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The Theory of X-ray Crystal Diffraction for Finite Polyhedral Crystals. II. The Laue–(Bragg)^m Cases

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(*Received* 18 *January* 1971 *and in revised form* 7 *July* 1971)

The wave fields specified by the Laue–(Bragg)^m cases are treated from the view points of the plane-wave and spherical-wave theory. The results are very similar to those in the Laue–Bragg case in Part I (*Acta Cryst.* (1972). A**28**, 102.). The diffraction phenomena for a finite polyhedral crystal and the experiment of Lehmann & Borrmann (*Z. Kristallogr.* (1967). **125**, 234) are discussed from the view point of the spherical-wave theory.

Introduction

When the exit surfaces, S_a and S_b, are close to each other the Laue–Bragg waves obtained previously may be reflected many times at them before leaving through any one of the exit surfaces. In this Part, this topic is treated from the stand points of both the plane-wave and spherical-wave theories. According to the terminology defined in Part I (Saka, Katagawa & Kato, 1972), this case is specified as the Laue–(Bragg)^m case. The same notations as in Part I are used in this Part, unless otherwise specified. The equations of Part I are cited by adding I to the equation number.

Here, again, two cases of Type I and II must be distinguished. In the former case, the crystal waves hit the exit surfaces in the sequence, S_a, S_b, S_a, ..., whereas the sequence starts from S_b in the latter case (see Fig. 1). In order to specify the quantities pertinent to the wave fields reflected m times, the suffix m is added to them, *e.g.* the wave vector $\mathbf{k}_{0,m}$ and Anpassung δ_m. Obviously, $\mathbf{k}_{0,0}$, $\mathbf{k}_{0,1}$ and δ_1 are $\mathbf{k}_0$, $\mathbf{k}_{0,r}$ and δ_r in Part I.

The wave fields of Type I

As shown in Fig. 1(*a*), the waves reflected $2n$ and $2n+1$ times fall on the exit surfaces S_a and S_b respectively. The boundary conditions for the totally reflected waves are read as,

$$0=d_{0,2n}\exp[i(\mathbf{k}_{0,2n}\cdot\mathbf{r}_{a,2n+1})]+d_{0,2n+1}\exp[i(\mathbf{k}_{0,2n+1}\cdot\mathbf{r}_{a,2n+1})] \quad (1a)$$

$$0=d_{g,2n+1}\exp[i(\mathbf{k}_{g,2n+1}\cdot\mathbf{r}_{b,2n+2})]+d_{g,2n+2}\exp[i(\mathbf{k}_{g,2n+2}\cdot\mathbf{r}_{b,2n+2})] \quad (1b)$$

where $\mathbf{r}_{a,2n+1}$ and $\mathbf{r}_{b,2n+2}$ denote position vectors on the surfaces S_a and S_b.

From these equations, one can obtain the recurrence formulae

$$d_{0,2n+1}=-d_{0,2n}\exp[i\{(\mathbf{k}_{0,2n}-\mathbf{k}_{0,2n+1})\cdot\mathbf{r}_{a,2n+1}\}] \quad (2a)$$

$$d_{0,2n+2}=-\frac{\Delta\eta_{0,2n+1}}{\Delta\eta_{0,2n+2}}d_{0,2n+1}\times\exp[i\{(\mathbf{k}_{0,2n+1}-\mathbf{k}_{0,2n+2})\cdot\mathbf{r}_{b,2n+2}\}]. \quad (2b)$$

In the last equation, the relations $\mathbf{k}_{g,m}=\mathbf{k}_{0,m}+2\pi\mathbf{g}$ and $d_{g,m}/d_{0,m}=2\Delta\eta_{0,m}/KC\chi_{-g}$ are used, where $\Delta\eta_{0,m}$ is the Resonanzfehler of the wave reflected m times. By combining these, it is easy to see that

$$d_{0,2n+2}=\frac{\Delta\eta_{0,2n+1}}{\Delta\eta_{0,2n+2}}\,d_{0,2n}\times\exp\left[i\{[(\mathbf{k}_{0,2n+1}-\mathbf{k}_{0,2n+2})\cdot\mathbf{r}_{b,2n+2}]+[(\mathbf{k}_{0,2n}-\mathbf{k}_{0,2n+1})\cdot\mathbf{r}_{a,2n+1}]\}\right]. \quad (3)$$

By repeating the same procedure the amplitudes are derived as

$$d_{0,2n}=\prod_{l=1}^{n}\frac{\Delta\eta_{0,2l-1}}{\Delta\eta_{0,2l}}\,C_0E_e\exp(i\varphi_{2n}) \quad (4a)$$

$$d_{0,2n+1}=-\prod_{l=1}^{n}\frac{\Delta\eta_{0,2l-1}}{\Delta\eta_{0,2l}}\,C_0E_e\exp(i\varphi_{2n+1}) \quad (4b)$$

where

$$\varphi_{2n}=[(\mathbf{K}_e-\mathbf{k}_0)\cdot\mathbf{r}_e]+\sum_{l=1}^{n}[(\mathbf{k}_{0,2l-2}-\mathbf{k}_{0,2l-1})\cdot\mathbf{r}_{a,2l-1}]+\sum_{l=1}^{n}[(\mathbf{k}_{0,2l-1}-\mathbf{k}_{0,2l})\cdot\mathbf{r}_{b,2l}] \quad (5a)$$

$$\varphi_{2n+1}=\varphi_{2n}+[(\mathbf{k}_{0,2n}-\mathbf{k}_{0,2n+1})\cdot\mathbf{r}_{a,2n+1}]. \quad (5b)$$

Here, the amplitude d_0 is replaced by the expression $C_0E_e\exp[i\{(\mathbf{K}_e-\mathbf{k}_0)\cdot\mathbf{r}_e\}]$, which is obtained from equation (I·6a). In equations (5a and b), $\mathbf{r}_{a,m}$ can be replaced by any position vector $\mathbf{r}_a$ on the surface S_a because the tangential continuity of the wave vectors requires that $\mathbf{k}_{0,2n-2}-\mathbf{k}_{0,2n-1}$ is perpendicular to S_a. For the same reason, $\mathbf{r}_{b,m}$ can be replaced by $\mathbf{r}_b$.

