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Effect of Heavy Atoms on the Two-Phase Structure Seminvariant $\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}$ in $P\bar{1}$*

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Abstract

A crystal structure in $P\bar{1}$ consisting of P heavy atoms and Q light atoms in the unit cell is considered, and the random variable vectors $\mathbf{h}$ and $\mathbf{k}$, subject to well defined restrictions, are uniformly and independently distributed in reciprocal space. The linear combination of two phases $\psi=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}$ is a structure seminvariant if and only if $\mathbf{h}+\mathbf{k}=0$ (mod $\boldsymbol{\omega}$) where $\boldsymbol{\omega}=(2, 2, 2)$. $E_{\mathbf{h}}$ and $E_{\mathbf{k}}$ are the two normalized structure factors associated with phases $\varphi_{\mathbf{h}}$ and $\varphi_{\mathbf{k}}$ and $E^P_{\mathbf{h}}$ and $E^P_{\mathbf{k}}$ are the contributions of the heavy atoms respectively. The first neighborhood of ψ consists of the four magnitudes $|E_{\mathbf{h}}|$, $|E_{\mathbf{k}}|$, $|E_{(\mathbf{h}+\mathbf{k})/2}|$, $|E_{(\mathbf{h}-\mathbf{k})/2}|$. The conditional probability distribution of ψ, given the four magnitudes $|E_{\mathbf{h}}|$, $|E_{\mathbf{k}}|$, $|E_{(\mathbf{h}+\mathbf{k})/2}|$, $|E_{(\mathbf{h}-\mathbf{k})/2}|$ and the known contributions $E^P_{\mathbf{h}}$, $E^P_{\mathbf{k}}$ from the heavy atoms, is derived to the approximation of $1/N$. In favorable cases, *i.e.* when phase indications from the four-magnitude neighborhood of the seminvariant and the heavy-atom contributions coincide, a reliable estimate for ψ is obtained. The result obtained is applied to the structure of a derivative of β-lactam and its usefulness is demonstrated.

1. Introduction

The use of the structure seminvariant in direct methods of crystal structure analysis is well known. The probability methods have been applied to derive the conditional distribution of the two-phase structure seminvariant (Hauptman, 1976; Green & Hauptman, 1976). Hauptman (1975) formulated the neighborhood concept in order to identify the small sets of magnitude $|E|$ on which the value of any structure seminvariant most sensitively depends. In a crystal in which one heavy atom or a few heavy atoms are present, it is often possible to locate the heavy atoms by the Patterson method, or a part of the structure can be recognized in the Fourier synthesis. The estimation of the structure seminvariants is likely to be more reliable when the contribution of the heavy atoms (or known fragment) is also taken into account.

In a recent paper Giacovazzo (1983) has applied the joint probability distribution method to estimate phases when part of the crystal structure is correctly positioned. In this paper we consider the effect of heavy atoms or known fragment on two normalized structure factors associated with the structure seminvariants to arrive at an expression that gives the probability that the sign of $E_{\mathbf{h}}E_{\mathbf{k}}$ is positive. The final result so obtained has been tested on the structure of a derivative of β-lactam and the anticipated improvement in the estimate of the seminvariants is in fact realized.

2. Derivation of the formula

In space group $P\bar{1}$ the linear combination

$$\psi=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}} \tag{1}$$

is a structure seminvariant if and only if

$$\mathbf{h}+\mathbf{k}=0 \ (\mathrm{mod}\ \boldsymbol{\omega}), \tag{2}$$

where $\boldsymbol{\omega}$ is the three-dimensional vector defined by

$$\boldsymbol{\omega}=(2, 2, 2). \tag{3}$$

Consider a crystal structure consisting of P heavy atoms (known) and Q light atoms (unknown) in the unit cell such that $P+Q=N$, where N is the total number of atoms in the unit cell. The normalized structure factors of reflections $\mathbf{h}$ (h_1, k_1, l_1) and $\mathbf{k}$ (h_2, k_2, l_2) can be written as

