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On Extinction. II. The Theory of Secondary Extinction

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The formalism developed in the previous paper [Kato, *Acta Cryst.* (1976), A32, 453–457] is applied to real crystals. If the correlation length of the lattice phase factor is sufficiently smaller than the extinction distance, the ensemble averages of the intensity fields, $\langle I_o \rangle$ and $\langle I_g \rangle$, satisfy a set of energy-transfer equations. Their form is essentially the same as that used in the conventional theory of secondary extinction. However, the physical meanings of the coupling constants connecting $\langle I_o \rangle$ and $\langle I_g \rangle$ are different, so that a modification to the theory of secondary extinction is suggested. The conventional model of mosaic blocks is merely a special case and the theoretical framework is free from the model of distorted crystals.

1. Introduction

The formalism presented in the previous paper is applied to real crystals. Mainly for the sake of concreteness, the Laue case is dealt with under the boundary conditions specified by equations (I.12).* The aim is to give a wave-optical justification of the energy-transfer equations of the type (I.4) on which the conventional theory of secondary extinction is based.

In conclusion, one can obtain fundamental equations similar to equations (I.4), under the condition $\tau \ll \Lambda$ where τ is the correlation length of the lattice phase factors and Λ is the extinction distance. However, the physical meanings of the coupling constants in the fundamental equations are different from those of equations (I.4). Thus, a modification to the theory of secondary extinction is suggested.

2. The correlation of the lattice phase factors

We shall assume an isotropic and homogeneous correlation regarding the phase factors $\exp \pm iG(m,n)$. The assumption is expressed explicitly by

$$\langle \exp iG(m+z,n) \,.\, \exp -iG(m,n) \rangle = f(z) \qquad (1a)$$

$$\langle \exp iG(m,n+z) \,.\, \exp -iG(m,n) \rangle = f(z)\,, \qquad (1b)$$

where $f(z)$ is a symmetric function for $\pm z$, the maximum value being unity at $z=0$. The correlation function $\langle\ \rangle$ may be complex in general but the conditions of isotropy and homogeneity eliminate the possibility of being complex. A few physically interesting examples of $f(z)$ will be given in Appendix *A*.

In the rigorous treatment of the averages $\langle \exp i(P_R - P_{R'}) \rangle$ and $\langle \exp i(Q_R - Q_{R'}) \rangle$ appearing in equations (I.16) one needs higher-order correlations, for example

$$\langle \exp iG(m+z,n) \,.\, \exp -iG(m,n) \times \exp iG(m'+z',n') \,.\, \exp -iG(m',n') \rangle \,.$$

If the positions (m,n) and (m',n') are sufficiently far apart, this expression can be reduced to the product of two second-order correlation functions (1), since then the phases at (m,n) and (m',n') are statistically independent.

The correlation length of the nth order is defined by

$$\tau_n = a \sum_{z=0}^{\infty} \{f(z)\}^n = \int_0^{\infty} \{f(s)\}^n \mathrm{d}s\,, \qquad (2)$$

where $f(s)$ is the smoothed function of $f(z)$. Since $f(z)$ is less than unity,

$$\tau_1 \geq \tau_2 \geq \ldots \qquad (3)$$

is always satisfied. When only the order of magnitude is referred to, the suffix n will be omitted.

Additionally, a few terminologies used in the following are explained.

(1) Separation number Δ of the kinks: We shall take a number Δ which is small enough but larger than (τ/a) so that $f(\Delta)$ is practically zero.

(2) Isolate kinks (IK): If a kink is separated by a number larger than Δ from the neighbours along a single zigzag route illustrated in Fig. I-2, such a kink is called IK.

(3) Kink pairs (KP): If a pair of the neighbouring kinks, of types (*a*) and (*b*), are closer than Δ, it is called KP.

In the following, we shall describe the details only for $\langle I_o \rangle$. The calculation of $\langle I_g \rangle$ can be performed along the same line of consideration so that only the results will be presented.

3. IK approximation

In this section, as a preparation for the next section, we shall consider a pair of route R_o and R_o', each of which is composed of only IK as illustrated in Fig. 1(*a*).* Their kink points are specified by sets of num-

* The equations and the figures of the previous paper are referred to by Roman number I.

* The segments of R_o and R_o' are drawn as either vertical or horizontal lines since only the topological features are of significance.

bers, (n_i,m_i) and (n_i',m_i') respectively as in equation (I-15a). They are assumed to differ by the numbers $(\bar{x}_i,\bar{y}_i)$ which are less than (Δ). Otherwise, there is no possibility that the route pair will contribute to the final expression for $\langle I_o\rangle$.

As the boundary conditions, $\bar{y}_0=0$ and $\bar{y}_r=0$. Thus, one can write down the phase factors for the pair of routes R_o and R_o' in the form

$$\begin{aligned}\exp i(P_{R_o}-P'_{R_o})=&\exp i[G(n_1+\bar{x}_1,0)-G(n_1,0)]\\ &\cdots\\ &\times\exp i[-G(n_i+\bar{x}_i,m_i+\bar{y}_i)+G(n_i,m_i)]\\ &\times\exp i[G(n_{i+1}+\bar{x}_{i+1},m_i+\bar{y}_i)\\ &-G(n_{i+1},m_i)]\\ &\cdots\\ &\times\exp i[-G(n_r+\bar{x}_r,m_r)+G(n_r,m_r)]. \quad (4)\end{aligned}$$

Here it is assumed that

$$\langle\exp iG(n+x,m+y)-G(n,m)\rangle=f(x)f(y)\,. \quad (5)$$

Thus, one obtains

$$\begin{aligned}&\langle\exp i(P_{R_o}-P'_{R_o})\rangle\\ &\quad=\{f(\bar{x}_1)f(\bar{y}_1)\cdots f(\bar{x}_{r-1})f(\bar{y}_{r-1})f(\bar{x}_r)\}^2. \quad (6)\end{aligned}$$

The amplitude of the routes R_o and R_o' are given by equation (I-14a). It is to be noted that the numbers of the kinks, r and r', must be identical. The averaged intensity, therefore, is given by

$$\begin{aligned}\langle I_o\rangle=&|A|^2\sum_{r=1}^{\infty}\alpha_r|\kappa_g\kappa_{-g}|^{2r}a^{4r-2}\\ &\times\prod_{i=1}^{r}S_{\bar{x}_i}\{f(\bar{x}_i)\}^2\cdot\prod_{i=1}^{r-1}S_{\bar{y}_i}\{f(\bar{y}_i)\}^2, \quad (7)\end{aligned}$$