By multiplying the amplitude ratio by equations (4a and b), G waves are obtained as follows,

$$d_{g,2n}=\frac{2\Delta\eta_{0,2n}}{KC\chi_{-g}}\prod_{l=1}^{n}\frac{\Delta\eta_{0,2l-1}}{\Delta\eta_{0,2l}}\,C_0E_e\exp(i\varphi_{2n}) \quad (6a)$$

$$d_{g,2n+1}=-\frac{2\Delta\eta_{0,2n+1}}{KC\chi_{-g}}\prod_{l=1}^{n}\frac{\Delta\eta_{0,2l-1}}{\Delta\eta_{0,2l}}\,C_0E_e\exp(i\varphi_{2n+1}). \quad (6b)$$

As explained in Appendix A, Resonanzfehler of the repeatedly reflected fields satisfy a set of recurrence formulae [*cf.* equations (A7)]. Thus, they can be represented by the Resonanzfehler of the initial Bloch waves, $\Delta\eta_0$ and $\Delta\eta_g$, as follows.

$$\Delta\eta_{0,2n}=\left(\frac{\gamma_g'}{\gamma_0'}\,\frac{\gamma_0''}{\gamma_g''}\right)^n\Delta\eta_0 \quad (7a)$$

$$\Delta\eta_{g,2n}=\left(\frac{\gamma_0'}{\gamma_g'}\,\frac{\gamma_g''}{\gamma_0''}\right)^n\Delta\eta_g \quad (7b)$$

$$\Delta\eta_{0,2n+1}=-\frac{\gamma_0'}{\gamma_g'}\left(\frac{\gamma_0'}{\gamma_g'}\,\frac{\gamma_g''}{\gamma_0''}\right)^n\Delta\eta_g \quad (7c)$$

$$\Delta\eta_{g,2n+1}=-\frac{\gamma_g'}{\gamma_0'}\left(\frac{\gamma_g'}{\gamma_0'}\,\frac{\gamma_0''}{\gamma_g''}\right)^n\Delta\eta_0. \quad (7d)$$

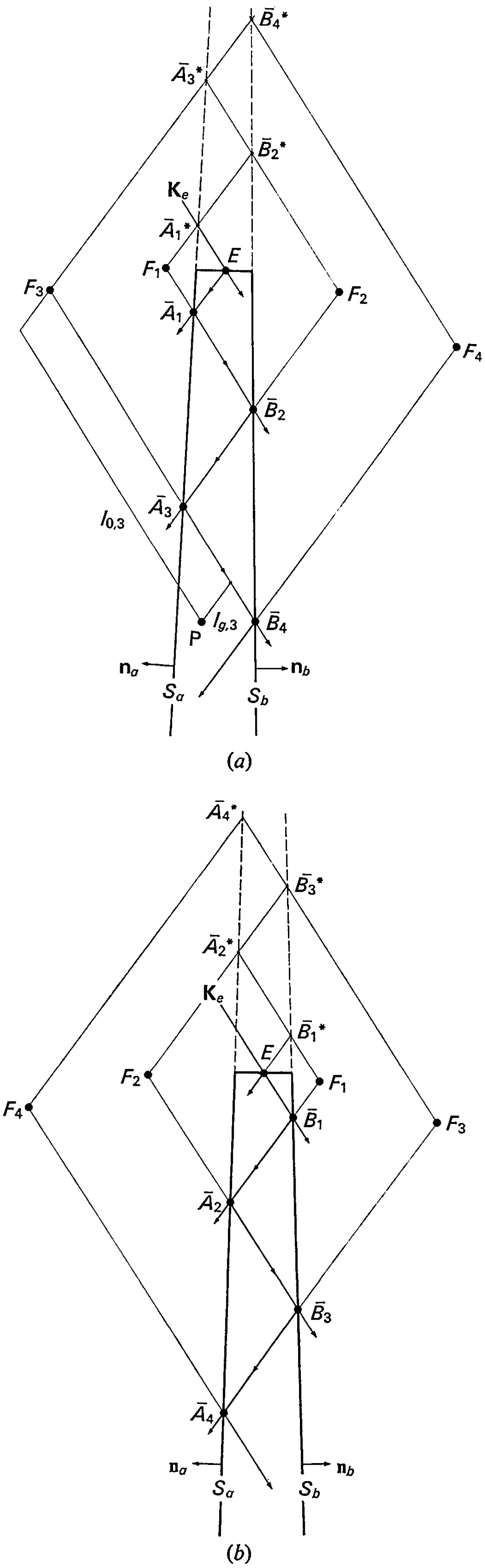

Fig. 1. The Laue-(Bragg)^m cases. (a) Type I, (b) Type II.

Since C_0, $\Delta\eta_0$ and $\Delta\eta_g$ are expressed in terms of the deviation parameter s (*cf.* Tables 1 and 4 of Part I), the wave fields can be written as,

$$d_{0,2n}(\mathbf{r})=\tfrac{1}{2}\Gamma_{0,n}\frac{(-s\pm\sqrt{s^2+\beta^2})^{2n+1}}{\beta^{2n}(\pm\sqrt{s^2+\beta^2})} \times \exp(i\varphi_{2n})\exp[i(\mathbf{k}_{0,2n}\cdot\mathbf{r})]E_e \tag{8a}$$

$$d_{0,2n+1}(\mathbf{r})=-\tfrac{1}{2}\Gamma_{0,n}\frac{(-s\pm\sqrt{s^2+\beta^2})^{2n+1}}{\beta^{2n}(\pm\sqrt{s^2+\beta^2})} \times \exp(i\varphi_{2n+1})\exp[i(\mathbf{k}_{0,2n+1}\cdot\mathbf{r})]E_e \tag{8b}$$

$$d_{g,2n}(\mathbf{r})=\tfrac{1}{2}\left(\frac{\chi_g}{\chi_{-g}}\right)^{\frac{1}{2}}\left(\frac{\gamma_0}{\gamma_g}\right)^{\frac{1}{2}}\Gamma_{g,n}\frac{(-s\pm\sqrt{s^2+\beta^2})^{2n}}{\beta^{2n-1}(\pm\sqrt{s^2+\beta^2})} \times \exp(i\varphi_{2n})\exp[i(\mathbf{k}_{g,2n}\cdot\mathbf{r})]E_e \tag{8c}$$

$$d_{g,2n+1}(\mathbf{r})=-\tfrac{1}{2}\left(\frac{\chi_g}{\chi_{-g}}\right)^{\frac{1}{2}}\left(\frac{\gamma_0}{\gamma_g}\right)^{\frac{1}{2}}\Gamma_{g,n+1} \times\frac{(-s\pm\sqrt{s^2+\beta^2})^{2n+2}}{\beta^{2n+1}(\pm\sqrt{s^2+\beta^2})}\exp(i\varphi_{2n+1}) \times\exp[i(\mathbf{k}_{g,2n+1}\cdot\mathbf{r})]E_e \tag{8d}$$

where

$$\Gamma_{0,n}=\left(-\frac{\gamma_0'}{\gamma_g'}\right)^n\left(\frac{\gamma_0'}{\gamma_g'}\frac{\gamma_g''}{\gamma_0''}\right)^{n^2}\left(\frac{\gamma_g}{\gamma_0}\right)^n \tag{9a}$$

$$\Gamma_{g,n}=\left(-\frac{\gamma_0'}{\gamma_g'}\right)^n\left(\frac{\gamma_0'}{\gamma_g'}\frac{\gamma_g''}{\gamma_0''}\right)^{n^2-n}\left(\frac{\gamma_g}{\gamma_0}\right)^n. \tag{9b}$$

