Table 1 (*cont.*)

hkl	F_c	F_o	*hkl*	F_c	F_o	*hkl*	F_c	F_o
$20\bar{2}$	−19	22	$29\bar{2}$	5	6	$31\bar{3}$	− 6	6
$21\bar{2}$	−12	12	$2,10,\bar{2}$	− 6	6	$32\bar{3}$	2	< 7
$22\bar{2}$	− 3	< 6	$2,11,\bar{2}$	− 3	6	$33\bar{3}$	− 8	9
$23\bar{2}$	25	25	$2,12,\bar{2}$	− 1	< 6	$34\bar{3}$	− 6	< 7
$24\bar{2}$	13	15	$2,13,\bar{2}$	− 6	6	$35\bar{3}$	16	15
$25\bar{2}$	16	20	$2,14,\bar{2}$	7	6	$36\bar{3}$	− 8	6
$26\bar{2}$	6	< 8	$2,15,\bar{2}$	2	< 6	$37\bar{3}$	4	6
$27\bar{2}$	−27	27	$2,16,\bar{2}$	2	< 5	$38\bar{3}$	3	6
$28\bar{2}$	− 3	< 6				$39\bar{3}$	8	10
						$3,10,\bar{3}$	− 6	6

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The Diffraction of X-rays by Distorted-Crystal Aggregates. IV. Diffraction by a Crystal with an Axial Screw Dislocation

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In the reciprocal-lattice representation, the regions of high intensity become discs perpendicular to the dislocation axis. The variation of amplitude of reflexion across a disc can be represented either as an integral or as a finite series involving Bessel functions. Expressions for the integral breadths of lines on powder photographs are obtained in closed form.

1. Introduction

The hypothesis of dislocations explains many of the properties of cold-worked metals and the ease of crystal growth from vapour or solution. At the time when the work described below was begun (Wilson 1949*a*) there was no direct evidence of their existence, and it was hoped that some might be found through study of the details of diffraction by cold-worked metals, preferably of single crystals deformed in a way that would make it reasonable to suppose that most of the dislocation axes were parallel. This interest in the effect of a dislocation on the X-ray diffraction patterns of a crystal has now largely disappeared, as growth spirals give an ample direct indication of the existence of dislocations, but it is perhaps worth while to place the results on record, as the dislocated crystal and the bent lamella (Wilson, 1949*b*; Blackman, 1951) appear to be the only models of distorted crystals for which detailed calculations exist.

The theory of diffraction by an elastically distorted crystal is not easy, and the elastic field of a Taylor–Burgers dislocation (Koehler, 1941; Eshelby, 1949) is particularly complex. For the 'screw' dislocations more recently postulated (Burgers, 1939; Burton, Cabrera & Frank, 1949), however, the displacement of the atoms is simpler, and some results on diffraction by a cylindrical crystal containing an axial screw dislocation can be obtained. Hall (1950) has pointed out that the leading term in the expressions for the displacements caused by 'edge' dislocations and intermediate types has the same form as that for a screw dislocation, and that the diffraction effects would be expected to be of the same general type. The modifications required when the displacement is not parallel to the dislocation axis, but is otherwise similar to that of a screw dislocation, have already been outlined (Wilson, 1950) and are not discussed further here.

2. Amplitude of reflexion

Consider a cylindrical crystal of radius A, with a screw dislocation axis along its centre. (In the application to cold-worked metals the radius A is to be identified with some sort of an average distance between dislocations.) In the undislocated crystal the jth cell is at

$$\mathbf{r}_j = j_1\mathbf{a}+j_2\mathbf{b}+j_3\mathbf{c}\,, \tag{1}$$

where the axes are chosen so that $\mathbf{c}$ is parallel to the dislocation axis, which will normally have some important crystallographic direction. With the screw dislocation present the jth cell will be shifted to

$$\mathbf{r}_j' = \mathbf{r}_j+\frac{n\psi}{2\pi}\mathbf{c}\,, \tag{2}$$

where ψ is an angle measured from some fixed direction perpendicular to $\mathbf{c}$, and n is an integer determining the 'pitch' of the screw (the displacement experienced in moving once round the dislocation axis on what appears to be a lattice plane). The amplitude of X-ray diffraction from the dislocated crystal is