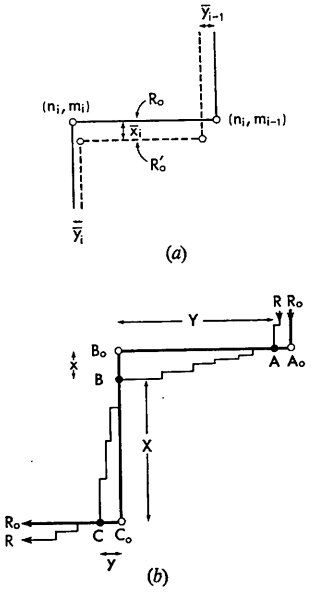


Fig. 1. (a) The optical routes for IK approximation. (b) The optical routes for IK plus KP approximation.

where α_r is given by (I-20a) with sufficient accuracy and the sum S is taken over $(-\Delta,\Delta)$. From the definition of the correlation length τ_2 [see equation (2)] we obtain

$$\langle I_o\rangle=|A|^2\sum_{r=1}^{\infty}\frac{1}{r!(r-1)!}|\kappa_g\kappa_{-g}|^{2r}(2\tau_2)^{2r-1}s_o^r s_g^{r-1} \quad (8a)$$

$$=|A|^2|\kappa_g\kappa_{-g}|\sqrt{s_o/s_g}\,I_1(4\tau_2|\kappa_g\kappa_{-g}|\sqrt{s_o s_g}) \quad (8b)$$

where I_1 is the modified Bessel function of the first order.

For the higher-order terms in equation (8a), the assumption of IK fails since the average distance l between IK is estimated to be s_o/r or s_g/r for a single route R_o containing r isolate kinks. Nevertheless, the sum of terms of higher order than $r\gg\bar{r}$ can be neglected provided that

$$\{2\tau_2|\kappa_g\kappa_{-g}|\}\sqrt{s_o s_g}\ll\bar{r}\,. \quad (9a)$$

The requirements for the IK approximation, $l>\Delta\,.\,a>\tau_2$ must be

$$\bar{r}<(s_o/\tau_2)\quad\text{and}\quad(s_g/\tau_2)\,. \quad (9b)$$

Combining the conditions (9a) and (9b), the necessary and sufficient condition is given by

$$2\tau_2^2|\kappa_g\kappa_{-g}|\ll\sqrt{s_o/s_g}\quad\text{and}\quad\sqrt{s_g/s_o}\,. \quad (9c)$$

This condition fails in the region where either s_o or s_g is nearly zero. There the routes with KP are of significance. Therefore, the discussion of equation (9c) will be postponed to the end of the next section.

By using similar procedures one can calculate $\langle I_g\rangle$. The results are given by

$$\langle I_g\rangle=|A|^2|\kappa_g|^2\sum_{r=0}^{\infty}\frac{1}{r!r!}|\kappa_g\kappa_{-g}|^{2r}(2\tau_2)^{2r}s_o^r s_g^r \quad (10a)$$

$$=|A|^2|\kappa_g|^2I_0(4\tau_2|\kappa_g\kappa_{-g}|\sqrt{s_o s_g}) \quad (10b)$$

where I_0 is the modified Bessel function of the zeroth order.

4. The improvement by taking into account KP

So far, only the routes $R_o(R_o')$ with isolate kinks have been considered. As shown in Fig. 1(b), however, there are many routes $R(R')$ having kink pairs in the vicinity of the route $R_o(R_o')$. They are called associated routes of the route $R_o(R_o')$.

Here, the assumption is made that KP on a route $R(R')$ are mutually independent. By the definition of IK, a KP is independent also of IK. The assumption is justified if KP are sufficiently rare. Thus, before taking the ensemble average $\langle\ \rangle_k$ over IK, it is allowable to take the ensemble averages $\langle\exp iP_R\rangle_P$ and $\langle\exp iP_{R'}\rangle_P$ over KP. By definition, $\langle\langle\exp iP_R\rangle_P\langle\exp -iP_{R'}\rangle_P\rangle_k$ means the ensemble average $\langle\ \rangle$ over all the kinks.

We shall consider the ith vertical segment of R_o and a segment of R which can be produced by adding p kink pairs to it. In Fig. 1(b), if the coordinate numbers of B are (n,m), those of C are $(n+X,m+y)$. The relevant part of the phase factor, therefore, is given by

$$\begin{aligned}\exp iP_R = \ldots &\exp iG(n,m)\\ &\times\exp i[G(n_1,m_1+y_1)-G(n_1,m_1)]\\ &\ldots\\ &\times\exp i[G(n_p,m_p+y_p)-G(n_p,m_p)]\\ &\times\exp -iG(n+X,m+y)\,,\end{aligned} \tag{11}$$

where the first and the last factors are responsible for IK of type (b) at the top and of type (a) at the tail of the segment, B and C respectively, and the other factors are due to KP between them. The indexes are j index, which specifies the order of KP. Here, the index i specifying the order of the segments is suppressed in the position numbers (n,m) and $(n+X,m+y)$.

The ensemble average over KP, therefore, is given by

$$\begin{aligned}\langle\exp iP_R\rangle_P = \ldots &\exp iG(n,m)\prod_{j=1}^{p} f(y_j)\\ &\times\exp -iG(n+X,m+y)\ \ldots\,.\end{aligned} \tag{12a}$$

Similarly, the ensemble average of the phase factor for R' is given by

$$\begin{aligned}\langle\exp -iP_{R'}\rangle_P = \ldots &\exp -iG(n',m')\prod_{j=1}^{p'} f(y'_j)\\ &\times\exp iG(n'+X',m'+y')\ \ldots\,.\end{aligned} \tag{12b}$$

Among the coordinate numbers appearing in equations (12), the following relations are satisfied.

$$(n'-x'_-) = (n-x_-)+\bar{x}_- \tag{13a}$$

$$m' = m+\bar{y} \tag{13b}$$

$$n'+X' = n+X+\bar{x}_+\,. \tag{13c}$$

Here, the suffix $(-)$ refers to the preceding horizontal segment and $(+)$ to the following one and $(\bar{x},\bar{y})$ are the vertical and horizontal differences in the coordinate numbers of the parallel segments of R_o and R'_o. In addition, (x,y) are related to $\{x_j\}$ and $\{y_j\}$ as

$$x = \sum_{j=1}^{q} x_j\,,\quad y = \sum_{j=1}^{p} y_j \tag{14a, b}$$

$$x' = \sum_{j=1}^{q'} x'_j\,,\quad y' = \sum_{j=1}^{p'} y'_j \tag{14c, d}$$

where $x_j(x'_j)$ is the vertical difference of the jth kink pair in a horizontal segment, and $q(q')$ is the number of KP in it.