As shown in Appendix *B*, the phase term $\{\varphi_m+(\mathbf{k}_{0,m}\cdot\mathbf{r})\}$ in equations (8) is expressed in terms of s in the simple form,

$$\varphi_m+(\mathbf{k}_{0,m}\cdot\mathbf{r})=P+K_yy+K_zz \pm\eta_{1,m}\sqrt{s^2+\beta^2}-\eta_{2,m}s \tag{10}$$

where $\eta_{1,m}\pm\eta_{2,m}$ have the same meanings as $\eta_1\pm\eta_2$ in the Laue–Bragg case and their explicit formulae are given by equations (*B*8).

So far the plane-wave theory has been developed. Now the spherical-wave theory will be described. The spherical-wave solution is given by the Fourier transform of the plane-wave solution, as in the case of Laue–Bragg. The required integrals are also represented by Bessel functions in the present case (see Appendix *A* of Part I). As a result, the wave fields have the following forms, similar to those in the Laue–Bragg case. In the region $\eta_1^2-\eta_2^2>0$:

$$\phi_{0,2n}(\mathbf{r})=(i)^{2n+2}\pi\beta\left(\frac{\eta_1-\eta_2}{\eta_1+\eta_2}\right)^{n+\frac{1}{2}} \times J_{2n+1}(\beta\sqrt{\eta_1^2-\eta_2^2})\Gamma_{0,n}\cdot B_0E_e \tag{11a}$$

$$\phi_{0,2n+1}(\mathbf{r})=(i)^{2n}\pi\beta\left(\frac{\eta_1-\eta_2}{\eta_1+\eta_2}\right)^{n+\frac{1}{2}} \times J_{2n+1}(\beta\sqrt{\eta_1^2-\eta_2^2})\Gamma_{0,n}\cdot B_0E_e \tag{11b}$$

$$\phi_{g,2n}(\mathbf{r})=(i)^{2n+1}\pi\beta_g\left(\frac{\chi_g}{\chi_{-g}}\right)^{\frac{1}{2}}\operatorname{sign}(\eta_1-\eta_2) \times\left(\frac{\eta_1-\eta_2}{\eta_1+\eta_2}\right)^n J_{2n}(\beta\sqrt{\eta_1^2-\eta_2^2})\Gamma_{g,n}\cdot B_gE_e \tag{11c}$$

$$\phi_{g,2n+1}(\mathbf{r})=(i)^{2n+1}\pi\beta_g\left(\frac{\chi_g}{\chi_{-g}}\right)^{\frac{1}{2}}\operatorname{sign}(\eta_1-\eta_2) \times\left(\frac{\eta_1-\eta_2}{\eta_1+\eta_2}\right)^{n+1} J_{2n+2}(\beta\sqrt{\eta_1^2-\eta_2^2}) \times\Gamma_{g,n+1}\cdot B_gE_e. \tag{11d}$$

In the region $\eta_1^2-\eta_2^2<0$:

$$\phi_{0,2n}(\mathbf{r})=0 \tag{12a}$$

$$\phi_{0,2n+1}(\mathbf{r})=0 \tag{12b}$$

$$\phi_{g,2n}(\mathbf{r})=0 \tag{12c}$$

$$\phi_{g,2n+1}(\mathbf{r})=0\quad. \tag{12d}$$

Here η_i is the abbreviation for $\eta_{i,2n}$ in equations (11*a* and *c*) and for $\eta_{i,2n+1}$ in equations (11*b* and *d*); $\Gamma_{0,n}$ and $\Gamma_{g,n}$ are given by equations (9*a* and *b*) and B_0 and B_g are given by equations (I·48*a* and *b*). As in the case of Laue–Bragg, we obtain

$$\eta_{1,m}^2-\eta_{2,m}^2=\frac{\gamma_0}{\gamma_g}x_{0,m}x_{g,m} \tag{13}$$

where $x_{0,m}$ and $x_{g,m}$ are the perpendiculars from an observation point to the lines $\bar{\mathbf{K}}_0$ and $\bar{\mathbf{K}}_g$ passing through the point F_m (see Appendix *B*).

Remembering that the wave fields given by equations (11) are constructed from the plane waves with the phase given by equation (10), and employing the stationary phase method, we can interpret each of the spherical-wave solutions as a bundle of rays. All of the rays which are reflected $2n$ or $2n+1$ times at the surfaces S_a and S_b pass through an imaginary source F_{2n} or F_{2n+1} and the bundle of the rays covers the triangular fan associated with the source F_{2n} or F_{2n+1}.

The wave field of Type II

The boundary conditions are given by

$$0=d_{0,2n-1}\exp[i(\mathbf{k}_{0,2n-1}\cdot\mathbf{r}_a)] +d_{0,2n}\exp[i(\mathbf{k}_{0,2n}\cdot\mathbf{r}_a)] \tag{14a}$$

$$0=d_{g,2n}\exp[i(\mathbf{k}_{g,2n}\cdot\mathbf{r}_b)] +d_{g,2n+1}\exp[i(\mathbf{k}_{g,2n+1}\cdot\mathbf{r}_b)]. \tag{14b}$$

By following the same procedure as for Type I, the wave fields are obtained. Since no new concept is required, only the final results are presented.

