i_{2,2}$. Thus, owing to the periodic dislocation structure of the boundary, extra reflections are involved, which increases the total reflectivity of a bicrystal. On the other hand, because of that structure, the integrated intensities of principal reflections decrease. At small A both factors compensate each other and $\varepsilon_n = 0$. With increasing A the extinction effect becomes important, and at some value of A the effect of the second factor is minimum. Thus, if the bicrystal thickness is such that extinction cannot be neglected, when the total reflectivity of a bicrystal is calculated, neglecting the boundary structure may cause an error. The smaller the block size y_b along a direction perpendicular to the boundary plane, the more significant is the error.

As is well known, in the theory of X-ray diffraction by mosaic crystals the model used is one in which the blocks of a mosaic crystal are considered as ideal, *i.e.* the structure of inter-block boundaries is ignored (Zachariasen, 1967). Proceeding from our results obtained in the present paper one may suppose that, if block sizes are such that primary extinction is to be taken into account, then the contributions of block boundaries to the integrated intensity of a mosaic crystal cannot be neglected.

APPENDIX *A*

We shall evaluate the integral

$$F_{l,n} = \frac{1}{2y_b} \int_{-y_b}^{y_b} M^2_{l,n}\, dy. \qquad (A1)$$

(*a*) For the $l \neq n$ reflections the integration limits can be extended to infinity, since with the increase of y $M_{l,n}$ decreases rapidly. Denoting $l = 2k$ and $n = 2r$ and transforming the integration variable from y to q defined by (6), we obtain

$$F_{l,n} = \frac{z_0}{8\pi y_b} \int_0^1 q^{k-r-1}(1-q)^2 [P^{(k-r,1)}_{r-1}(1-2q)]^2\, dq. \qquad (A2)$$

After substitution of $x = 1 - 2q$ into $(A2)$ it becomes

$$F_{l,n} = \frac{z_0}{8\pi y_b} \frac{1}{2^{k-r+2}} \times \left\{ 2 \int_{-1}^{1} (1-x)^{k-r-1}(1+x)[P^{(k-r,1)}_{r-1}(x)]^2\, dx - \int_{-1}^{1} (1-x)^{k-r}(1+x)[P^{(k-r,1)}_{r-1}(x)]^2\, dx \right\}. \qquad (A3)$$

These integrals are tabulated (Proudnikov, Brychkov & Marichev, 1981), and the result is

$$F_{l,n} = \frac{z_0}{8\pi y_b} \frac{2n^2}{|l|(l^2 - n^2)}. \qquad (A4)$$

Using $(4b)$ for $|l| < |n|$ we find

$$F_{l,n} = \frac{z_0}{8\pi y_b} \frac{2|n|}{l^2 - n^2}. \qquad (A5)$$

(*b*) For the $l = n = 2r$ principal reflections, from $(5b)$ we have

$$M_{n,n} = (1-q) P^{(0,1)}_{r-1}(1-2q). \qquad (A6)$$

Substituting $(A6)$ into $(A1)$ and noting that $x = 1 - 2q$, we obtain

$$F_{n,n} = \frac{z_0}{32\pi y_b} \int_{-1}^{1-2x_0} (1+x)^2(1-x)^{-1}[P^{(0,1)}_{r-1}(x)]^2\, dx \qquad (A7)$$

where

$$x_0 = \exp(-4\pi y_b / z_0) \ll 1. \qquad (A8)$$

Using the relation

$$(1+x) P^{(0,1)}_{r-1}(x) = P_{r-1}(x) + P_r(x)$$

where $P_r(x)$ are the Legendre polynomials and using tabulated integrals (Bateman & Erdelyi, 1953) we find

$$F_{n,n} = \frac{z_0}{32\pi y_b} [2P_{r-1}(\gamma) Q_{r-1}(\gamma) + 2P_r(\gamma) Q_r(\gamma) + 4P_r(\gamma) Q_{r-1}(\gamma) - 4/r], \qquad (A9)$$