At the next stage, we shall take $\langle\ \rangle_k$ after multiplying equations (12a, b). From the approximation (5) and the relations (13), the phase correlations relevant to IK are given by

$$\langle\exp iG(n,m)\,.\exp -iG(n',m')\rangle = f(\bar{x}_- + x'_- - x_-)f(\bar{y}) \tag{15a}$$

$$\langle\exp iG(n'+X',m'+y')\,.\exp -iG(n+X,m+y)\rangle = f(\bar{x}_+)f(\bar{y}+y'-y)\,. \tag{15b}$$

For the horizontal segments, the factors due to IK do not appear because they are already included in the expressions (12) for a vertical segment. Therefore, the horizontal segments introduce only the factors

$$\prod_{j=1}^{q} f(x_j)\prod_{j=1}^{q'} f(x'_j)\,.$$

Thus, one can write the ensemble average of the phase factor in the form

$$\begin{aligned}\langle\exp i(P_R-P_{R'})\rangle = \ldots\\ \times f(\bar{y})\prod_{j=1}^{p} f(y_j)\prod_{j=1}^{p'} f(y'_j)f(\bar{y}+\textstyle\sum y'_j-\sum y_j)\\ \times f(\bar{x})\prod_{j=1}^{q} f(x_j)\prod_{j=1}^{q'} f(x'_j)f(\bar{x}+\textstyle\sum x'_j-\sum x_j)\\ \times\ldots\,,\end{aligned} \tag{16}$$

where the relations (14) have been employed for x,y *etc.*, and the suffix $(\pm)$ in $\bar{x}$, x and x' can be dropped since now they refer to the same horizontal segment. The relation (16) is an extension of the relation (6) where $\{x_j\},\{y_j\}$ *etc.* are neglected.

For the first and the last (vertical) segments, a special care must be paid. In the former, $f(\bar{y})$ is unity because $\bar{y}=0$ always. Similarly, in the last $(r+1)$th segment, $f(\bar{y}+\sum y'_j-\sum y_j)$ is unity because then the argument must be zero.

The amplitudes of R and R' are given by

$$A_R = \left(\frac{A}{a}\right)(-\kappa_g\kappa_{-g})^{r+\sum p_i+\sum q_i}(a)^{2(r+\sum p_i+\sum q_i)} \tag{17a}$$

$$A_{R'} = \left(\frac{A}{a}\right)(-\kappa_g\kappa_{-g})^{r+\sum' i+\sum q'_i}(a)^{2(r+\sum p'_i+\sum q'_i)} \tag{17b}$$

where r is the number of IK of one type. Again, the number must be identical for the routes R and R'. Here, for clarity, the index i of the segment is explicitly retained.

Now, we shall sum over R', fixing the route R. This implies summing over p'_i and q'_i after taking the sum over the variables (x'_{ij},y'_{ij}) and $(\bar{x}_i,\bar{y}_i)$. Next we shall sum over the associate route R, fixing the route R_o. This implies summation over p_i and q_i after taking the sum over (x_{ij},y_{ij}). All of these summations can be done independently of the different segments of the route R_o and R'_o. Finally, one has to sum over the possible route R_o.

Thus, one can obtain the averaged intensity in the form

$$\langle I_o\rangle=|A|^2\sum_{R_o}|\kappa_g\kappa_{-g}|^{2r}a^{4r-2}\times(\text{First Vert. Seg.})\times\cdots\times(i\text{th Vert. Seg.})\times(i\text{th Horiz. Seg.})\times\cdots\times[(r+1)\text{th Vert. Seg.}]\,, \quad (18)$$

where

(ith Vert. Seg.)

$$=\sum_{p=0}\sum_{p'=0}\bar{\alpha}_{p,X}\bar{\alpha}_{p',X'}\times(-\kappa_g\kappa_{-g})^p(-\kappa_g^*\kappa_{-g}^*)^{p'}a^{2(p+p')}F(p,p') \quad (19a)$$

(ith Horiz. Seg.)

$$=\sum_{q=0}\sum_{q'=0}\bar{\alpha}_{q,Y}\bar{\alpha}_{q',Y'}\times(-\kappa_g\kappa_{-g})^q(-\kappa_g^*\kappa_{-g}^*)^{q'}a^{2(q+q')}F(q,q') \quad (19b)$$

where $\bar{\alpha}_{p,X}(\bar{\alpha}_{q,Y})$ is the number of the possible routes with $p(q)$ kink pairs associated with a vertical (horizontal) segment of length $l_o=Xa(l_g=Ya)$. They are given by

$$\bar{\alpha}_{p,X}=\frac{1}{p!}(l_o/a)^p,\quad \bar{\alpha}_{q,Y}=\frac{1}{q!}(l_g/a)^q. \quad (20a,b)$$

The function $F(p,p')$ is defined by

$$F(p,p')=S_{\bar{y}}\sum y_1\cdots\sum y_1'\cdots\{f(y_1)\cdots f(y_p)\cdot f(y_1')\cdots f(y_{p'}')\}\times f(\bar{y})f(\bar{y}+\sum y_j'-\sum y_j) \quad (21a)$$

$$F(q,q')=S_{\bar{x}}\sum x_1\cdots\sum x_1'\cdots\{f(x_1)\cdots f(x_q)\cdot f(x_1')\cdots f(x_{q'}')\}\times f(\bar{x})f(\bar{x}+\sum x_j'-\sum x_j)\,. \quad (21b)$$

In these formulae the summation $\sum$ covers from zero to Δ and the summation S covers from $-\Delta$ to $+\Delta$ except when it applies to the first and the last segments. As will be seen below, these cases are treated with a special care.

The summations appearing in equations (21) are a kind of conditional summation. Here, we shall use the approximation

$$f(\bar{x}+\sum x_j'-\sum x_j)=f(\bar{x})\prod_{j=1}^{q}f(x_j)\prod_{j=1}^{q'}f(x_j') \quad (22a)$$

$$f(\bar{y}+\sum y_j'-\sum y_j)=f(\bar{y})\prod_{j=1}^{p}f(y_j)\prod_{j=1}^{p'}f(y_j')\,. \quad (22b)$$

The justification will be discussed in Appendix *B*. Under this approximation, one can regard $\bar{y}$, $\{y_j\}$, $\bar{x}$ and $\{x_j\}$ as independent variables. Then one obtains

$$F(p,p')\simeq(1/a)^{p+p'+1}(\tau_2)^{p+p'}(2\tau_2) \quad (23a)$$

$$F(q,q')\simeq(1/a)^{q+q'+1}(\tau_2)^{q+q'}(2\tau_2)\,. \quad (23b)$$

For the first vertical segment, the summation $S_{\bar{y}}$ can be omitted since $\bar{y}=0$. Similarly, in the last vertical segment, $f(\bar{y})$ can be replaced by $f(\sum y_j'-\sum y_j)$ because $\bar{y}+\sum y_j'-\sum y_j$ is zero. Again the summation $S_{\bar{y}}$ can be omitted. Thus,

$$F_1(p,p')\simeq(1/a)^{p+p'}(\tau_2)^{p+p'} \quad (23c)$$

$$F_{r+1}(p,p')\simeq(1/a)^{p+p'}(\tau_2)^{p+p'}. \quad (23d)$$

Substituting from the relations (20) and (23) into (19), we shall have

(First Vert. Seg.)