(i) *Plane-wave solution*:

$$d_{0,2n}(\mathbf{r})=\tfrac{1}{2}\Gamma_{0,n}\frac{(s\pm\sqrt{s^2+\beta^2})^{2n-1}}{\beta^{2n-2}(\pm\sqrt{s^2+\beta^2})}\exp(i\varphi_{2n})\times\exp[i(\mathbf{k}_{0,2n}\cdot\mathbf{r})]E_e \quad (15a)$$

$$d_{0,2n+1}(\mathbf{r})=-\tfrac{1}{2}\Gamma_{0,n+1}\frac{(s\pm\sqrt{s^2+\beta^2})^{2n+1}}{\beta^{2n}(\pm\sqrt{s^2+\beta^2})}\times\exp(i\varphi_{2n+1})\exp[i(\mathbf{k}_{0,2n+1}\cdot\mathbf{r})]E_e \quad (15b)$$

$$d_{g,2n}(\mathbf{r})=\tfrac{1}{2}\left(\frac{\chi_g}{\chi_{-g}}\right)^{\frac{1}{2}}\left(\frac{\gamma_0}{\gamma_g}\right)^{\frac{1}{2}}\Gamma_{g,n}\frac{(s\pm\sqrt{s^2+\beta^2})^{2n}}{\beta^{2n-1}(\pm\sqrt{s^2+\beta^2})}\times\exp(i\varphi_{2n})\exp[i(\mathbf{k}_{g,2n}\cdot\mathbf{r})]E_e \quad (15c)$$

$$d_{g,2n+1}(\mathbf{r})=-\tfrac{1}{2}\left(\frac{\chi_g}{\chi_{-g}}\right)^{\frac{1}{2}}\left(\frac{\gamma_0}{\gamma_g}\right)^{\frac{1}{2}}\times\Gamma_{g,n}\frac{(s\pm\sqrt{s^2+\beta^2})^{2n}}{\beta^{2n-1}(\pm\sqrt{s^2+\beta^2})}\times\exp(i\varphi_{2n+1})\exp[i(\mathbf{k}_{g,2n+1}\cdot\mathbf{r})]E_e \quad (15d)$$

where

$$\Gamma_{0,n}=\left(-\frac{\gamma_g''}{\gamma_0''}\right)^n\left(\frac{\gamma_0'}{\gamma_g'}\frac{\gamma_g''}{\gamma_0''}\right)^{n2-n}\left(\frac{\gamma_0}{\gamma_g}\right)^n \quad (16a)$$

$$\Gamma_{g,n}=\left(-\frac{\gamma_g''}{\gamma_0''}\right)^n\left(\frac{\gamma_0'}{\gamma_g'}\frac{\gamma_g''}{\gamma_0''}\right)^{n2}\left(\frac{\gamma_0}{\gamma_g}\right)^n \quad (16b)$$

$$\varphi_{2n}=[(\mathbf{K}_e-\mathbf{k}_0)\cdot\mathbf{r}_e]+\sum_{l=1}^{n}[(\mathbf{k}_{0,2l-2}-\mathbf{k}_{0,2l-1})\cdot\mathbf{r}_b]+\sum_{l=1}^{n}[(\mathbf{k}_{0,2l-1}-\mathbf{k}_{0,2l})\cdot\mathbf{r}_a] \quad (17a)$$

$$\varphi_{2n+1}=\varphi_{2n}+[(\mathbf{k}_{0,2n}-\mathbf{k}_{0,2n+1})\cdot\mathbf{r}_b]\,. \quad (17b)$$

The phase term $\{\varphi_m+(\mathbf{k}_{0,m}\cdot\mathbf{r})\}$ in equations (15) is given in the same form as in equation (10) in the case of Type I. The explicit forms of $\eta_{1,m}\pm\eta_{2,m}$ in the present case are given by equations (B9).

(ii) *Spherical-wave solution*:

In the region $\eta_1^2-\eta_2^2>0$:

$$\phi_{0,2n}(\mathbf{r})=(i)^{2n}\pi\beta\left(\frac{\eta_1+\eta_2}{\eta_1-\eta_2}\right)^{n-\frac{1}{2}}\times J_{2n-1}(\beta\sqrt{\eta_1^2-\eta_2^2})\Gamma_{0,n}\cdot B_0E_e \quad (18a)$$

$$\phi_{0,2n+1}(\mathbf{r})=(i)^{2n}\pi\beta\left(\frac{\eta_1+\eta_2}{\eta_1-\eta_2}\right)^{n+\frac{1}{2}}\times J_{2n+1}(\beta\sqrt{\eta_1^2-\eta_2^2})\Gamma_{0,n+1}\cdot B_0E_e \quad (18b)$$

$$\phi_{g,2n}(\mathbf{r})=(i)^{2n+1}\pi\beta_g\left(\frac{\chi_g}{\chi_{-g}}\right)^{\frac{1}{2}}\operatorname{sign}(\eta_1+\eta_2)\left(\frac{\eta_1+\eta_2}{\eta_1-\eta_2}\right)^n\times J_{2n}(\beta\sqrt{\eta_1^2-\eta_2^2})\Gamma_{g,n}\cdot B_gE_e \quad (18c)$$

$$\phi_{g,2n+1}(\mathbf{r})=(i)^{2n+3}\pi\beta_g\left(\frac{\chi_g}{\chi_{-g}}\right)^{\frac{1}{2}}\operatorname{sign}(\eta_1+\eta_2)\left(\frac{\eta_1+\eta_2}{\eta_1-\eta_2}\right)^n\times J_{2n}(\beta\sqrt{\eta_1^2-\eta_2^2})\Gamma_{g,n}\cdot B_gE_e\,. \quad (18d)$$

In the region $\eta_1^2-\eta_2^2<0$:

$$\phi_{0,2n}(\mathbf{r})=0 \quad (19a)$$

$$\phi_{0,2n+1}(\mathbf{r})=0 \quad (19b)$$

$$\phi_{g,2n}(\mathbf{r})=0 \quad (19c)$$

$$\phi_{g,2n+1}(\mathbf{r})=0\,. \quad (19d)$$

In equations (18) the subscript $2n$ or $2n+1$ in η_i is omitted. These solutions, again, have the properties described in the case of Type I.

Vacuum waves

The vacuum wave fields in the Laue–(Bragg)^m cases are easily obtained for both Types I and II. The procedures are similar to those in the case of Laue–Bragg. The vacuum wave field specified by m is the transmitted wave of the G or O component of the crystal wave specified by $m-1$.

In the plane-wave theory, writing the transmitted waves through the surfaces S_a and S_b as

$$E_{g,t,m}\exp[i(\mathbf{K}_{g,t,m}\cdot\mathbf{r})]$$

and

$$E_{0,t,m}\exp[i(\mathbf{K}_{0,t,m}\cdot\mathbf{r})]$$

respectively, the amplitudes are determined by the additional boundary conditions;

$$E_{g,t,m}\exp[i(\mathbf{K}_{g,t,m}\cdot\mathbf{r}_a)]=d_{g,m-1}\exp[i(\mathbf{k}_{g,m-1}\cdot\mathbf{r}_a)]+d_{g,m}\exp[i(\mathbf{k}_{g,m}\cdot\mathbf{r}_a)] \quad (20a)$$

$$E_{0,t,m}\exp[i(\mathbf{K}_{0,t,m}\cdot\mathbf{r}_b)]=d_{0,m-1}\exp[i(\mathbf{k}_{0,m-1}\cdot\mathbf{r}_b)]+d_{0,m}\exp[i(\mathbf{k}_{0,m}\cdot\mathbf{r}_b)]\,. \quad (20b)$$

From these relations, it turns out that the transmitted wave $E_{g,t,m}(\mathbf{r})$ is represented by the wave fields $d_{g,m-1}(\mathbf{r}_a)$ and $d_{g,m}(\mathbf{r}_a)$. Similarly, $E_{0,t,m}(\mathbf{r})$ is represented by $d_{0,m-1}(\mathbf{r}_b)$ and $d_{0,m}(\mathbf{r}_b)$.