$$G = F\Sigma_j \exp\{2\pi i\mathbf{S}.\mathbf{r}_j'\}\,, \tag{3}$$

where $\mathbf{S}$ is the position vector in reciprocal space and F the corresponding structure factor. With

$$\mathbf{S} = H\mathbf{a}^*+K\mathbf{b}^*+L\mathbf{c}^*\,, \tag{4}$$

where H, K, L are not necessarily integral, the amplitude may be written

$$G=F\Sigma_j \exp\{2\pi i(j_1H+j_2K+j_3L)+nLi\psi\}\,. \tag{5}$$

The angle ψ depends on j_1 and j_2, but not on j_3, so that the sum over j_3 may be performed immediately, giving

$$G = F\cdot\frac{\sin(\pi N_3L)}{\sin\pi L}\cdot\Sigma_j \exp\{2\pi i(j_1H+j_2K)+nLi\psi\}\,, \tag{6}$$

where N_3 is the number of unit cells in the $\mathbf{c}$ direction. Since N_3 is large, the factor containing L is appreciable only in the immediate neighbourhood of the integral values l of L. Any spreading of the regions of high intensity in reciprocal space is thus confined to planes parallel to $\mathbf{a}^*$, $\mathbf{b}^*$. In other words, the spreading takes place perpendicular to the axis of the dislocation. The amplitude of diffraction is then

$$G = FZ\Sigma_j \exp\{2\pi i(j_1H+j_2K)+nli\psi\}\,, \tag{7}$$

where Z represents the factor depending on L in equation (6). With

$$\mathbf{r}' = j_1\mathbf{a}+j_2\mathbf{b} \tag{8}$$

and

$$\boldsymbol{\rho} = (H-h)\mathbf{a}^*+(K-k)\mathbf{b}^*\,, \tag{9}$$

this becomes

$$G = FZ\Sigma_j \exp\{2\pi i\boldsymbol{\rho}.\mathbf{r}'+nli\psi\}\,, \tag{10}$$

where the integers h and k have been chosen so that $|H-h|$ and $|K-k|$ are less than $\frac{1}{2}$. The expression to be summed is now a slowly varying function of $\mathbf{r}'$, so that the summation over j_1 and j_2 can be replaced by integration over the cross-section of the crystal. Also, because of the symmetry of the problem, G depends only on the magnitude of ϱ, not on its direction, and it may be supposed parallel to the fixed direction from which ψ is measured. Then $\boldsymbol{\rho}.\mathbf{r}' = \varrho r\cos\psi$, where r is the projection of $\mathbf{r}'$ on the plane of $\mathbf{a}^*$, $\mathbf{b}^*$, and equation (10) becomes

$$G = FZC^{-1}\int_0^{2\pi}\int_0^A \exp\{2\pi i\varrho r\cos\psi+nli\psi\}rdrd\psi \tag{11}$$

$$= 2\pi i^{nl}FZC^{-1}\int_0^A J_{nl}(2\pi\varrho r)rdr\,, \tag{12}$$

where J_{nl} is the Bessel function of order nl (Jahnke & Emde, 1938, p. 149) and C is the area of the base of the unit cell projected on the plane of $\mathbf{a}^*$, $\mathbf{b}^*$. For $n = 0$ (no dislocation) this becomes

$$G = 2\pi FZC^{-1}\int_0^A J_0(2\pi\varrho r)rdr \tag{13}$$

$$= FZAC^{-1}\varrho^{-1}J_1(2\pi\varrho A)\,. \tag{14}$$

This is also the form assumed by G for $l = 0$, whatever the value of n. Reflexions with $l = 0$, therefore, are unaffected by a screw dislocation, and for $\varrho = 0$ have an amplitude

$$G_0 = FZ\pi A^2/C\,, \tag{15}$$

proportional to the cross-sectional area of the crystal. For all other reflexions from a screw-dislocated crystal the amplitude is zero for $\varrho = 0$. This appears curious at first sight; Frank (1949) has given an elementary argument to make it plausible.