$$=\exp-\tau_2[(\kappa_g\kappa_{-g})l_{o,1}+(\kappa_g^*\kappa_{-g}^*)l_{o,1}'] \quad (24a)$$

(ith Vert. Seg.)

$$=\exp-\tau_2[(\kappa_g\kappa_{-g})l_{o,i}+(\kappa_g^*\kappa_{-g}^*)l_{o,i}'](2\tau_2/a) \quad (24b)$$

(ith Horiz. Seg.)

$$=\exp-\tau_2[(\kappa_g\kappa_{-g})l_{g,i}+(\kappa_g^*\kappa_{-g}^*)l_{g,i}'](2\tau_2/a) \quad (24c)$$

[$(r+1)$th Vert. Seg.]

$$=\exp-\tau_2[(\kappa_g\kappa_{-g})l_{o,r+1}+(\kappa_g^*\kappa_{-g}^*)l_{o,r+1}']\,. \quad (24d)$$

Since

$$\sum_{i=1}^{r+1}l_{o,i}=\sum_{i=1}^{r+1}l_{o,i}'=s_o \quad\text{and}\quad \sum_{i=1}^{r}l_{g,i}=\sum_{i=1}^{r}l_{g,i}'=s_g\,,$$

one obtains from equation (18) that

$$\langle I_o\rangle=|A|^2\exp-2\tau_2\,\mathrm{Re}\,(\kappa_g\kappa_{-g})\,(s_o+s_g)\times\sum_{R_o}|\kappa_g\kappa_{-g}|^{2r}a^{4r-2}(2\tau_2/a)^{2r-1}. \quad (25)$$

As in the case of equation (8), $\sum_{R_o}$ can be replaced by $\sum_{r=1}^{\infty}\alpha_r$ so that we shall have finally

$$\langle I_o\rangle=|A|^2\exp-2\tau_2\,\mathrm{Re}\,(\kappa_g\kappa_{-g})\,(s_o+s_g)\times|\kappa_g\kappa_{-g}|\sqrt{s_o/s_g}I_1(4\tau_2|\kappa_g\kappa_{-g}|\sqrt{s_os_g})\,. \quad (26a)$$

By similar procedures one can obtain the average intensity for the Bragg-reflected wave as

$$\langle I_g\rangle=|A|^2\exp-2\tau_2\,\mathrm{Re}\,(\kappa_g\kappa_{-g})\,(s_o+s_g)\times|\kappa_g|^2I_0(4\tau_2|\kappa_g\kappa_{-g}|\sqrt{s_os_g})\,. \quad (26b)$$

In deriving these results, the essential approximation is to represent the correlation of the lattice phases by the product of the second-order correlation function defined by equations (1). This approximation can be justified when the IK and KP are separated by a distance more than $\Delta\,.\,a$, namely when the number of KP along all vertical segments, $\bar{p}$, and the number of IK of (a) type, $\bar{r}$, satisfy the condition

$$\bar{p}+\bar{r}<s_o/\Delta\,.\,a<s_o/\tau_2\,. \quad (27a)$$

Similarly, for the number of KP along all horizontal segments, $\bar{q}$, the condition

$$\bar{q}+\bar{r}<s_g/\Delta\,.\,a<s_g/\tau_2 \quad (27b)$$

must be satisfied. Accordingly, if a set of numbers, $\bar{p}$, $\bar{q}$ and $\bar{r}$, exist and the higher-order terms than $\bar{p}$, $\bar{q}$ and $\bar{r}$ in the power series expansions of $\exp-2\tau_2\times\mathrm{Re}\,(\kappa_g\kappa_{-g})s_o$, $\exp-2\tau_2\,\mathrm{Re}\,(\kappa_g\kappa_{-g})s_g$, and I_1 (or I_o) are

negligibly small respectively, the approximation mentioned above would not harm the final results, equations (26). These conditions are obviously

$$2\tau_2|\kappa_g\kappa_{-g}|s_o<\bar{p} \tag{28a}$$

$$2\tau_2|\kappa_g\kappa_{-g}|s_g<\bar{q} \tag{28b}$$

$$2\tau_2|\kappa_g\kappa_{-g}|\sqrt{s_o s_g}<\bar{r}\,, \tag{28c}$$

where $\mathrm{Re}\,(\kappa_g\kappa_{-g})$ and $|\kappa_g\kappa_{-g}|$ are not distinguished. The necessary and sufficient condition for such $\bar{p}$, $\bar{q}$ and $\bar{r}$ to be found is

$$2\tau_2|\kappa_g\kappa_{-g}|(\sqrt{s_o}+\sqrt{s_g})^2<(\bar{p}+\bar{q}+2\bar{r})<(s_o+s_g)/\tau_2\,,$$

namely

$$\tau_2^2|\kappa_g\kappa_{-g}|\ll\frac{\frac{1}{2}(s_o+s_g)}{s_o+s_g+2\sqrt{s_o s_g}}<\frac{1}{2}\,. \tag{29a}$$

This implies that

$$\tau_2\ll\tfrac{1}{2}|\kappa_g\kappa_{-g}|^{-1/2}\sim\Lambda\,, \tag{29b}$$

where Λ is the Pendellösung fringe spacing or primary extinction distance in order of magnitude.

5. Discussion and conclusions: mainly on secondary extinction

The formulae (26*a*, *b*) are a good approximation of $\langle I_o\rangle$ and $\langle I_g\rangle$ under the condition (29*b*) and the prescribed boundary conditions (I.12). It is a straightforward matter to show that they satisfy the differential equations

$$\frac{\partial\langle I_o\rangle}{\partial s_o}=-2\tau_2\,\mathrm{Re}\,(\kappa_g\kappa_{-g})\langle I_o\rangle+2\tau_2|\kappa_{-g}|^2\langle I_g\rangle \tag{30a}$$

$$\frac{\partial\langle I_g\rangle}{\partial s_g}=-2\tau_2\,\mathrm{Re}\,(\kappa_g\kappa_{-g})\langle I_g\rangle+2\tau_2|\kappa_g|^2\langle I_o\rangle\,. \tag{30b}$$

These are nothing but a set of energy-transfer equations. Neglecting the difference between $\mathrm{Re}\,(\kappa_g\kappa_{-g})$, $|\kappa_g|^2$ and $|\kappa_{-g}|^2$ the equations are identical in form to equations (I.4) on which the conventional theory of secondary extinction is based. The difference is of significance when the dispersion effect on the structure factor F_g is appreciable. From the physical meaning of the coupling constants, the present form is more reasonable than the conventional one.