In the spherical-wave theory, the situation is exactly the same as that in the plane-wave theory. The transmitted wave fields are a projection of the crystal wave fields on the exit surface concerned along either the $\overline{\mathbf{K}}_0$ or $\overline{\mathbf{K}}_g$ direction.

Discussion

In this paper, the crystal and vacuum wave fields in the Laue–(Bragg)^m cases ($m=2,3,\ldots$) have been worked out. In the spherical-wave theory, as in the case of Laue–Bragg, each wave field is confined in a triangular fan, emitted from an imaginary focal point F_m. The wave fields for different m are very similar. The Bessel functions involved in the expression for the wave fields are listed in Table 1. Real crystal waves are the sum of the various wave fields. For instance, the wave field in the triangle $\bar{A}_1\bar{B}_2\bar{A}_3$ in Fig. 1(a) is the superposition of the Laue–Bragg waves and the wave emitted from the entrance point E under the Laue condition. Similarly the vacuum waves are also the superposition of many waves, each being specified by Laue–(Bragg)^m. A few experimental topics related to the present theory will be discussed in the following sections.

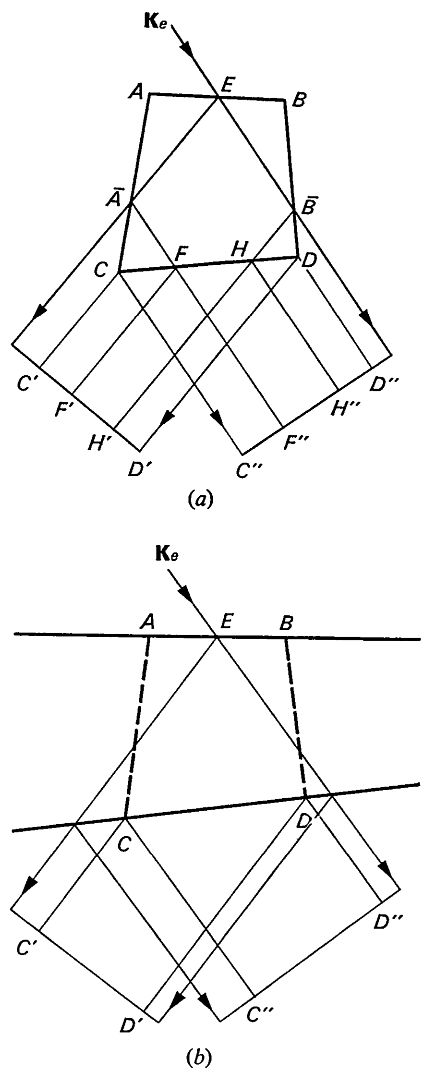

Fig. 2. Diffraction for a polyhedral crystal. (a) real case, (b) hypothetical case.

Table 1. *Bessel functions appearing in the wave fields of the Laue–(Bragg)^m cases*

	Type I		Type II	
	O	G	O	G
Laue	J_1	J_0	J_1	J_0
Laue–(Bragg)^{2n}	J_{2n+1}	J_{2n}	J_{2n-1}	J_{2n}
Laue–(Bragg)$^{2n+1}$	J_{2n+1}	J_{2n+2}	J_{2n+1}	J_{2n}

(a) *Diffraction phenomena in a finite polyhedral crystal*

In this section, we shall consider a crystal which has a polyhedral form. In Fig. 2(a), G waves come out from the crystal surface AC under the Laue–Bragg condition and from FH under the Laue–Laue condition. They can be treated straightforwardly using the formulations discussed under the heading 'The Laue–Bragg case; spherical-wave theory' in Part I and in the paper of Kato (1968) respectively. G waves penetrating the surface CF are a superposition of the Laue–Laue waves and the Laue–Bragg–Laue (Type I) waves in our present terminology. Similarly, G waves coming out from the surface HD are the Laue–Laue and the Laue–Bragg–Laue (Type II) waves. It is obvious that the Laue–Bragg–Laue waves are nothing more than the projected G waves of the Laue–Bragg waves on the final exit surface CD. In the same way, O waves coming through the surfaces BD and CD can be understood as the Laue–Bragg waves and a superposition of the Laue–Laue and the Laue–Bragg–Laue waves respectively. In more general cases, where the Laue–Bragg waves hit another crystal surface under the Bragg condition similar arguments can be applied.

A question may arise as to what integrated powers are expected in the case of Fig. 2(a). Since the wave fields mentioned above are rather complicated, the interference terms are neglected. In another words, the ray-optical viewpoint will be adopted in the following. In the non-absorbing crystal, the total powers of both O and G beams must be equal to those for the hypothetical crystal without lateral surfaces as shown in Fig. 2(b). This conclusion is obtained because energy conservation must hold on the surface in the Bragg case for both O and G waves.

In absorbing crystals the situation is different because, firstly, the optical distance of the reflected beam in the real crystal is different from that of the transmitted beam in the hypothetical crystal, and, secondly, the linear absorption coefficients of the Bloch waves concerned are different.* In the symmetrical case (with the surfaces AC and BD parallel to the lattice plane and the surface CD perpendicular to the lattice plane), the absorption coefficients and the optical distances in the real and hypothetical crystals become identical. Only in this special case, therefore, can the conclusion for the non-absorbing crystal be retained.

* The attenuation of the crystal wave is represented (Kato, 1968) by $\exp\{-K[I_m(\chi_0)\pm CI_m[(\chi_g\chi_{-g})^{1/2}](1-p^2)^{1/2}](l_0+l_g)\}$ in which $p=\tan\theta/\tan\theta_B$, θ being the angle between the ray direction and the lattice plane.