where $Q_n(x)$ are associated Legendre functions of the second kind, and

$$\gamma = (1 + x_0)/(1 - x_0) \simeq 1 + 2x_0.$$

Since $P_n(\gamma) \simeq 1$, from $(A9)$ we obtain

$$F_{n,n} = \frac{z_0}{32\pi y_b} \left[4 \ln \frac{\gamma+1}{\gamma-1} - 8 \sum_{i=1}^{r-1} \frac{1}{i} - \frac{6}{r} \right] = \frac{1}{2} - \frac{z_0}{4\pi y_b} \sum_{i=1}^{r-1} \frac{1}{i} - \frac{3z_0}{16\pi r y_b}. \qquad (A10)$$

APPENDIX *B*

We shall evaluate the integral

$$G_{l,n} = \frac{1}{2y_b} \int_{-y_b}^{y_b} M_{l,n} \bar{J}_0(2\pi A M_{l,n})\, dy. \qquad (B1)$$

Using the expansion

$$\bar{J}_0(x)=\sum_{m=0}^{\infty}\frac{(-1)^m x^{2m+1}}{2^{2m}(2m+1)(m!)^2} \qquad (B2)$$

from ($B1$) we obtain

$$G_{l,n}=\frac{1}{2y_b}\sum_{m=0}^{\infty}\frac{(-1)^m x^{2m+1}}{2^{2m}(2m+1)(m!)^2}\int\limits_{-y_b}^{y_b}(M_{l,n})^{2m+2}\,\mathrm{d}y. \qquad (B3)$$

(a) For the $l=0$ reflection

$$M_{0,n}=q^{|n|/4}$$

and from ($B3$) we obtain

$$G_{0,n}=\frac{z_0}{2\pi n y_b}\sum_{m=0}^{\infty}\frac{(-1)^m(2\pi A)^{2m+1}}{2^{2m}(m!)^2}\left(\frac{2}{2m+1}-\frac{1}{m+1}\right)$$
$$=\frac{z_0}{\pi n y_b}[\bar{J}_0(2\pi A)-J_1(2\pi A)]. \qquad (B4)$$

(b) For the $l\neq n=2$ reflections, substituting (28) into ($B3$) and using ($B2$) we obtain

$$G_{l,2}=\frac{z_0}{2\pi y_b(|l|+2)}\times\sum_{m=0}^{\infty}\frac{(-1)^m\Gamma(2m+1)\Gamma[\frac{1}{2}(|l|-2)(m+1)]}{2^{2m}\Gamma(m+1)\Gamma[\frac{1}{2}(|l|+2)(m+1)]}\times(2\pi A)^{2m+1}. \qquad (B5)$$

Using the expansion (Abramowitz & Stegun, 1965)

$$J_\nu(\eta)J_{-\nu}(\eta)=\sum_{m=0}^{\infty}\frac{(-1)^m(\eta/2)^{2m}\Gamma(2m+1)}{(m!)^2\Gamma(m+1+\nu)\Gamma(m+1-\nu)}$$

one can obtain (30) and (31).

(c) For the $l=2$ principal reflection

$$M_{2,2}=1-q$$

and from ($B3$) we obtain

$$G_{2,2}-\tfrac{1}{2}\bar{J}_0(2\pi A)=-\frac{z_0}{8\pi y_b}\sum_{m=0}^{\infty}\frac{(-1)^m(2\pi A)^{2m+1}}{2^{2m}(m!)^2(2m+1)}\times\int\limits_0^1\frac{1-(1-q)^{2m+2}}{q}\,\mathrm{d}q$$
$$=-\frac{z_0}{8\pi y_b}\sum_{m=0}^{\infty}\frac{(-1)^m(2\pi A)^{2m+1}}{2^{2m}(m!)^2(2m+1)}\times\sum_{i=1}^{2m+2}\frac{1}{i}. \qquad (B6)$$

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