Here a few significant remarks will be additionally mentioned.

(1) Equations (30) refer to the intensities taken over an ensemble of real crystals, rather than the intensities in the individual experiments.

(2) Equations (30) are derived from the spherical-wave theory. This implies that the intensity fields concerned are an angularly integrated intensity. For this reason, the coupling constants are irrelevant to the direction of the incident beam. This is the most significant difference between equations (30) and (I.4). The correlation length τ_2 depends purely on the characters of the medium or the assumed statistical ensemble of distorted crystals.

(3) To obtain the integrated power, one does not need the integration over the direction of the incident beam. In the experiments using a crystal bathed in the incident beam, if the solution is given for the incident wave of δ-function type, what one needs is spatial integrations on both the incident surface and the exit surface of the crystal. The procedures have already been discussed in a general way in § 5 of the first paper.

In the conventional theory of secondary extinction, first a kind of angular integration is performed to find the coupling constant $\bar{\sigma}(\varepsilon)$ [see equations (I.5)] and next another angular integration is required to obtain the integrated power. The correctness of these double integrations is doubtful.

(4) The conventional theory of secondary extinction is based on the model of mosaic blocks in which the diffraction theory for perfect crystals can be used. As to the model of the crystals, the present theory is more flexible. In Appendix *A* the correlation length τ_2 is discussed for a few models of the ensemble of distorted crystals. In the first model only a distribution of elastic strain is assumed. In the second model, a size distribution of the mosaic blocks is assumed in the sense of the conventional theory of secondary extinction. Although the characters of τ_2 (λ or θ_B dependence) depend on the specified model, the framework of the present theory is not confined to the mosaic block model.

This paper has dealt with only the fundamental problems on the energy-transfer equations. A few remarks on further developments will be given here.

(1) From the standpoint of the present theory it is necessary to consider correctly the higher-order correlation of the lattice phase, if the correlation length τ_2 is larger than the extinction distance.

(2) To obtain the spatial integrations mentioned in (3) above, one needs the intensity fields not only in the Laue case but also in the other cases, such as Laue–Bragg and Bragg cases. It is desirable to obtain the intensities in these cases by combinatorial calculation, as in the Laue case. In practice, however, once we admit the energy-transfer equations (30), it is more convenient to solve them under suitable boundary conditions. Some of the calculations based on equations (I.4) (Werner & Arrott, 1965; Werner, Arrott, King & Kendrick, 1966; Becker & Coppens, 1974) are useful for this purpose, although the physical meanings are different.

(3) To avoid the mathematical difficulty in solving equations (30) for crystal of arbitrary shape it is advisable to do the experiments for a parallel-slab crystal under the conditions of the Laue or the Bragg case. Nevertheless, to find the ensemble average of the intensities, the experiments must be done with a fairly wide incident beam.

The present theory can be regarded as a dynamical theory for distorted crystals. In the past decade, several

types of theory have been proposed for the understanding of the diffraction phenomena of crystal defects. Limited to X-ray cases, for example, one can list Penning & Polder (1961, 1964), Takagi (1962, 1969), Kato (1963*a*, *b*, *c*, 1964*a*, *b*, 1973), Bonse (1964), Kambe (1965, 1968), Kuriyama (1967, 1968, 1970, 1971, 1972, 1973), Kuriyama & Early (1974) and Dederichs (1966, 1967). Furthermore, it would be worth mentioning the work of Kuriyama & Miyakawa (1969, 1970) who dealt with the problem of extinction for vibrating crystals. Also Katagawa & Kato (1974) & Chukovskii (1974) presented the exact analytical solution for the crystal having a constant strain gradient of arbitrary magnitude. In these theories, except for the theory of Dederichs studying the statistical nature of point defects and clusters, all authors are interested in the cases where the lattice distortion is definitely specified. In the result, even in highly distorted crystals, the wave fields obtained must be regarded as perfectly coherent with the incident waves.

In the problems of highly distorted crystals, if only statistical information about lattice distortions is available, one cannot obtain both the wave fields and the intensity fields for a specified lattice distortion. What one can discuss is the averaged intensity for an ensemble of lattice distortions. It must be emphasized that incoherence of waves is merely a result, usually an approximate one, of the ensemble average. The present approach is the first step in developing the dynamical diffraction theory to take into account the statistical nature of lattice distortions of displacement type.

APPENDIX A
Correlation function $f(s)$

1. *Misorientation model*

The rectangular coordinates (x_1, x_2) normal and parallel to the net plane within the reflexion plane are given by

$$(x_1, x_2) = (-\sin\theta_B, \cos\theta_B)s_o + (\sin\theta_B, \cos\theta_B)s_g \,. \quad (A.1)$$

Then, one can write the **g** component of the displacement vector **u** in the vicinity of $s=0$ in the form

$$u(s) = u(0) + \varepsilon s \quad (A.2)$$

where s stands for s_o or s_g and

$$\varepsilon = \pm \left(\frac{\partial u}{\partial x_1}\right)_o \sin\theta_B + \left(\frac{\partial u}{\partial x_2}\right)_o \cos\theta_B \,. \quad (A.3)$$

The lattice phase, therefore, is given by

$$G = 2\pi(\mathbf{g} \,.\, \mathbf{u}) = G_o + \alpha\varphi s \quad (A.4)$$

where

$$\alpha = 2\pi|\mathbf{g}|\cos\theta_B = 2\pi(\sin 2\theta_B/\lambda) \quad (A.5)$$

and

$$\varphi = \left(\frac{\partial u}{\partial x_2}\right)_o \pm \left(\frac{\partial u}{\partial x_1}\right)_o \tan\theta_B \quad (A.6)$$

is the deviation angle from the exact Bragg condition for a beam which satisfies exactly the condition when $\varepsilon=0$. In the following, we shall take φ as a statistical variable and assume that the crystalline state is characterized by a normalized distribution function $\Phi(\varphi)$. The model is called the misorientation model.

