sequence creates 321123 out of $(22)_3$. It is to be noted that a scheme similar to ours has been put forward by Mardix, Kalman & Steinberger (1969) to explain the growth of ZnS polytypes. However, their work relates to transformation of polytypes in the same crystal and not to the growth of different polytypes. Also, their scheme always envisages stacking faults at equal intervals and up to a certain step the layers slip in a clockwise direction and for the rest of the steps in an anticlockwise direction, and this sequence of slip repeats periodically. The present scheme assumes only periodic stacking faults; the faults may not be at equal intervals as for example in the case of 32*H*. Moreover, the slip of layers is always alternately in clockwise and anticlockwise directions. Such a scheme of layer transposition is possible only when suitable partial dislocations, which nucleate stacking faults, sweep the basal plane; the sweeping occurs in the sequence after certain regular period in the parent structure. In order to find out whether chains of basal stacking faults occur in cadmium iodide crystals, we tried to observe the crystals directly in the electron microscope. Since cadmium iodide crystals are extremely susceptible to electron beam damage, it is not usually possible to observe the dislocation pattern in these crystals. However, by improving the thermal contact of the crystal with the specimen grid and employing full excitation of condenser lenses, we were able to observe the dislocation patterns in nearly 60% of the crystals. It is, however, not always possible to study completely each individual crystal. We found that dissociation of basal dislocations producing twofold, threefold and fourfold ribbons usually took place in all the crystals observed. Fig. 5 represents a typical example of twofold, threefold and fourfold partial ribbons. Thus it seems reasonable to believe that sequences of partial ribbons producing stacking faults occur in the cadmium iodide crystals and a regular sequence of stacking faults creating a polytype can easily occur. This lends support to the scheme of the growth of the polytypes that we have presented. Finally the determination of probable structure of a polytype based on calculation of theoretical stacking fault energy seems to be a new approach which needs to be explored further. Also the minimum stacking fault energy criterion lends credence to the above explanation of growth of polytypes in terms of creation and ordering of stacking faults.

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Calculation of the Intensity of Secondary Scattering of X-rays by Non-crystalline Materials

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Equations that require numerical integration over only one variable were derived for calculating the intensity of secondary scattering of X-rays for non-crystalline samples of finite thickness. Both the reflection and transmission geometry cases were considered. Tables are given that allow the intensity ratio of secondary to primary scattering to be determined without making lengthy calculations. Modification of the normalization procedure when secondary scattering is important is discussed.

Introduction

In studies of high molecular weight, petroleum-related, non-crystalline organic solids it was necessary to correct for secondary scattering. Warren & Mozzi's (1966) method of calculating secondary intensity for reflection geometry using samples of effective infinite thickness could not be used, because it was desired to use thin samples to avoid certain smearing corrections (Bragg & Packer, 1963; Keating & Warren, 1952) in the high angle scattering region. It also was desired to make secondary scattering corrections for trans-

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mission data in angular ranges for which the small-angle approximations do not apply. Thus the method of Chonacky & Beeman (1968, 1969) that applies only in the small-angle scattering region could not be used.

Thus equations were derived that allow calculation of secondary intensity in the reflection case for samples of any thickness and that allow calculation of secondary intensity in the transmission case for high- as well as low-scattering angles. It was desired to obtain working equations in a form convenient for evaluation using a computer.

Little more than starting and final equations can be given, because the derivations are extremely long. Those needing more details concerning the derivations should contact the authors.

Symbols used in different sections should not be exchanged unless they are listed in the nomenclature section or it is otherwise indicated that they can be exchanged.

General theory

Smearing corrections will be neglected here, but they will be considered in the Appendix concerning normalization.

The general equation for primary scattering, either coherent or incoherent, can be expressed as

$$I_{xp}=\frac{I_0 n}{R^2}\int_{V_{12}} J_x\sigma_{ex}\exp\left(-\mu l_0-\mu'\{2\theta\}l\right)\mathrm{d}V_{12}\,. \quad (1)$$

The subscript x is replaced by i for incoherent scattering. For coherent scattering the subscript x is replaced by c and the exponential argument reduces to $-\mu L_1$.

The differential electron cross sections include the polarization correction and, in the case of incoherent scattering, the recoil correction.