(b) Borrmann and Lehmann fringes

This study can be applied to the experiment reported by Borrmann & Lehmann (1963) and Lehmann & Borrmann (1967). They were concerned with highly absorbing crystals and they obtained the fringe patterns in the regions $C'F'$ and $C''F''$ in Fig. 2(*a*). The fringes were interpreted as the interference of Laue–Laue and Laue–Bragg–Laue (Type I) waves, using the present terminology. From the plane-wave theory they calculated the fringe spacing in a special case, *i.e.* AB, CD perpendicular to the lattice plane, AC parallel to the lattice plane. Using the results, they determined the structure factors from the spacing of fringes. The Pendellösung phenomena were neglected because of the rapid attenuation of branch (2) waves.* Our calculation is general for all magnitudes of absorption and for all geometrical relations between the lattice plane and the crystal surfaces.

Strictly speaking, moreover, the experiments of Lehmann & Borrmann should be interpreted by the spherical-wave theory developed in this article. In the spherical-wave theory, the wave fields are expressed as follows;

Laue–Laue

$$O:\ -J_1(\varrho_1)\simeq\sqrt{1/2\pi\varrho_1}\ (x_g/x_0)^{\frac{1}{2}}\,[\exp\{i(\varrho_1+\tfrac{1}{4}\pi)\}+\exp\{-i(\varrho_1+\tfrac{1}{4}\pi)\}] \tag{21a}$$

$$G:\ iJ_0(\varrho_1)\simeq\sqrt{1/2\pi\varrho_1}\ [\exp\{i(\varrho_1+\tfrac{1}{4}\pi)\}+\exp\{-i(\varrho_1+\tfrac{1}{4}\pi)\}] \tag{21b}$$

Laue–Bragg–Laue

$$O:\ J_1(\varrho_2)\simeq\sqrt{1/2\pi\varrho_2}(x_{0,r}/x_{g,r})^{\frac{1}{2}}\ [\exp\{i(\varrho_2-\tfrac{3}{4}\pi)\}+\exp\{-i(\varrho_2-\tfrac{3}{4}\pi)\}] \tag{21c}$$

$$G:\ iJ_2(\varrho_2)\simeq\sqrt{1/2\pi\varrho_2}(x_{0,r}/x_{g,r})\ [\exp\{i(\varrho_2-\tfrac{3}{4}\pi)\}+\exp\{-i(\varrho_2-\tfrac{3}{4}\pi)\}] \tag{21d}$$

where

$$\varrho_1=\beta_g\sqrt{x_0x_g} \tag{22a}$$

$$\varrho_2=\beta_g\sqrt{x_{0,r}x_{g,r}}\,. \tag{22b}$$

Here, the common phase factors and constant factors are omitted. For highly absorbing crystals, only the first terms in the brackets of equations (21) are to be considered. In O and G waves, the phase differences between the Laue–Laue and the Laue–Bragg–Laue waves are commonly given by $\varrho_1-\varrho_2+\pi$. Thus, it is concluded that O and G waves have maxima or minima of intensity at the same position. Furthermore, since ϱ_1 is equal to ϱ_2 on the exit surface AC, the O and G waves have a minimum at the crystal surface. The minimum value is zero for the O wave, whereas it is a finite value for the G wave. These arguments justify Lehmann & Borrmann's conclusions. The same situation holds in the case of Type II in the Laue–Bragg case and in more general cases discussed in the previous sections of this paper.

Finally, it seems worthwhile mentioning that the exit surfaces need not be vacuum-crystal boundaries. When the boundary is a stacking fault in which no total reflexion occurs, the crystal wave fields can be obtained by similar treatments. In the Laue case for the crystal–crystal boundary, Kato, Usami & Katagawa (1967) have already discussed the problem. The Bragg case will be reported in another paper.

* The authors have been informed that Uragami (1971) has succeeded in obtaining Pendellösung phenomena experimentally.

APPENDIX *A*

Resonanzfehler and Anpassungen of the wave fields reflected many times

(a) Type I

From the tangential continuity of the wave vectors at the exit surfaces, the following conditions must be satisfied for both O and G waves,

$$\mathbf{k}_{2n+1}=\mathbf{k}_{2n}+K\delta_{2n+1}\mathbf{n}_a \tag{A1a†}$$

$$\mathbf{k}_{2n}=\mathbf{k}_{2n-1}+K\delta_{2n}\mathbf{n}_b\,. \tag{A1b†}$$

The Resonanzfehler of the wave fields are defined by

$$\Delta\eta_{0,m}=[\mathring{\mathbf{K}}_0\,.\,(\mathbf{k}_m-\bar{\mathbf{k}})] \tag{A2a†}$$

$$\Delta\eta_{g,m}=[\mathring{\mathbf{K}}_g\,.\,(\mathbf{k}_m-\bar{\mathbf{k}})]\,. \tag{A2b†}$$

From equation (A1a) the following relations are obtained

$$\Delta\eta_{0,2n+1}=\Delta\eta_{0,2n}+K\delta_{2n+1}\gamma_0' \tag{A3a}$$

$$\Delta\eta_{g,2n+1}=\Delta\eta_{g,2n}+K\delta_{2n+1}\gamma_g'\,. \tag{A3b}$$

By virtue of the dispersion relation, $\Delta\eta_{0,2n+1}\,.\,\Delta\eta_{g,2n+1}=\Delta\eta_{0,2n}\,.\,\Delta\eta_{g,2n}$, $K\delta_{2n+1}$ is given by

$$K\delta_{2n+1}=-(\Delta\eta_{0,2n}/\gamma_0'+\Delta\eta_{g,2n}/\gamma_g')\,. \tag{A4}$$

Substituting equation (A4) into equations (A3a and b), one obtains the recurrence formulae of the Resonanzfehler

$$\Delta\eta_{0,2n+1}=-\frac{\gamma_0'}{\gamma_g'}\Delta\eta_{g,2n} \tag{A5a}$$

$$\Delta\eta_{g,2n+1}=-\frac{\gamma_g'}{\gamma_0'}\Delta\eta_{0,2n}\,. \tag{A5b}$$

From equation (A1b) $K\delta_{2n}$ is given by

$$K\delta_{2n}=-(\Delta\eta_{0,2n-1}/\gamma_0''+\Delta\eta_{g,2n-1}/\gamma_g'')\,. \tag{A6}$$

† Here, the subscript 0 or g of $\mathbf{k}_m$ and $\bar{\mathbf{k}}$ is omitted.

From this, another set of recurrence formulae is obtained as follows,

$$\Delta\eta_{0,2n} = -\frac{\gamma_0''}{\gamma_g''}\Delta\eta_{g,2n-1} \quad (A7a)$$

$$\Delta\eta_{g,2n} = -\frac{\gamma_g''}{\gamma_0''}\Delta\eta_{0,2n-1}\,. \quad (A7b)$$

By using equations ($A5$) and ($A7$) repeatedly, $\Delta\eta_{0,m}$ and $\Delta\eta_{g,m}$ are expressed in terms of the Resonanzfehler of the initial Bloch wave as shown in equations (7).