With this model, the correlation function can be calculated by

$$f(s) = \int_{-\infty}^{+\infty} \Phi(\varphi) \exp\left[2\pi i(\sin 2\theta_B/\lambda)\varphi s\right] \mathrm{d}\varphi \,. \quad (A.7)$$

It is reasonable to assume that $\Phi(\varphi)$ is a symmetric function. Then, $f(s)$ is also a real symmetric function. The Fourier transform of $f(s)$ is given by

$$g(\xi) = \frac{1}{\sqrt{2\pi}} (\lambda/\sin 2\theta_B)\Phi(\xi\lambda/2\pi \sin 2\theta_B) \,. \quad (A.8)$$

The correlation length defined by equation (2) is given by

$$\tau_1 = \sqrt{\frac{\pi}{2}}\, g(0) = \tfrac{1}{2}(\lambda/\sin 2\theta_B)\Phi(0) \quad (A.9a)$$

$$\tau_2 = \tfrac{1}{2}\int_{-\infty}^{+\infty} [g(\xi)]^2 \mathrm{d}\xi = \tfrac{1}{2}(\lambda/\sin 2\theta_B) \times \int_{-\infty}^{+\infty} \{\Phi(\varphi)\}^2 \mathrm{d}\varphi \,. \quad (A.9b)$$

2. *Block model*

If the displacement vector **u** is constant within a distance l and at random outside it, the correlation function must be $C(|s|-l)$, the function $C(x)$ being defined by

$$C(x) = 1 \quad x<0$$
$$= 0 \quad x>0 \,. \quad (A.10)$$

If such regions occur with a probability density $L(l)$, one obtains the correlation function

$$f(s) = \int_0^\infty L(l) C(|s|-l) \mathrm{d}l \,. \quad (A.11)$$

The Fourier transform of $f(s)$ is given by

$$g(\xi) = \sqrt{\frac{2}{\pi}} \int_0^\infty L(l) \frac{\sin \xi l}{\xi} \mathrm{d}l \,. \quad (A.12)$$

The correlation length can be calculated by

$$\tau_1 = \int_0^\infty L(l) \,.\, l \mathrm{d}l \quad (A.13a)$$

$$\tau_2 = 2\int_0^\infty L(l) \int_0^l l' L(l') \mathrm{d}l' \mathrm{d}l \,. \quad (A.13b)$$

Unlike the misorientation model, τ_1 and τ_2 are independent of λ and the Bragg angle θ_B.

3. *Combination model*

A more realistic model would be a combination of models 1 and 2. Then the correlation function can be written down as

$$f(s)=\int_{-\infty}^{+\infty}\Phi(\varphi)\mathrm{d}\varphi\int_0^{\infty}L(l)C(|s|-l)\exp i\alpha\varphi s\,\mathrm{d}l\,. \tag{A.14}$$

The Fourier transform of $f(s)$ is

$$g(\xi)=\sqrt{\frac{2}{\pi}}\int_{-\infty}^{+\infty}\Phi(\varphi)\mathrm{d}\varphi\int_0^{\infty}L(l)\frac{\sin\xi' l}{\xi'}\,\mathrm{d}l, \tag{A.15}$$

where

$$\xi'=\xi+\alpha\varphi\,. \tag{A.16}$$

By the use of this expression, one can see that

$$\tau_1=\int_{-\infty}^{+\infty}\Phi(\varphi)\mathrm{d}\varphi\int_0^{\infty}\frac{\sin\alpha\varphi l}{\alpha\varphi}L(l)\mathrm{d}l \tag{A.17a}$$

$$\tau_2=\frac{1}{\pi}\int_{-\infty}^{+\infty}\Phi(\varphi')\mathrm{d}\varphi\int_{-\infty}^{+\infty}\Phi(\varphi'')\mathrm{d}\varphi''\int_0^{\infty}L(l')\mathrm{d}l'$$
$$\times\int_0^{\infty}L(l'')\mathrm{d}l''\int_{-\infty}^{+\infty}\frac{\sin\xi' l'}{\xi'}\frac{\sin\xi'' l''}{\xi''}\,\mathrm{d}\xi\,.$$

The last integral can be calculated easily by contour integration so that

$$\tau_2=2\int_{-\infty}^{+\infty}\Phi(\varphi')\mathrm{d}\varphi'\int_{-\infty}^{+\infty}\Phi(\varphi'')\mathrm{d}\varphi''\int_0^{\infty}L(l')\mathrm{d}l'$$
$$\times\int_0^{l'}L(l'')\,\frac{\sin\alpha(\varphi'-\varphi'')l''}{\alpha(\varphi'-\varphi'')}\,\mathrm{d}l''\,. \tag{A.17b}$$

Model 1 is the special case where $\alpha\varphi l$ is effectively infinity so that

$$\frac{\sin\alpha(\varphi'-\varphi'')l''}{\alpha(\varphi'-\varphi'')}\sim\pi\frac{1}{\alpha}\,\delta(\varphi'-\varphi'')\,. \tag{A.18a}*$$

Model 2 is the case where $\alpha\varphi l$ is effectively small, so that

$$\frac{\sin\alpha(\varphi'-\varphi'')l''}{\alpha(\varphi'-\varphi'')}\sim l''-\frac{1}{3!}[\alpha(\varphi'-\varphi'')]^2(l'')^3+\ldots\,. \tag{A.18b}$$

The transition occurs under the condition

$$2\pi\sin 2\theta_B=\lambda/(\bar{l}\,.\,\bar{\varphi}) \tag{A.19}$$

where $\bar{l}$ and $\bar{\varphi}$ are the average block size and the average misorientation angle. In a sense, models 1 and 2 correspond to the types I and II in Zachariasen's classification of mosaic crystals but the correspondence is not exact.

In general, the λ and θ_B dependence is rather complicated. From the above analysis, however, one can conclude that:

(1) Model 1 is adequate in practice when $(\bar{l}\,.\,\bar{\varphi})\gg\lambda$.

(2) In principle, if the Bragg angle is small, all crystals behave as if they are crystals of model 2.

* Notice:
$\int_0^{\infty}L(l')\mathrm{d}l'\int_0^{l'}L(l'')\mathrm{d}l''=\frac{1}{2}\int_0^{\infty}L(l')\mathrm{d}l'\int_0^{\infty}L(l'')\mathrm{d}l''=\frac{1}{2}$.

APPENDIX B

The function $F(p,p')$ and related topics

First, we shall consider $F(p,p')$ defined by equation (21*a*). Replacing the coordinate numbers $\{\bar{y},y_j,y_j'\}$ by the continuous variables $\{\bar{s},s_j,s_j'\}$ as in equation (2) and introducing a dummy variable s, one can write $F(p,p')$ in the form

$$F(p,p')=\left(\frac{1}{a}\right)^{p+p'+1}\int_{-\infty}^{+\infty}\mathrm{d}s\int_{-\infty}^{+\infty}\mathrm{d}\bar{s}$$
$$\times\left\{\prod_{j=1}^{p}\int_0^{\infty}f(s_j)\mathrm{d}s_j\right\}\left\{\prod_{j=1}^{p'}\int_0^{\infty}f(s_j')\mathrm{d}s_j'\right\}$$
$$\times f(\bar{s})f(s)\delta(s-\bar{s}-\textstyle\sum s_j'+\sum s_j)\,. \tag{B.1}$$