Because electron cross sections are nearly the same for coherent and incoherent scattering, they can be assumed to be the same for calculating the intensity of secondary scattering. Also incoherent frequency shifts can be approximated so that the absorption term $\exp(-\mu L_2)$ can be used. Using these simplifications, the intensity for secondary scattering is

$$I_2=\frac{I_0 n^2}{R^2}\int_{V_1}\int_{V_2}\frac{1}{r^2}\,\sigma_{e2}J\{2\theta_1\}\,J\{2\theta_2\} \times \exp\left(-\mu L_2\right)\mathrm{d}V_1\mathrm{d}V_2\,. \quad (2)$$

The differential electron cross section for secondary scattering can be obtained for nearly any case of interest using the matrix methods of McMaster (1961) and appropriate simplifications. The J terms in equation (2) are

$$J\{2\theta_j\}=J_c\{2\theta_j\}+\left(\frac{\nu'_{2\theta_j}}{\nu}\right)^3 J_i\{2\theta_j\}\,. \quad (3)$$

The term $\nu'_{2\theta_j}$ is the incoherent frequency resulting from scattering at the point j through a scattering angle of $2\theta_j$. Usually the frequency ratio term in equation (3) can be completely neglected for secondary scattering. It was used as given because of the manner in which the authors store incoherent intensity data for computer use.

The results for both the transmission and reflection geometry cases will be presented in the form of the Q function that is related to the ratio of secondary to primary intensity by

$$\frac{I_2}{I_1}=\frac{(\sum Z_j^2)^2 Q}{J\{2\theta\}\sum A_j\mu_j\{m\}}\,. \quad (4)$$

Transmission geometry theory

The geometry considered is that of a slab of sample having faces normal to the incident X-ray beam. The six position variables of equation (2) were transformed to a set of three cartesian coordinates and to a set of three spherical coordinates in terms of the vector **r**. After introduction of boundary conditions for the sample shape and explicit expression of the terms in equation (2), it was possible to integrate analytically over five of the six position variables. It is assumed that the detector views a portion of the sample larger than V_1.

The Q function and terms that are contained in it are given in the equations that follow. These are the final working equations.

$$Q\{b,q,2\theta,\mu t\}=G\left[\int_{\gamma=-\pi/2}^{0} W_- M\,\mathrm{d}\gamma+\int_{\gamma=0}^{\pi/2} W_+ M\,\mathrm{d}\gamma\right] \quad (5)$$

$$W_+=\left[\frac{\cos\gamma}{1-\sin\gamma\sec 2\theta}\right]\times\left[\frac{1-\exp(-\mu t\{1-\sec 2\theta\})}{1-\sec 2\theta} - \frac{\exp(-\mu t\{1-\sec 2\theta\})-\exp(-\mu t\{\csc\gamma-\sec 2\theta\})}{\csc\gamma-1}\right]$$

$$W_-=\left[\frac{\cos\gamma}{1-\sin\gamma\sec 2\theta}\right]\left[\frac{1-\exp(-\mu t\{1-\sec 2\theta\})}{1-\sec 2\theta} - \frac{\exp(-\mu t\{1-\csc\gamma\})-1}{\csc\gamma-1}\right]$$

$$G=\left[\frac{e^4}{m^2c^4}\right]\times\left[\frac{2N(1-\sec 2\theta)}{(1+\cos^2 2\theta)(1-\exp\{-\mu t\,[1-\sec 2\theta]\})}\right]$$

$$M=2\pi\left[q+\frac{2(1-q)}{2+b(1-\sin\gamma)}\right]\times\left[qA+\frac{qC}{2}-EB+\frac{E}{\sqrt{F^2-1}}(A+BF+CF^2)-ECF\right]$$

$$A=[\sin^2\gamma+\cos^2 2\theta\,(1-\sin^2\gamma+\sin^4\gamma)]/2$$

$$B=\sin 2\theta\cos 2\theta\sin^3\gamma\cos\gamma$$

$$C=[\sin^2 2\theta\cos^2\gamma\,(1+\sin^2\gamma)]/2$$

$$E=\frac{2(1-q)}{b\sin 2\theta\cos\gamma}$$

$$F=\frac{2+b(1-\cos 2\theta\sin\gamma)}{b\sin 2\theta\cos\gamma}.$$

Care must be taken to consider indeterminate forms in calculating the Q function. Indeterminate forms can be avoided by careful selection of the increments in γ for the numerical integration, or l'Hospital's law can be used.

Reflection geometry theory

The paper of Warren & Mozzi (1966) should be consulted for the derivation of equations for a sample of infinite thickness. Conversion of equation (2) to the coordinate system used by Warren & Mozzi results in their expression for the differential of secondary intensity except for the absorption term that must be modified for a sample of finite thickness. It was possible to analytically integrate over five of the six position variables.