For convenience of mathematical discussion equation (12) may be put in the form

$$G = i^m . FZ . \pi A^2 C^{-1} . K_m(x) , \tag{16}$$

where

$$m = nl , \tag{17}$$

$$x = 2\pi\varrho A , \tag{18}$$

and

$$K_m(x) = 2x^{-2} \int_0^x \xi J_m(\xi) d\xi . \tag{19}$$

By writing $\xi = \xi^m . \xi^{-m+1}$ and integrating by parts the integral becomes

$$\int_0^x \xi J_m(\xi) d\xi = -x J_m(x) + m \int_0^x J_{m-1}(\xi) d\xi \tag{20}$$

$$= -x J_{m-1}(x) + 2m \sum_{g=0}^{\infty} J_{m+2g}(x) \tag{21}$$

(Jahnke & Emde, 1938, p. 145). It may however be expressed as a finite sum by repeated use of the recurrence relation

$$J_n = -2J'_{n-1} + J_{n-2} ,$$

giving

$$J_{m-1} = -2 \sum_{g=1}^{\frac{1}{2}m-1} J'_{m-2g} + J_1 \tag{22}$$

form m even, and

$$J_{m-1} = -2 \sum_{g=1}^{\frac{1}{2}(m-1)} J'_{m-2g} + J_0 \tag{23}$$

for m odd. Equation (20) thus becomes

$$\int_0^x \xi J_m(\xi) d\xi = -x J_{m-1}(x) - 2m \sum_{g=1}^{\frac{1}{2}m-1} J_{m-2g}(x) - mJ_0(x) + m \tag{24}$$

when m is even, and

$$\int_0^x \xi J_m(\xi) d\xi$$

$$= -x J_{m-1}(x) - 2m \sum_{g=1}^{\frac{1}{2}(m-1)} J_{m-2g}(x) + m \int_0^x J_0(\xi) d\xi \tag{25}$$

when m is odd. The integral terminating the series for m odd has been tabulated by Lowan & Abramowitz (1943). For small x it may be more convenient to use the power series

$$K_m(x) = \sum_{g=0}^{\infty} \frac{(-)^g x^{2g+m}}{(2g+m+2)g!(g+m)!2^{2g+m-1}} \tag{26}$$

obtained by expanding $J_m(x)$ in equation (19) and integrating term-by-term. For large values of x convergence is not rapid.

3. Apparent particle sizes

The expressions for G are complicated when $nl \neq 0$, so that it seems impracticable to derive the line profiles on a Debye–Scherrer photograph. Series for the integral breadths can however be obtained. If $H(\varrho) \equiv G(\varrho)G^*(\varrho)$ is the intensity distribution near the point hkl of the reciprocal lattice, the intensity of the Debye–Scherrer line for $s \equiv 2(\sin\theta - \sin\theta_0)/\lambda = 0$, where θ_0 is the Bragg angle for the undislocated crystal, is proportional to

$$H_0 \equiv C \int_{-\frac{1}{2}}^{\frac{1}{2}} \int_{-\infty}^{\infty} H(\varrho) d\varrho dL . \tag{27}$$

Because of geometrical foreshortening of the discs for which $l \neq 0$ there is also a factor depending on $\sin\theta_0$ and l (compare Wilson, 1949c, p. 71), so that

$$I_0 ds = \sqrt{\left\{\frac{4\sin^2\theta_0}{4\sin^2\theta_0 - l^2\lambda^2/c^2}\right\}} \cdot H_0 . ds . \tag{28}$$

It is only for $nl = 0$ that H_0 can be expressed simply. In this case $G(\varrho) = FZAC^{-1}\varrho^{-1}J_1(2\pi\varrho A)$ (equation (14)), so that

$$H_0 = 2F^2A^2C^{-1} \int_0^{\infty} \varrho^{-2} J_1^2(2\pi\varrho A) d\varrho \cdot \int_{-\frac{1}{2}}^{\frac{1}{2}} Z^2 dL \tag{29}$$

$$= \frac{16}{3} F^2 A^3 C^{-1} \int_{-\frac{1}{2}}^{\frac{1}{2}} Z^2 dL \tag{30}$$

on making use of an equation given by Watson (1922, p. 403, equation (2)). The integral of Z^2 gives N_3, so that

$$H_0 = \frac{16}{3} F^2 A^3 C^{-1} N_3$$

$$= \frac{16A}{3\pi} \cdot NF^2 , \tag{31}$$

where N is the total number of cells in the crystal. The integrated intensity of the reflexion is NF^2, so that the apparent particle size is

$$\varepsilon = I_0/I = \frac{16A}{3\pi} \cdot \sqrt{\left\{\frac{4\sin^2\theta_0}{4\sin^2\theta_0 - l^2\lambda^2/c^2}\right\}} . \tag{32}$$