By the use of the well-known expression

$$\delta(s-\bar{s}-\textstyle\sum s_j'+\sum s_j)$$
$$=(2\pi)^{-1}\int_{-\infty}^{+\infty}\exp i\xi(s-\bar{s}-\textstyle\sum s_j'+\sum s_j)\mathrm{d}\xi\,, \tag{B.2}$$

equation (*B*.1) can be rewritten as

$$F(p,p')=(\sqrt{2\pi})^{p+p'}(2/a)^{p+p'+1}$$
$$\times\int_{-\infty}^{+\infty}g(\xi)g^*(\xi)\{g^+(\xi)\}^p\{g^-(\xi)\}^{p'}\mathrm{d}\xi \tag{B.3}$$

where

$$g(\xi)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}f(s)\exp i\xi s\mathrm{d}s \tag{B.4a}$$

$$g^*(\xi)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}f(\bar{s})\exp -i\xi\bar{s}\mathrm{d}\bar{s} \tag{B 4b}$$

$$g^+(\xi)=\frac{1}{\sqrt{2\pi}}\int_0^{\infty}f(s_j)\exp i\xi s_j\mathrm{d}s_j \tag{B.4c}$$

$$g^-(\xi)=\frac{1}{\sqrt{2\pi}}\int_0^{\infty}f(s_j')\exp -i\xi s_j'\mathrm{d}s_j'\,. \tag{B.4d}$$

Since $f(s)$ is a symmetric function, one can see that

$$g(\xi)=g^*(\xi) \tag{B.5a}$$

is real and has the maximum at $\xi=0$ and tends to zero as ξ increases. Moreover,

$$g(\xi)=g^+(\xi)+g^-(\xi) \tag{B.5b}$$

and

$$h(\xi)=(i)^{-1}\{g^+(\xi)-g^-(\xi)\} \tag{B.5c}$$

is real and $h(0)$ is zero.

The other useful properties of $g(\xi)$ are listed below:

$$g(0)=\sqrt{\frac{2}{\pi}}\tau_1 \qquad (B.6a)$$

$$\int_{-\infty}^{+\infty} g(\xi)\mathrm{d}\xi=\sqrt{2\pi}f(0)=\sqrt{2\pi} \qquad (B.6b)$$

$$\int_{-\infty}^{+\infty}\{g(\xi)\}^2\mathrm{d}\xi=\int_{-\infty}^{+\infty}\{f(s)\}^2\mathrm{d}s=2\tau_2\,. \qquad (B.6c)$$

Substituting from the expression (*B*.3) into equations (19), one can write the contribution of the ith vertical and horizontal segment as

$$V_i=\left(\frac{1}{a}\right)\int_{-\infty}^{+\infty}\{g(\xi)\}^2\exp-\{\Gamma_o g(\xi)+\gamma_o h(\xi)\}\mathrm{d}\xi \qquad (B.7a)$$

$$H_i=\left(\frac{1}{a}\right)\int_{-\infty}^{+\infty}\{g(\xi)\}^2\exp-\{\Gamma_g g(\xi)+\gamma_g h(\xi)\}\mathrm{d}\xi \qquad (B.7b)$$

where

$$\Gamma_o=\sqrt{2\pi}\,\mathrm{Re}\,(\kappa_g\kappa_{-g})l_{o,i}\,,$$
$$\gamma_o=\sqrt{2\pi}\,\mathrm{Im}\,(\kappa_g\kappa_{-g})l_{o,i} \qquad (B.8a, b)$$

$$\Gamma_g=\sqrt{2\pi}\,\mathrm{Re}\,(\kappa_g\kappa_{-g})l_{g,i}\,,$$
$$\gamma_g=\sqrt{2\pi}\,\mathrm{Im}\,(\kappa_g\kappa_{-g})l_{g,i}\,, \qquad (B.8c, d)$$

so that $\Gamma_{o,g}\gg\gamma_{o,g}$ are always satisfied. In deriving equations (*B*.7), the minute approximations $l_{o,i}=l'_{o,i}$ and $l_{g,i}=l'_{o,i}$ are employed.

Here, we shall consider the function

$$Z=\left(\frac{1}{a}\right)\int_{-\infty}^{+\infty} g(\xi)\exp-\{\Gamma g(\xi)+\gamma h(\xi)\}\mathrm{d}\xi\,. \qquad (B.9)$$

Since we are interested in the case of appreciable values of V_i and H_i, it is safe to assume that $\Gamma g(0)$ is not too large. Then, remembering both that $h(0)$ is zero and the properties listed in equations (6), one can obtain the main contribution to the integral from the region in the vicinity of $\xi\sim 0$, so that one can approximate (*B*.9) as

$$\begin{aligned}Z&=\left(\frac{1}{a}\right)\exp-\Gamma g(0)\\&\quad\times\int_{-\infty}^{+\infty} g(\xi)\exp-\Gamma[g(\xi)-g(0)]\,\mathrm{d}\xi\\&\simeq\left(\frac{1}{a}\right)\exp-\Gamma g(0)\\&\quad\times\int_{-\infty}^{+\infty} g(\xi)\{1-\Gamma[g(\xi)-g(0)]+\ldots\}\mathrm{d}\xi \qquad (B.10a)\\&=\left(\frac{1}{a}\right)\exp-\sqrt{2/\pi}\Gamma\tau_1\,.\{\sqrt{2\pi}-2\Gamma(\tau_2-\tau_1)+\ldots\}\\&\simeq\sqrt{2\pi}\left(\frac{1}{a}\right)\exp-\sqrt{2/\pi}\Gamma\tau_2\,. \qquad (B.10b)\end{aligned}$$

From equations (*B*.7*a*) and (*B*.9), one obtains

$$\begin{aligned}V_i&=-\left[\frac{\partial}{\partial\Gamma}Z\right]_{\Gamma=\Gamma_o}\\&\simeq(2\tau_2/a)\exp-2\,\mathrm{Re}\,(\kappa_g\kappa_{-g})\tau_2 l_{o,i}\,. \qquad (B.12a)\end{aligned}$$

By a similar calculation,

$$H_i\simeq(2\tau_2/a)\exp-2\,\mathrm{Re}\,(\kappa_g\kappa_{-g})\tau_2 l_{g,i}\,. \qquad (B.12b)$$

The results (*B*.12) are identical to equations (24*b*, *c*) obtained in the text. Thus, it turns out that the approximations (22) are equivalent to those used in (*B*.10).