By the use of equations ($A4$), ($A6$) and (7), the Anpassungen $K\delta_m$ are also expressed in terms of $\Delta\eta_0$ and $\Delta\eta_g$, and consequently in terms of the deviation parameter s.

(*b*) *Type* II

The relations obtained for the wave fields in Type I are converted to the relations in Type II when $\mathbf{n}_a$ and $\mathbf{n}_b$ are interchanged. The modification required, therefore, is simply interchanging the single and double primes of γ_0 and γ_g in equations (7). The final results are read as

$$\Delta\eta_{0,2n} = \left(\frac{\gamma_0'}{\gamma_g'}\frac{\gamma_g''}{\gamma_0''}\right)^n\Delta\eta_0 \quad (A8a)$$

$$\Delta\eta_{g,2n} = \left(\frac{\gamma_g'}{\gamma_0'}\frac{\gamma_0''}{\gamma_g''}\right)^n\Delta\eta_g \quad (A8b)$$

$$\Delta\eta_{0,2n+1} = -\frac{\gamma_0''}{\gamma_g''}\left(\frac{\gamma_g'}{\gamma_0'}\frac{\gamma_0''}{\gamma_g''}\right)^n\Delta\eta_g \quad (A8c)$$

$$\Delta\eta_{g,2n+1} = -\frac{\gamma_g''}{\gamma_0''}\left(\frac{\gamma_0'}{\gamma_g'}\frac{\gamma_g''}{\gamma_0''}\right)^n\Delta\eta_0\,. \quad (A8d)$$

APPENDIX *B*

The evaluation of $\eta_{1,m}\pm\eta_{2,m}$ in the Laue-(Bragg)^m cases

(*a*) *Type* I

We shall define the points F_m as shown in Fig. 1(*a*) and the oblique coordinate system $\mathring{\mathbf{K}}_0$ and $\mathring{\mathbf{K}}_g$ whose origin is F_m. The coordinates are denoted by ($l_{0,m}$, $l_{g,m}$). For example, $l_{0,3}$ and $l_{g,3}$ are shown in Fig. 1(*a*).

The phases $\bar{\varphi}_m = \varphi_m + (\mathbf{k}_{0,m}\,.\,\mathbf{r})$ in equations (8*a* and *b*) are expressed in the following forms.

$$\bar{\varphi}_{2n+1} = \bar{\varphi}_{2n} + \{(\mathbf{k}_{0,2n+1} - \mathbf{k}_{0,2n})\,.\,(\mathbf{r}-\mathbf{r}_a)\} \quad (B1a)$$

$$\bar{\varphi}_{2n} = \bar{\varphi}_{2n-1} + \{(\mathbf{k}_{0,2n} - \mathbf{k}_{0,2n-1})\,.\,(\mathbf{r}-\mathbf{r}_b)\}\,. \quad (B1b)$$

The vectors $\mathbf{r}-\mathbf{r}_a$ and $\mathbf{r}-\mathbf{r}_b$ are expressed in terms of the oblique coordinates as follows [*cf.* equations (I.$B3a$ and b)].

$$\mathbf{r}-\mathbf{r}_a = l_{0,2n+1}\mathring{\mathbf{K}}_0 + l_{g,2n}\mathring{\mathbf{K}}_g \quad (\mathbf{r}_a \text{ fixed at } \bar{A}^*_{2n+1}) \quad (B2a)$$

$$= l_{0,2n}\mathring{\mathbf{K}}_0 + l_{g,2n+1}\mathring{\mathbf{K}}_g \quad (\mathbf{r}_a \text{ fixed at } \bar{A}_{2n+1}) \quad (B2b)$$

$$\mathbf{r}-\mathbf{r}_b = l_{0,2n-1}\mathring{\mathbf{K}}_0 + l_{g,2n}\mathring{\mathbf{K}}_g \quad (\mathbf{r}_b \text{ fixed at } \bar{B}^*_{2n}) \quad (B3a)$$

$$= l_{0,2n}\mathring{\mathbf{K}}_0 + l_{g,2n-1}\mathring{\mathbf{K}}_g \quad (\mathbf{r}_b \text{ fixed at } \bar{B}_{2n}) \quad (B3b)$$

Operating $[\,]_+$ on equations ($B1a$ and b) as in equation (I.$B7$) we obtain

$$[\bar{\varphi}_{2n+1}]_+ - [\bar{\varphi}_{2n}]_+ = \Delta\eta_{0,2n+1}l_{0,2n+1} - \Delta\eta_{g,2n}l_{g,2n} \quad (B4a)$$

$$[\bar{\varphi}_{2n}]_+ - [\bar{\varphi}_{2n-1}]_+ = \Delta\eta_{g,2n}l_{g,2n} - \Delta\eta_{0,2n-1}l_{0,2n-1}\,. \quad (B4b)$$

In deriving these, equations ($B2a$) and ($B3a$) are used. Repeating the same procedures we obtain

$$[\bar{\varphi}_{2n+1}]_+ = \Delta\eta_{0,2n+1}l_{0,2n+1} \quad (B5a)$$

$$[\bar{\varphi}_{2n}]_+ = \Delta\eta_{g,2n}l_{g,2n}\,. \quad (B5b)$$

Substituting equations ($B2b$) and ($B3b$) into equations ($B1$) and operating $[\,]_-$, we have

$$[\bar{\varphi}_{2n+1}]_- - [\bar{\varphi}_{2n}]_- = \Delta\eta_{g,2n+1}l_{g,2n+1} - \Delta\eta_{0,2n}l_{g,2n} \quad (B6a)$$

$$[\bar{\varphi}_{2n}]_- - [\bar{\varphi}_{2n-1}]_- = \Delta\eta_{0,2n}l_{0,2n} - \Delta\eta_{g,2n-1}l_{g,2n-1}\,. \quad (B6b)$$

Thus, $[\bar{\varphi}_m]_-$ are given by

$$[\bar{\varphi}_{2n+1}]_- = \Delta\eta_{g,2n+1}l_{g,2n+1} \quad (B7a)$$

$$[\bar{\varphi}_{2n}]_- = \Delta\eta_{0,2n}l_{0,2n}\,. \quad (B7b)$$

Finally, using equations (7) for $\Delta\eta_{0,m}$ and $\Delta\eta_{g,m}$ we obtain the forms for $\eta_{1,m}\pm\eta_{2,m}$ as follows.