For $l = 0$ (the only case in which it applies to dislocated crystals) this becomes

$$\varepsilon = 16A/3\pi . \tag{33}$$

Equation (32) gives also the apparent particle size for long cylindrical non-dislocated crystals, a result which does not appear to have been previously obtained. In terms of the 'true' particle size $p = \sqrt{(\pi A^2)}$ it becomes

$$\varepsilon = \frac{16}{3\pi^{\frac{3}{2}}} \cdot p \cdot \sqrt{\left\{\frac{4\sin^2\theta_0}{4\sin^2\theta_0 - l^2\lambda^2/c^2}\right\}} . \tag{34}$$

The numerical factor has the value 0·957..., which is of the order of unity, as usual (Wilson, 1949c p. 40, Table 1). In general (equation (12))

$$H(\varrho) = 4\pi^2F^2Z^2C^{-2} \int_0^A \int_0^A J_{nl}(2\pi\varrho r) J_{nl}(2\pi\varrho t) r dr t dt , \tag{35}$$

so that

$$H_0 = 8\pi^2 F^2 N_3 C^{-1} \times \int_0^A \int_0^A \left\{ \int_0^\infty J_{nl}(2\pi r\varrho) J_{nl}(2\pi t\varrho) d\varrho \right\} r dr t dt . \quad (36)$$

The integral in curly brackets gives a hypergeometric function (Watson, 1922, p. 401):

$$\int_0^\infty J_{nl}(2\pi r\varrho) J_{nl}(2\pi t\varrho) d\varrho \quad (37)$$

$$= \frac{1}{2\pi t} \cdot \left(\frac{r}{t}\right)^{nl} \cdot \frac{\Gamma(nl+\frac{1}{2})}{\Gamma(nl+1)\Gamma(\frac{1}{2})} \cdot {}_2F_1\left(nl+\tfrac{1}{2}, \tfrac{1}{2}; nl+1; \frac{r^2}{t^2}\right),$$

provided that $t > r$; r and t are interchanged for $r > t$. In order to perform the integrations over r and t the hypergeometric function must be expressed as a series:

$$H_0 = 4F^2 N_3 C^{-1} \sum_{m=0}^\infty \frac{\Gamma(m+nl+\frac{1}{2})\Gamma(m+\frac{1}{2})}{\Gamma(m+nl+1)m!} \times \int_0^A \left\{ \int_0^t \frac{r^{2m+nl}}{t^{2m+nl+1}} \cdot r dr + \int_t^A \frac{t^{2m+nl}}{r^{2m+nl+1}} \cdot r dr \right\} t dt \quad (38)$$

$$= \frac{8}{3} A^3 F^2 N_3 C^{-1} \sum_{m=0}^\infty \frac{\Gamma(m+nl+\frac{1}{2})\Gamma(m+\frac{1}{2})}{(2m+nl+2)\Gamma(m+nl+1)m!} \quad (39)$$

$$= \frac{8A}{3\pi} \cdot NF^2 \sum_{m=0}^\infty \frac{\Gamma(m+nl+\frac{1}{2})\Gamma(m+\frac{1}{2})}{(2m+nl+2)\Gamma(m+nl+1)m!} . \quad (40)$$

The series in equation (40) is, except for the factor $(2m+nl+2)$ and a constant factor, a hypergeometric function of argument unity, which has simple values given by (Whittaker & Watson, 1935, pp. 281–282).

$$\sum_{m=0}^\infty \frac{\Gamma(m+a)\Gamma(m+b)}{\Gamma(m+c)m!} = \frac{\Gamma(a)\Gamma(b)\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)} . \quad (41)$$