In order to see how acceptable the approximations (*B*.10) are, we shall examine two special cases in which: case I:

$$\begin{aligned}g(\xi)&=E(1-|\xi|/\xi_o) &&|\xi|\le\xi_o\\&=0 &&|\xi|>\xi_o \qquad (B.13a)\\&\{\text{normalization: } E\xi_o=\sqrt{2\pi}\}\end{aligned}$$

case II:

$$g(\xi)=E\exp-\alpha|\xi| \qquad (B.13b)$$

$$\left\{\text{normalization: } E/\alpha=\sqrt{\frac{\pi}{2}}\right\}.$$

In these cases, one can obtain the exact function Z and V or H in the forms (let $x=\Gamma E$; dropping the suffix i)

$$Z(x)=a^{-1}\sqrt{2\pi}F(x) \qquad (B.14a)$$

$$V(x)=a^{-1}\sqrt{2\pi}E\left\{-\frac{\mathrm{d}}{\mathrm{d}x}F(x)\right\}, \qquad (B.14b)$$

where the function $F(x)$ is given by:

case I:

$$F(x)=\frac{2}{x^2}\{1-(1+x)\exp(-x)\} \qquad (B.15a)$$

case II:

$$F(x)=\frac{1}{x}\{1-\exp(-x)\}\,. \qquad (B.15b)$$

On the other hand, the approximate results are

$$Z_{\mathrm{app}}=a^{-1}\sqrt{2\pi}G(x) \qquad (B.14c)$$

$$V_{\mathrm{app}}=a^{-1}\sqrt{2\pi}E\left\{-\frac{\mathrm{d}}{\mathrm{d}x}G(x)\right\}, \qquad (B.14d)$$

where the function $G(x)$ is given by

case I:

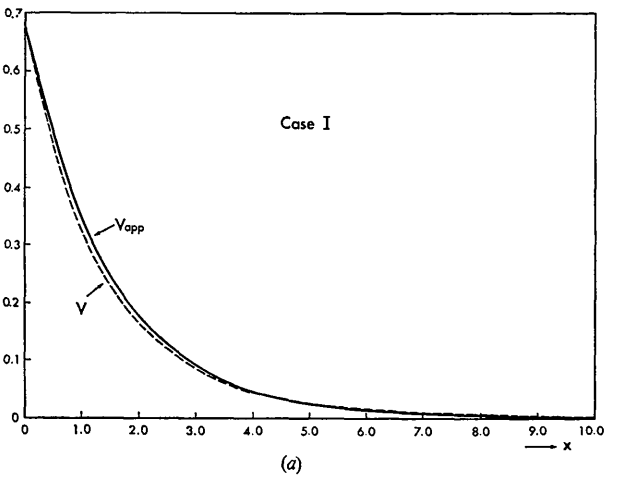
$$G(x)=\exp-\tfrac{2}{3}x \qquad (B.15c)$$

case II:

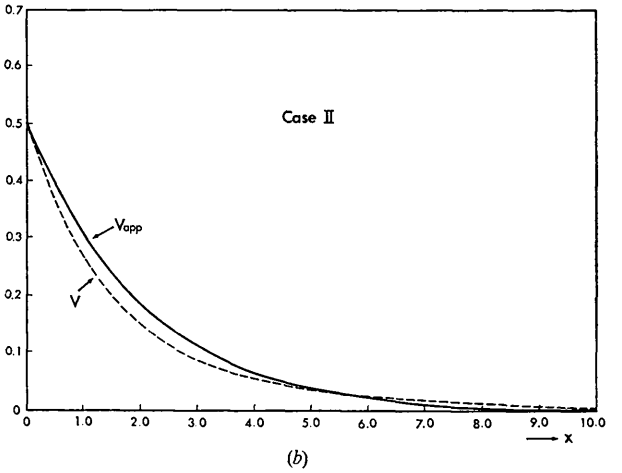
$$G(x)=\exp-x\,. \qquad (B.15d)$$

In Fig. 2, the functions $\mathrm{d}F/\mathrm{d}x$ and $\mathrm{d}G/\mathrm{d}x$ are compared in the respective cases. From this analysis, the approximations are reasonably satisfactory in the wide

range of ΓE, irrespective of the functional form. In particular, it is easily seen that the present treatment is exact when $g(\xi)$ is a rectangular form. However, it is clear that the approximations are worse in the second case than the first case. In the second case, the correlation function $f(s)$, the Fourier transform of $g(\xi)$, is Lorentzian, so that $f(s)$ has a long tail for large values of s. For such a case, the present approximations would not be very satisfactory.



(*a*)



(*b*)

Fig. 2. The comparison of the exact function V and the function V_{app} calculated with the approximations (*B*.10). (*a*) The case I. (*b*) The case II.

References

BECKER, J. P. & COPPENS, P. (1974). *Acta Cryst.* A**30**, 129–147.

BONSE, U. (1964). *Z. Phys.* **177**, 385–423.

CHUKOVSKII, F. N. (1974). *Kristallografiya*, **19**, 482–488.

DEDERICHS, P. H. (1966). *Phys. Kondens. Mater.* **4**, 347–363.

DEDERICHS, P. H. (1967). *Phys. Stat. Sol.* **23**, 377–386.

KAMBE, K. (1965). *Z. Naturforsch.* **20a**, 770–786.

KAMBE, K. (1968). *Z. Naturforsch.* **23a**, 25–43.

KATAGAWA, T. & KATO, N. (1974). *Acta Cryst.* A**30**, 830–836.

KATO, N. (1963*a*). *Acta Cryst.* **16**, 276–281.

KATO, N. (1963*b*). *Acta Cryst.* **16**, 282–290.

KATO, N. (1963*c*). *J. Phys. Soc. Japan*, **18**, 1785–1791.

KATO, N. (1964*a*). *J. Phys. Soc. Japan*, **19**, 67–77.

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

KATO, N. (1973). *Z. Naturforsch.* **28a**, 604–609.

KURIYAMA, M. (1967). *J. Phys. Soc. Japan*, **23**, 1369–1379.

KURIYAMA, M. (1968). *J. Phys. Soc. Japan*, **25**, 846–855.

KURIYAMA, M. (1970). *Acta Cryst.* A**26**, 56–59.

KURIYAMA, M. (1971). *Acta Cryst.* A**27**, 634–647.

KURIYAMA, M. (1972). *Acta Cryst.* A**28**, 588–593.

KURIYAMA, M. & EARLY, J. G. (1974). *Acta Cryst.* A**30**, 525–535.

KURIYAMA, M. & MIYAKAWA, T. (1969). *J. Appl. Phys.* **40**, 1697–1702.

KURIYAMA, M. & MIYAKAWA, T. (1970). *Acta Cryst.* A**26**, 667–673.

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

PENNING, P. & POLDER, D. (1964). *Acta Cryst.* **17**, 950–955.

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

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

WERNER, S. A. & ARROTT, A. (1965). *Phys. Rev.* **140A**, 675–686.

WERNER, S. A., ARROTT, A., KING, J. S. & KENDRICK, H. (1966). *J. Appl. Phys.* **37**, 2343–2350.