The Q function and terms in it are given in equations that follow. These are the final working equations.

$$Q\{b,q,\theta,\mu t\}=G\int_{\varepsilon=0}^{\pi/2} WM\,d\varepsilon \qquad (6)$$

$$G=\left(\frac{e^4}{m^2c^4}\right)\cdot\left(\frac{8N\sin\theta}{[1+\cos^2 2\theta][1-\exp(-2\mu t\csc\theta)]}\right)$$

$$X=\frac{[\exp(-\mu t\csc\theta)][2|\sin\varepsilon|\exp(-\mu t|\csc\varepsilon|)-(\sin\theta+|\sin\varepsilon|)\exp(-\mu t\csc\theta)]}{\sin^2\theta-\sin^2\varepsilon}$$

$$W=X+X'$$

$$X'=1/(\sin\theta+|\sin\varepsilon|)$$

$$M=[q^2(AY_1+BY_2+CY_3)+qE(AY_4+BY_5+CY_6)+E^2(AY_7+BY_8+CY_9)]\cos\varepsilon$$

$$A=\sin^2\theta\sin^2\varepsilon+(\sin^2\theta\sin^2\varepsilon+\cos 2\theta)^2/2$$

$$B=\cos^2\theta\cos^2\varepsilon(1-\sin^2\theta\sin^2\varepsilon-\cos 2\theta)$$

$$C=\cos^4\theta\cos^4\varepsilon/2$$

$$E=2(1-q)/(b\cos\theta\cos\varepsilon)$$

$$Y_1=\pi;\ Y_2=\pi/2;\ Y_3=3\pi/8;\ Y_4=T_1+T_2$$
$$Y_5=F_1^2T_1+F_2^2T_2-\pi(F_1+F_2)$$
$$Y_6=F_1^4T_1+F_2^4T_2-\pi(F_1+F_2)/2-\pi(F_1^3+F_2^3)$$
$$Y_7=(T_2-T_1)/(F_1-F_2)$$
$$Y_8=\pi+(F_2^2T_2-F_1^2T_1)/(F_1-F_2)$$
$$Y_9=\pi/2+(F_2^4T_2-F_1^4T_1)/(F_1-F_2)+\pi[(F_1+F_2)^2-F_1F_2]$$

$$F_1=[2+b(1+\sin\theta\sin\varepsilon)]/b\cos\theta\cos\varepsilon$$
$$F_2=[2+b(1-\sin\theta\sin\varepsilon)]/b\cos\theta\cos\varepsilon$$
$$T_1=\pi/(F_1^2-1)^{1/2};\ T_2=\pi/(F_2^2-1)^{1/2}.$$

Care must be taken to consider indeterminate forms in calculating the Q function.

Results

Values of the Q function for the reflection geometry case are given in Table 1, and values for the transmission geometry case are given in Table 2. The parameters b and q that are necessary to determine Q are defined in the *Nomenclature* section by an equation relating them to the total atomic intensity J for the selected structural unit. Values of b and q are selected that give the best fit between the equation and J values calculated from the squares of structure factors and, when incoherent radiation is detected, incoherent intensities. A trial-and-error method can be used. If a computer is available, it often is faster to solve for b and q using either a successive-approximations or a least-squares method. Using b, q, and μt, interpolation between values given in the tables should give values of Q that are sufficiently accurate for most purposes. When Q is obtained, the intensity ratio of secondary to primary intensity can be determined using equation (4).

Double precision source programs for calculating Q that are written in 360 Fortran IV (H level) are available from the authors. Only 81 seconds of computing time were required to compile the source program and calculate 576 values of Q in the reflection geometry case, and only 85 seconds were required in the transmission geometry case. However it also was possible to calculate Q values on a drum memory computer having a memory of only 2000 words.

If the intensity ratio I_2/I_1 is calculated for infinite thickness in the reflection case using the Q_∞ values of Warren & Mozzi (1966), then the percentage error in I_2/I_1 on assuming that a sample of finite thickness is of infinite thickness is $100(Q_\infty-Q)/Q$. As typical examples, for $b=20$, $q=0$, and $2\theta=120°$, the error is 22 per cent for $\mu t=1$ and 70 percent for $\mu t=0{\cdot}5$.

Typical values of I_2/I_1 in both the transmission and reflection cases have ranged from 1 to 10 percent in the authors' work with materials containing mainly hydrocarbons for μt values of 0·3 to 3 in the reflection case and for μt values of 0·3 to 1 in the transmission case. A calculation of I_2/I_1 for vitreous silica agreed with that of Warren & Mozzi (1966) for the reflection geometry case in the limit of infinite thickness. Using the scattering coefficient for water given by Chonacky & Beeman (1969), I_2/I_1 was about 0·095 for $\mu t=1$ in the transmission case at zero scattering angle. This is in reasonably good agreement with the value of 0·08 given by Chonacky & Beeman (1969) who determined I_2/I_1 using experimental coherent intensities rather than an approximation based on atomic coherent intensities.