For the special case $nl=3$ the factor $(2m+5)=2(m+2\frac{1}{2})$ in the denominator of equation (40) can be cancelled with the first factor of $\Gamma(m+3\frac{1}{2})=(m+2\frac{1}{2})\Gamma(m+2\frac{1}{2})$, so that

$$H_0 = \frac{4A}{3\pi} \cdot NF^2 \sum_{m=0}^\infty \frac{\Gamma(m+2\frac{1}{2})\Gamma(m+\frac{1}{2})}{\Gamma(m+4)m!} = \frac{16A}{15\pi} \cdot NF^2 . \quad (42)$$

This suggests a general method of reducing equation (40) to a finite sum for $nl = 3, 5, 7, \ldots$, by dividing $(2m+nl+2)$ into $\Gamma(m+nl+\frac{1}{2})$. Let

$$nl = 2p+1, \quad \text{where} \quad p = 1, 2, 3, \ldots , \quad (43)$$

and represent the sum in equation (40) by S_{nl}. By repeated division

$$\frac{\Gamma(m+2p+\frac{3}{2})}{m+p+\frac{3}{2}} = \Gamma(m+2p+\tfrac{1}{2}) + (p-1)\frac{\Gamma(m+2p+\frac{1}{2})}{m+p+\frac{3}{2}}$$
$$= \Gamma(m+2p+\tfrac{1}{2}) + (p-1)\Gamma(m+2p-\tfrac{1}{2}) + (p-1)(p-2)\frac{\Gamma(m+2p-\frac{1}{2})}{m+p+\frac{3}{2}}$$
$$= \ldots$$
$$= \sum_{k=0}^{p-1} \frac{(p-1)!}{(p-k-1)!} \Gamma(m+2p-k+\tfrac{1}{2}) , \quad (44)$$

and

$$S_{nl} = \tfrac{1}{2} \sum_{k=0}^{p-1} \frac{(p-1)!}{(p-k-1)!} \sum_{m=0}^\infty \frac{\Gamma(m+2p-k+\frac{1}{2})\Gamma(m+\frac{1}{2})}{\Gamma(m+2p+2)m!}$$
$$= \frac{(p-1)!\Gamma(\frac{1}{2})}{2\Gamma(2p+\frac{3}{2})} \sum_{k=0}^{p-1} \frac{\Gamma(2p-k+\frac{1}{2})k!}{(p-k-1)!\Gamma(k+\frac{3}{2})} . \quad (45)$$

For nl even the factor $(2m+nl+2)$ can be absorbed into $m!$, the missing factors being inserted in both the numerator and the denominator. Then, on writing $2p$ for nl and g for $m+p+1$,

$$S_{nl} = \tfrac{1}{2} \sum_{g=p+1}^\infty \frac{\Gamma(g+p-\frac{1}{2})(g-1)(g-2)\ldots(g-p)\Gamma(g-p-\frac{1}{2})}{\Gamma(g+p)g!} . \quad (46)$$

The sum is from $g = p+1$ to ∞, but terms constructed on the same model for $g = 1$ to $g = p$ are all zero, so that writing the sum from $g = 1$ to ∞ does not change its value. A term for $g = 0$ is, however, finite, and has the value $-2p\pi/(4p^2-1)$. Equation (46) thus becomes

$$S_{nl} = \frac{2p\pi}{4p^2-1} + \tfrac{1}{2} \sum_{g=0}^\infty \frac{\Gamma(g+p-\frac{1}{2})(g-1)(g-2)\ldots(g-p)\Gamma(g-p-\frac{1}{2})}{\Gamma(g+p)g!} . \quad (47)$$

Consider the product

$$P_j = (g-p+j-1)\ldots(g-p+1)(g-p)\Gamma(g-p-\tfrac{1}{2}) . \quad (48)$$

Since $(g-p) = (g-p-\frac{1}{2}+\frac{1}{2})$

the last two factors may be written

$$(g-p)\Gamma(g-p-\tfrac{1}{2}) = \Gamma(g-p+\tfrac{1}{2}) + \tfrac{1}{2}\Gamma(g-p-\tfrac{1}{2}) ,$$

and by a continuation of this process P_j may be expressed as a finite series

$$P_j = \sum_{k=0}^{j} A_{j,k}\Gamma(g-p+k-\tfrac{1}{2}) , \quad (49)$$

where clearly $A_{j,j} = 1$ and $A_{j,0} = \Gamma(j+\frac{1}{2})/\Gamma(\frac{1}{2})$. Since