$$\eta_{1,2n}+\eta_{2,2n} = \left(\frac{\gamma_0'}{\gamma_g'}\frac{\gamma_g''}{\gamma_0''}\right)^n x_{0,2n} \quad (B8a)$$

$$\eta_{1,2n+1}+\eta_{2,2n+1} = -\frac{\gamma_0'}{\gamma_g'}\left(\frac{\gamma_0'}{\gamma_g'}\frac{\gamma_g''}{\gamma_0''}\right)^n x_{g,2n+1} \quad (B8b)$$

$$\eta_{1,2n}-\eta_{2,2n} = \frac{\gamma_0}{\gamma_g}\left(\frac{\gamma_g'}{\gamma_0'}\frac{\gamma_0''}{\gamma_g''}\right)^n x_{g,2n} \quad (B8c)$$

$$\eta_{1,2n+1}-\eta_{2,2n+1} = -\frac{\gamma_0}{\gamma_g}\frac{\gamma_g'}{\gamma_0'}\left(\frac{\gamma_g'}{\gamma_0'}\frac{\gamma_0''}{\gamma_g''}\right)^n x_{0,2n+1} \quad (B8d)$$

where $x_{0,m}$ and $x_{g,m}$ are the perpendiculars to the coordinate axes, $\mathring{\mathbf{K}}_0$ and $\mathring{\mathbf{K}}_g$ respectively.

(*b*) *Type* II

In this case, the points F_m are defined as shown in Fig. 1(*b*). The quantities $l_{0,m}$ and $l_{g,m}$ have the same meanings as for Type I. In those oblique coordinates the vectors $\mathbf{r}_a$ and $\mathbf{r}_b$ must be interchanged in equations ($B1$), ($B2$) and ($B3$). Thus, the results for Type I can be converted to the case of Type II by interchanging the single and double primes. Finally $\eta_{1,m}\pm\eta_{2,m}$ are given by

$$\eta_{1,2n}+\eta_{2,2n} = \left(\frac{\gamma_g'}{\gamma_0'}\frac{\gamma_0''}{\gamma_g''}\right)^n x_{0,2n} \quad (B9a)$$

$$\eta_{1,2n+1}+\eta_{2,2n+1} = -\frac{\gamma_0''}{\gamma_g''}\left(\frac{\gamma_g'}{\gamma_0'}\frac{\gamma_0''}{\gamma_g''}\right)^n x_{g,2n+1} \quad (B9b)$$

$$\eta_{1,2n}-\eta_{2,2n} = \frac{\gamma_0}{\gamma_g}\left(\frac{\gamma_0'}{\gamma_g'}\frac{\gamma_g''}{\gamma_0''}\right)^n x_{g,2n} \quad (B9c)$$

$$\eta_{1,2n+1}-\eta_{2,2n+1}=-\frac{\gamma_0}{\gamma_g}\frac{\gamma_g''}{\gamma_0''}\left(\frac{\gamma_0'}{\gamma_g'}\frac{\gamma_g''}{\gamma_0''}\right)^n x_{0,2n+1}\,. \quad (B9d)$$

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The One-Dimensional Anti-phase Domain Structures. II. Refinement of Fujiwara's Method of the Analysis of the Structure with a Non-integral Value for the Half Period, $\tilde{M}$

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(*Received* 15 *May* 1971 *and in revised form* 19 *August* 1971)

One-dimensional anti-phase domain structures with an out-of-step vector $\mathbf{u}=(\mathbf{a}+\mathbf{b})/2$ sometimes have half periods of non-integral value. Fujiwara interpreted this structure as a disordered structure (a *statistical assembly*) deviating from a *standard structure* which he defined by a step function. In the present paper, it is pointed out that the unitary intensity of a superlattice reflexion for the standard structure is obtained in a much simpler form than that given by Fujiwara. By the use of this intensity formula we verify the fact that a pair of intensities with special l-indices, ν and $-\nu$, is very strong while the others are extremely weak, so that we apparently obtain a non-integral value for the half period from the strongest pair. The statistical assembly, *i.e.* the disordered structure presented by Fujiwara, is interpreted using an easily understandable model, and a simple form of the corresponding intensity formula is obtained, which indicates that the intensities other than the pair, $\bar{I}_\nu$ and $\bar{I}_{\bar{\nu}}$, practically vanish. This fact implies that the non-integral half period, $\tilde{M}$, may be obtained experimentally from a pair of satellites corresponding to $\bar{I}_\nu$ and $\bar{I}_{\bar{\nu}}$. Some important remarks are made in the Appendix concerning the Fourier expansion of the step function.

1. Introduction

In part I of this series (Kakinoki & Minagawa, 1971) the one-dimensional anti-phase domain structures, with an out-of-step vector $\mathbf{u}=(\mathbf{a}+\mathbf{b})/2$ and the corresponding phase factor $\varepsilon=(-1)^{h+k}$, were classified into three kinds, and they were denoted by the layer sequence symbols which are similar to the Zhdanov symbol for the close-packed structures, as follows:

(1) the complex out-of-step structure, denoted by

$$(a_1\bar{b}_1a_2\bar{b}_2\ldots a_t\bar{b}_t) \text{ with } P=\sum_{i=1}^{t}(a_i+b_i)\,,$$

(2) the complex *APD* (anti-phase domain) structure, denoted by

$$([M]|[\bar{M}]) \text{ with } [M]=(a_1\bar{b}_1a_2\bar{b}_2\ldots a_s\bar{b}_sa_{s+1})$$

and

$$P/2=M=\sum_{i=1}^{s+1}a_i+\sum_{i=1}^{s}b_i\,,$$

(3) the simple *APD* structure, denoted by

$$(M|\bar{M}) \text{ with } P=2M,$$

where P is the period and a_i and b_i are the numbers of successive positive and negative layers respectively, where the positive and negative layers indicate the layers without and with the out-of-step vector, as shown in Fig. 1. The vertical and horizontal short lines in the symbols $([M]|[\bar{M}])$ and $(M|\bar{M})$ mean that the last M layers are obtained by changing all the signs of the corresponding layers of the first M layers.

The unitary intensities of superlattice reflexions in the case of simple APD structure are given by†

$$\left.\begin{aligned}&\begin{cases}I_l=0 & \text{for } l\text{: even}\\ I_l=4I_l^* & \text{for } l\text{: odd}\end{cases}\\ &\text{with}\quad I_l^*=\frac{1}{\sin^2\frac{\pi l}{P}}\,.\end{aligned}\right\} \quad (1)$$

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† Refer to equations (I.16), (I.18) and (I.19). In order to avoid confusion, the equation number in part I of this series is written as (I.1), (I.2) *etc.*, and that in Fujiwara's (1957) paper as (F1), (F2) *etc.*