Table 1. *Values of* $Q\{b,q,2\theta,\mu t\}\times 10^4$ *for reflection geometry*

$\mu t=0{\cdot}10$

2θ	$b=10$	$b=20$	$b=40$	$b=60$	$b=80$	$b=100$
			($q=0$)			
30	87·38	49·44	24·74	15·43	10·71	7·93
60	64·42	28·87	11·05	5·91	3·71	2·56
90	41·30	15·73	5·26	2·65	1·61	1·08
120	25·27	8·74	2·75	1·35	0·81	0·54
150	19·31	6·40	1·96	0·96	0·57	0·38
179	17·95	5·87	1·78	0·87	0·52	0·35
			($q=0{\cdot}05$)			
30	97·98	58·30	31·88	21·62	16·26	13·02
60	76·54	38·64	18·36	11·96	8·97	7·28
90	53·53	24·96	11·80	7·94	6·17	5·17
120	36·13	16·57	8·15	5·71	4·57	3·92
150	29·32	13·47	6·79	4·86	3·95	3·42
179	27·74	12·75	6·48	4·66	3·80	3·30
			($q=0{\cdot}10$)			
30	110·34	69·30	41·47	30·41	24·51	20·86
60	90·48	50·67	28·29	20·77	17·09	14·93
90	67·57	36·47	20·94	15·98	13·57	12·14
120	48·70	26·51	15·95	12·58	10·92	9·92
150	40·98	22·56	13·92	11·14	9·77	8·94
179	39·16	21·63	13·43	10·80	9·49	8·70
			($q=0{\cdot}20$)			
30	140·33	97·73	68·01	55·80	49·08	44·83
60	123·81	81·47	55·95	46·69	41·91	38·98
90	101·12	66·27	47·04	40·31	36·86	34·74
120	78·96	52·74	38·76	33·88	31·36	29·80
150	69·24	46·82	35·01	30·88	28·74	27·42
179	66·92	45·41	34·11	30·16	28·11	26·84

$\mu t=0{\cdot}20$

2θ	$b=10$	$b=20$	$b=40$	$b=60$	$b=80$	$b=100$
			($q=0$)			
30	128·78	71·92	35·66	22·20	15·40	11·41
60	99·17	44·42	17·09	9·20	5·80	4·01
90	66·05	25·31	8·55	4·34	2·64	1·79
120	41·67	14·58	4·64	2·30	1·39	0·93
150	32·16	10·79	3·35	1·65	0·99	0·66
179	29·92	9·93	3·06	1·50	0·90	0·60
			($q=0{\cdot}05$)			
30	145·19	85·54	46·57	31·63	23·86	19·16
60	118·49	59·98	28·76	18·86	14·22	11·58
90	86·06	40·49	19·34	13·09	10·20	8·56
120	59·70	27·67	13·72	9·63	7·72	6·62
150	48·79	22·64	11·50	8·22	6·68	5·78
179	46·17	21·45	10·97	7·88	6·42	5·57
			($q=0{\cdot}10$)			
30	164·32	102·48	61·27	45·08	36·46	31·15
60	140·69	79·10	44·55	32·90	27·16	23·77
90	108·97	59·29	34·31	26·25	22·30	19·96
120	80·46	44·15	26·67	21·02	18·22	16·54
150	68·02	37·71	23·30	18·63	16·29	14·88
179	65·00	36·15	22·48	18·03	15·81	14·46
			($q=0{\cdot}20$)			
30	210·74	146·29	102·03	84·01	74·14	67·89
60	193·70	128·02	88·46	74·05	66·57	61·98
90	163·50	107·77	76·77	65·82	60·15	56·67
120	130·14	87·27	64·14	55·97	51·72	49·09
150	114·32	77·53	57·87	50·92	47·29	45·04
179	110·40	75·11	56·30	49·65	46·17	44·02

Table 1 (*cont.*)