$$P_{j+1} = (g-p+j)P_j = \{(g-p+k-\tfrac{1}{2}) + (j-k+\tfrac{1}{2})\}P_j , \quad (50)$$

the coefficients $A_{j,k}$ can be built up by use of the relation

$$A_{j+1,k} = (j-k+\tfrac{1}{2})A_{j,k} + A_{j,k-1} . \quad (51)$$

Thus for $k = 1$

$$A_{j+1,1} = (j-\tfrac{1}{2})A_{j,1}+A_{j,0}$$

$$= (j-\tfrac{1}{2})A_{j,1}+\frac{\Gamma(j+\frac{1}{2})}{\Gamma(\frac{1}{2})}, \quad (52)$$

$$A_{j,1} = \frac{j\Gamma(j-\frac{1}{2})}{\Gamma(\frac{1}{2})}; \quad (53)$$

for $k = 2$

$$A_{j+1,2} = (j-\tfrac{3}{2})A_{j,2}+\frac{j\Gamma(j-\frac{1}{2})}{\Gamma(\frac{1}{2})}, \quad (54)$$

$$A_{j,2} = \frac{j(j-1)\Gamma(j-\frac{3}{2})}{2\Gamma(\frac{1}{2})}; \quad (55)$$

and ultimately

$$A_{j,k} = \frac{j!\,\Gamma(j-k+\frac{1}{2})}{k!\,(j-k)!\,\Gamma(\frac{1}{2})}. \quad (56)$$

The product in equation (47) is P_p, so that

$$S_{nl} = \frac{2\pi p}{4p^2-1} + \tfrac{1}{2}\sum_{k=0}^{p}\frac{p!\,\Gamma(p-k+\frac{1}{2})}{k!\,(p-k)!\,\Gamma(\frac{1}{2})}\sum_{g=0}^{\infty}\frac{\Gamma(g+p-\frac{1}{2})\Gamma(g-p+k-\frac{1}{2})}{\Gamma(g+p)\,g!}$$

$$= \frac{2\pi p}{4p^2-1} + \frac{p!}{2\pi}\Gamma(p-\tfrac{1}{2})\sum_{k=0}^{p}\frac{\Gamma(p-k+\frac{1}{2})\Gamma(-p+k-\frac{1}{2})}{\Gamma(2p-k+\frac{1}{2})k!}$$

$$= \frac{2\pi p}{4p^2-1} + \frac{(2p)!\sqrt{\pi}}{2^{2p-1}(2p-1)}\sum_{k=0}^{p}\frac{(-)^{p-k+1}}{(2p-2k+1)\,k!\,\Gamma(2p-k+\frac{1}{2})}. \quad (57)$$

4. Variation of line breadths with l

The series in equations (45) and (57) readily give S_{nl} for small nl, except $nl = 1$. There seems no easy way of calculating this, but direct use of the series in equation (40) (not very rapidly convergent) gives $S_1 > 0{\cdot}744$, and probably about $0{\cdot}78$. The line breadths, for constant foreshortening factor, are proportional to $1/S_{nl}$, and are shown plotted against nl in Fig. 1 for nl up to 7. In spite of the complexity of the expressions for S_{nl} they lie remarkably close to the straight line

$$\beta_{nl} = \beta_0(1+1{\cdot}30nl). \quad (58)$$

Frank's simple argument (1949) would give

$$\beta_{nl} = \beta_0(1+1{\cdot}17nl). \quad (59)$$

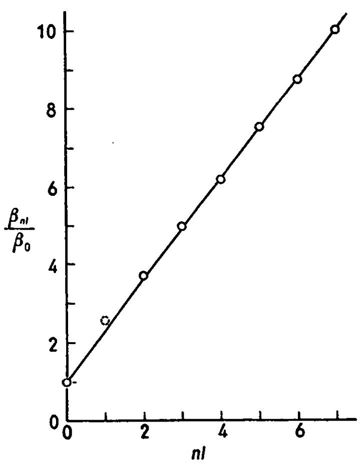

Fig. 1. The line breadth, corrected for foreshortening, as a function of nl. The straight line is $\beta_{nl} = \beta_0(1+1{\cdot}3nl)$.

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