2θ	$b=10$	$b=20$	$b=40$	$b=60$	$b=80$	$b=100$
			$\mu t=0{\cdot}50$			
			$(q=0)$			
30	178·45	97·86	47·90	29·69	20·58	15·24
60	155·09	69·29	26·82	14·53	9·21	6·40
90	111·51	43·11	14·76	7·56	4·64	3·16
120	74·33	26·43	8·56	4·29	2·61	1·76
150	58·40	20·01	6·33	3·15	1·90	1·28
179	54·48	18·47	5·80	2·88	1·74	1·17
			$(q=0{\cdot}05)$			
30	202·72	117·82	63·72	43·32	32·77	26·41
60	187·01	94·92	46·07	30·51	23·17	18·97
90	146·50	69·80	33·88	23·11	18·09	15·21
120	106·81	50·30	25·26	17·80	14·28	12·23
150	88·49	41·75	21·42	15·35	12·45	10·76
179	83·87	39·61	20·45	14·72	11·98	10·37
			$(q=0{\cdot}10)$			
30	231·02	142·68	85·15	62·87	51·08	43·83
60	223·62	126·35	72·03	53·61	44·48	39·06
90	186·40	102·62	60·07	46·16	39·27	35·15
120	143·89	79·93	48·58	38·28	33·13	30·00
150	122·93	68·93	42·74	34·09	29·72	27·06
179	117·56	66·11	41·21	32·98	28·81	26·27
			$(q=0{\cdot}20)$			
30	299·69	207·12	144·80	119·76	106·11	97·48
60	310·95	206·67	144·08	121·16	109·18	101·78
90	280·88	186·67	133·70	114·72	104·82	98·67
120	231·87	156·48	115·04	100·16	92·33	87·46
150	204·92	139·64	104·01	91·18	84·41	80·18
179	197·84	135·19	101·05	88·75	82·26	78·20

2θ	$b=10$	$b=20$	$b=40$	$b=60$	$b=80$	$b=100$
			$\mu t=1{\cdot}00$			
			$(q=0)$			
30	190·62	103·86	50·58	31·30	21·67	16·05
60	186·42	83·03	32·19	17·50	11·12	7·75
90	145·57	56·55	19·53	10·07	6·21	4·23
120	102·57	36·91	12·11	6·12	3·73	2·53
150	82·29	28·63	9·19	4·61	2·80	1·90
179	77·10	26·57	8·48	4·24	2·57	1·74
			$(q=0{\cdot}05)$			
30	217·17	125·60	67·76	46·06	34·86	28·12
60	226·15	114·83	56·08	37·34	28·47	23·38
90	192·44	92·42	45·33	31·10	24·41	20·56
120	147·72	70·38	35·68	25·22	20·24	17·33
150	124·56	59·53	30·81	22·11	17·93	15·47
179	118·48	56·70	29·52	21·27	17·30	14·95
			$(q=0{\cdot}10)$			
30	248·13	152·72	91·06	67·30	54·76	47·05
60	271·71	153·84	88·27	65·99	54·92	48·31
90	245·72	136·32	80·41	61·96	52·77	47·24
120	198·97	111·52	68·10	53·68	46·39	41·96
150	172·60	97·66	60·74	48·38	42·09	38·24
179	165·52	93·94	58·72	46·91	40·88	37·19
			$(q=0{\cdot}20)$			
30	323·27	223·05	156·06	129·25	114·66	105·45
60	380·32	253·49	177·59	149·73	135·14	126·09
90	371·49	248·22	178·44	153·22	139·97	131·72
120	319·78	216·83	159·49	138·64	127·60	120·67
150	285·93	195·65	145·56	127·26	117·52	111·40
179	276·58	189·74	141·61	124·00	114·62	108·72

Table 2. *Values of* $Q\{b, q, 2\theta, \mu t\} \times 10^4$ *for transmission geometry*

$\mu t = 0{\cdot}20$

2θ	$b=10$	$b=20$	$b=40$	$b=60$	$b=80$	$b=100$
			($q=0$)			
0·20	59·64	29·44	14·61	9·74	7·31	5·86
15	60·12	29·13	13·82	8·80	6·32	4·86
30	59·53	27·12	11·56	6·77	4·55	3·31
45	60·46	25·97	10·12	5·59	3·60	2·54
60	62·89	25·97	9·59	5·13	3·24	2·25
75	66·20	27·03	9·88	5·27	3·32	2·30
			($q=0{\cdot}05$)			
0·20	73·50	39·42	21·64	15·51	12·37	10·45
15	74·23	39·36	21·08	14·79	11·59	9·65
30	74·37	38·03	19·35	13·19	10·18	8·41
45	76·58	38·01	18·76	12·67	9·78	8·12
60	80·87	39·67	19·48	13·22	10·26	8·56
75	86·43	42·82	21·50	14·83	11·64	9·78
			($q=0{\cdot}10$)			
0·20	90·06	52·67	32·33	25·09	21·33	19·00
15	91·05	52·87	32·01	24·60	20·76	18·40
30	91·91	52·22	30·84	23·48	19·77	17·54
45	95·40	53·35	31·13	23·69	20·00	17·80
60	101·52	56·68	33·16	25·32	21·43	19·09
75	109·27	61·91	36·93	28·46	24·17	21·56
			($q=0{\cdot}20$)			
0·20	131·28	88·97	64·67	55·71	50·96	47·99
15	132·78	89·71	64·87	55·71	50·86	47·84
30	135·09	90·44	64·89	55·63	50·81	47·84
45	141·09	93·93	67·12	57·51	52·54	49·48
60	150·83	100·64	71·94	61·57	56·16	52·81
75	162·82	109·96	79·28	67·91	61·84	58·01

$\mu t = 0{\cdot}50$

2θ	$b=10$	$b=20$	$b=40$	$b=60$	$b=80$	$b=100$
			($q=0$)			
0·20	130·39	67·73	34·82	23·54	17·80	14·33
15	129·83	65·79	32·15	20·71	14·97	11·55
30	128·60	61·39	27·05	16·06	10·87	7·94
45	128·70	57·62	23·16	12·95	8·41	5·96
60	131·41	56·01	21·21	11·47	7·29	5·09
75	137·60	56·94	20·98	11·21	7·07	4·91
			($q=0{\cdot}05$)			
0·20	155·38	86·24	48·12	34·52	27·45	23·09
15	155·34	84·82	45·94	32·15	25·04	20·71
30	155·67	81·91	42·06	28·52	21·82	17·88
45	158·43	80·49	39·93	26·81	20·53	16·90
60	164·95	82·17	40·43	27·30	21·07	17·48
75	176·07	87·37	43·50	29·78	23·24	19·44
			($q=0{\cdot}10$)			
0·20	184·94	110·32	67·72	52·11	43·87	38·74
15	185·43	109·45	66·05	50·22	41·92	36·79
30	187·34	108·05	63·45	47·69	39·67	34·83
45	192·76	109·05	63·22	47·56	39·73	35·06
60	203·12	114·13	66·37	50·26	42·21	37·39
75	219·17	123·70	72·95	55·75	47·07	41·81
			($q=0{\cdot}20$)			
0·20	257·79	175·26	125·85	107·13	97·07	90·72
15	259·33	175·49	125·24	106·26	96·10	89·72
30	264·40	177·22	125·40	106·18	96·07	89·81
45	275·22	183·26	129·35	109·68	99·40	93·06
60	293·33	195·44	138·37	117·52	106·57	99·77
75	319·28	214·08	152·62	129·87	117·75	110·12

Table 2 (*cont.*)

$\mu t = 1{\cdot}00$

2θ	$b=10$	$b=20$	$b=40$	$b=60$	$b=80$	$b=100$
			($q=0$)			
0·20	232·89	126·24	66·82	45·69	34·78	28·10
15	231·52	122·33	61·52	40·08	29·16	22·57
30	227·94	113·17	51·23	30·75	20·94	15·36
45	226·35	104·91	43·22	24·43	15·96	11·34
60	229·82	100·56	38·81	21·16	13·51	9·45
75	241·94	101·35	37·52	20·05	12·65	8·78
			($q=0{\cdot}05$)			
0·20	269·94	154·51	87·58	62·96	49·98	41·91
15	269·50	151·58	83·21	58·22	45·18	37·17
30	268·69	145·08	75·15	50·77	38·59	31·37
45	271·76	140·96	70·26	46·94	35·68	29·15
60	282·10	142·40	70·08	47·06	36·09	29·76
75	303·75	151·02	74·52	50·58	39·18	32·58
			($q=0{\cdot}10$)			
0·20	313·24	190·54	117·20	89·56	74·79	65·51
15	313·75	188·59	113·78	85·74	70·85	61·59
30	315·73	184·81	108·07	80·32	66·06	57·41
45	323·55	185·00	106·56	79·29	65·58	57·36
60	340·89	192·53	111·08	83·34	69·44	61·10
75	372·23	209·38	121·89	92·25	77·32	68·28
			($q=0{\cdot}20$)			
0·20	418·64	285·83	202·98	170·76	153·21	142·06
15	421·05	285·89	201·56	168·85	151·13	139·92
30	428·69	287·77	200·89	167·95	150·44	139·53
45	446·24	297·08	206·98	173·54	155·94	145·02
60	478·01	317·65	222·27	187·06	168·48	156·88
75	529·25	352·21	247·75	209·01	188·39	175·43

$\mu t = 2{\cdot}00$

2θ	$b=10$	$b=20$	$b=40$	$b=60$	$b=80$	$b=100$
			($q=0$)			
0·20	410·23	232·67	127·12	88·05	67·52	54·82
15	407·09	224·74	116·51	76·85	56·30	43·78
30	400·42	207·12	96·47	58·58	40·16	29·58
45	397·46	190·83	80·57	46·00	30·22	21·57
60	404·67	181·68	71·31	39·15	25·08	17·59
75	413·96	175·52	65·29	34·90	22·00	15·26
			($q=0{\cdot}05$)			
0·20	462·75	274·40	158·67	114·57	90·95	76·12
15	461·30	268·25	149·80	105·02	81·29	66·58
30	459·66	255·52	133·93	90·29	68·23	55·08
45	465·29	246·85	123·76	82·28	62·10	50·36
60	485·48	248·42	122·19	81·50	62·06	50·82
75	510·88	254·90	124·90	84·08	64·69	53·46
			($q=0{\cdot}10$)			
0·20	523·20	326·13	201·85	153·44	127·16	110·50
15	523·45	321·78	194·76	145·61	119·15	102·53
30	526·91	314·11	183·30	134·73	109·49	94·11
45	541·35	313·43	179·44	131·97	107·93	93·47
60	574·94	326·47	186·62	138·47	114·29	99·74
75	616·90	346·47	199·37	149·39	124·24	109·04
			($q=0{\cdot}20$)			
0·20	667·88	459·57	323·07	268·27	237·96	218·50
15	671·58	458·94	319·71	264·05	233·45	213·92
30	685·49	461·82	317·78	261·75	231·63	212·74
45	718·19	478·29	328·30	271·56	241·44	222·66
60	779·80	516·46	356·13	296·28	264·52	244·66
75	856·23	566·22	392·89	328·35	293·96	272·33

Discussion

The derivations in this paper and in the references cited do not consider use of a monochromator crystal. The equations for primary and secondary intensity both must be modified when a crystal is used, and much more complicated polarization factors result. A preliminary consideration of this problem indicates that it can be solved and that the intensity of secondary scattering obtained when a crystal is used is not directly proportional to the intensity obtained when a crystal is not used. However such a solution would result in extremely complex equations. Because the primary and secondary intensities are changed in the same direction when a crystal is used, it usually should be sufficient to use Q values given if the intensity of secondary scattering is kept small. Crystals now need not be used for much X-ray scattering work. Improved pulse height analyzers used with the newer solid state detectors often give resolution as good as that produced by a crystal for energies of about 20 keV and greater (Campbell, 1970). Since radiation of about 20 keV or slightly less is needed to obtain high resolution radial distribution functions, the new detectors should serve as well as crystals in many cases.

The approximation for primary scattering based on atomic coherent intensity that is used to calculate secondary scattering intensities is most likely to give trouble for small angle data in the transmission case when μt is large. This is because the integration over the primary scattering curve, obtained using the approximation, is weighted heavily at fairly small scattering angles where the deviations of atomic coherent intensity from the true coherent intensity are the greatest. Thus, when collecting small angle transmission data, the value of μt should be made as small as possible. The value of μt usually should not exceed 1 because primary intensity decreases and the ratio of secondary to primary intensity increases for values greater than 1.

Nomenclature

- A_j Atomic weight of element j.
- b, q Parameters used to approximate scattering (Warren & Mozzi, 1966) in $J=[\sum Z_j^2][q+(1-q)/(1+b\sin^2\theta)]$.
- c Velocity of light.
- e Electronic charge.
- I_0 Intensity of X-ray beam incident to the sample.
- I_1 Total intensity of primary scattering.
- I_2 Total intensity of secondary scattering.
- I_{cp} Intensity of primary coherent scattering.
- I_{ip} Intensity of primary incoherent scattering.
- J_c Coherent intensity per structural unit in electron units.
- J_i Incoherent intensity per structural unit in electron units (without recoil correction).
- l_0, l Distance traveled by X-ray beam in sample before and after scattering, respectively, for primary scattering.
- L_1 Total distance traveled by X-ray beam in sample for primary scattering $=l_0+l$.
- L_2 Total distance traveled by X-ray beam in sample in the case of secondary scattering $=s+r+s_1$.
- m Rest mass of electron.
- N Avogadro's number.
- n Number of structural units per unit volume.
- R Distance from sample to detector face.
- $\mathbf{r}$ Vector from first to second scattering point in the case of secondary scattering.
- r Distance between first and second scattering points in the case of secondary scattering.
- s Distance traveled by X-ray beam in sample before scattering at first scattering point in the case of secondary scattering.
- s_1 Distance traveled by X-ray beam in sample after scattering at second scattering point in the case of secondary scattering.
- t Sample thickness.
- V_1 Volume of sample illuminated by incident X-ray beam.
- V_2 Volume of sample viewed by detector.
- V_{12} Volume of sample contained in both V_1 and V_2.
- Z_j Atomic number of element j.
- 2θ Total scattering angle for primary scattering.
- $2\theta_1$ Total scattering angle at first scattering point in the case of secondary scattering.
- $2\theta_2$ Total scattering angle at the second scattering point in the case of secondary scattering.
- μ Linear absorption coefficient at the wavelength of incident radiation.
- $\mu'\{2\theta\}$ Linear absorption coefficient at the wavelength of incoherent radiation as a function of scattering angle.
- $\mu_j\{m\}$ Mass absorption coefficient of element j.
- ν, ν' Frequency of coherent and incoherent radiation, respectively.
- σ_{ec} Differential cross section for coherent primary scattering by an electron.
- σ_{ei} Differential cross section for incoherent primary scattering by an electron.
- σ_{e2} Coherent electron cross section for double scattering.

APPENDIX

It is desired to obtain the intensity of primary scattering normalized to electron units. It will not be possible to give detailed derivations here, but working equations will be given.

The experimental counting rate R_{ex} can be expressed as

$$R_{\text{ex}} \propto \left[I_{cp}+I_{ip}\left(\frac{\nu'}{\nu}\right)+I_2\right]. \qquad (7)$$

The experimental counting rate measured using a radiation counter is proportional to the total number of photons detected per unit time and is not proportional to intensity when more than one frequency of radiation is present. Thus a frequency ratio must appear in equation (7) to obtain counting rate from intensity, because the derivations are based on intensity in units of erg.cm^{-2} per unit time. Uncorrected incoherent intensities J_i must be multiplied by a frequency ratio taken to the third power to make the recoil correction if intensity is desired. If a quantity proportional to the probability of scattering or detection of a photon is desired, the recoil correction is a frequency ratio taken to the second power.

Upon integration of equation (1) for both the coherent and incoherent cases and by slight manipulation of the equations for secondary scattering, an equation for a normalization constant K can be obtained.

$$K=R_{\text{ex}}/([\mathscr{F}_2 J_c+\mathscr{F}_3 J_i + \mathscr{F}_2 Q\{\sum Z_j^2\}^2/\sum A_j\mu_j\{m\}]\mathscr{F}_1) \quad (8)$$

$$\mathscr{F}_1=1+\cos^2 2\theta$$

$$\mathscr{F}_2=[\exp(-\mu t \sec 2\theta)-\exp(-\mu t)]/[(1-\sec\theta)\times\sum A_j\mu_j\{m\}] \quad \text{(transmission)}$$

$$\mathscr{F}_2=[1-\exp(-2\mu t \csc\theta)]/2\sum A_j\mu_j\{m\} \quad \text{(reflection)}$$

$$\mathscr{F}_3=\frac{\exp(-\mu' t\sec 2\theta)-\exp(-\mu t)}{\sum A_j\mu_j\{m\}-\sum A_j\mu_j'\{m\}\sec 2\theta}\left(\frac{\nu'}{\nu}\right)^2 \quad \text{(transmission)}$$

$$\mathscr{F}_3=\frac{1-\exp[-(\mu+\mu')t\csc\theta]}{\sum A_j\mu_j\{m\}+\sum A_j\mu_j'\{m\}}\left(\frac{\nu'}{\nu}\right)^2. \quad \text{(reflection)}$$

It should be noted that the denominator in the expression for $\mathscr{F}_3$ simplifies if it is assumed that the incoherent wavelength shift can be neglected in making the absorption correction. However, such an assumption can result in at least three per cent error for radiation of short wavelength at high scattering angles, so it may not be justified for all experiments.

Normalization is done in the usual manner using high-angle data except equation (8) is used to determine the normalization constant. Once the normalization constant is obtained, equation (8) can be solved for the intensity of primary coherent scattering at all scattering angles.

If both high and small-angle scattering data are collected using different equipment, the normalization procedure must be modified somewhat. The experimental intensity data for both experiments are overlapped in a region where intensities are changing only slowly with scattering angle so that any smearing corrections will be small. The high-angle scattering data, collected under conditions for which smearing is not important, is then normalized as described. The small-angle data then are multiplied by a constant so that the small and high-angle intensity data are equal in the overlap region. The small angle data then is unsmeared using any appropriate method. If the intensities for the two experiments in the overlap region do not agree after unsmearing, the unsmeared small-angle data are again multiplied by a constant that produces agreement in the overlap region.

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