$$\sigma_2^{1/2}E_{\mathbf{h}}=\sigma_{2P}^{1/2}E^P_{\mathbf{h}}+\sigma_{2Q}^{1/2}E^Q_{\mathbf{h}} \tag{4}$$

$$\sigma_2^{1/2}E_{\mathbf{k}}=\sigma_{2P}^{1/2}E^P_{\mathbf{k}}+\sigma_{2Q}^{1/2}E^Q_{\mathbf{k}}, \tag{5}$$

where

$$\sigma_n=\sum_{j=1}^{N} f_j^n,\ \sigma_{nP}=\sum_{j=1}^{P} f_j^n,\ \sigma_{nQ}\sum_{j=P+1}^{N} f_j^n,$$
$$n=1, 2, 3, \ldots. \tag{6}$$

$f_1, \ldots, f_N$ are the atomic numbers and E^P and E^Q are the heavy- and light-atom contributions to E, respectively. The first neighborhood of ψ consists of the four magnitudes $|E_{\mathbf{h}}|$, $|E_{\mathbf{k}}|$, $|E_{(\mathbf{h}+\mathbf{k})/2}|$, $|E_{(\mathbf{h}-\mathbf{k})/2}|$ (Hauptman, 1976).

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2.1. *The joint probability distribution of the six normalized structure factors* $E_{\mathbf{h}}$, $E_{\mathbf{k}}$, $E_{(\mathbf{h}+\mathbf{k})/2}$, $E_{(\mathbf{h}-\mathbf{k})/2}$, $E^P_{\mathbf{h}}$, $E^P_{\mathbf{k}}$

The joint probability distribution of the six normalized structure factors $E_{\mathbf{h}}$, $E_{\mathbf{k}}$, $E_{(\mathbf{h}+\mathbf{k})/2}$, $E_{(\mathbf{h}-\mathbf{k})/2}$, $E^P_{\mathbf{h}}$, $E^P_{\mathbf{k}}$ is denoted by

$$\mathcal{P}=\mathcal{P}(S_1, S_2, S_{12/2}, S_{1\bar{2}/2}, S_{1P}, S_{2P}), \qquad (7)$$

where $S_1=R_1\cos\varphi_1$, $S_2=R_2\cos\varphi_2$, $S_{12/2}=R_{12/2}\cos\varphi_{12/2}$, $S_{1\bar{2}/2}=R_{1\bar{2}/2}\cos\varphi_{1\bar{2}/2}$, $S_{1P}=R_{1P}\cos\varphi_{1P}$, $S_{2P}=R_{2P}\cos\varphi_{2P}$. Following a method suggested by Hauptman (1983), it is found that, retaining terms up to the approximation of $1/N$,

$$\begin{aligned}\mathcal{P}=(\tfrac{1}{2}\pi)^3\Big\{\exp\Big[&-\tfrac{1}{2}(S_1^2+S_2^2+S_{12/2}^2+S_{1\bar{2}/2}^2+S_{1P}^2+S_{2P}^2)\\
&-\frac{13\sigma_4}{8\sigma_2^2}+\frac{\sigma_4}{\sigma_2^2}(5S_1^2+5S_2^2+7S_{12/2}^2+7S_{1\bar{2}/2}^2)\\
&-\frac{\sigma_4}{8\sigma_2^2}(S_1^4+S_2^4+S_{12/2}^4+S_{1\bar{2}/2}^4+4S_1^2S_{12/2}^2\\
&+4S_1^2S_{1\bar{2}/2}^2+4S_2^2S_{12/2}^2+4S_1^2S_{1\bar{2}/2}^2+8S_{12/2}^2S_{1\bar{2}/2}^2)\\
&+\frac{\sigma_3}{\sigma_2^{3/2}}S_1S_{12/2}S_{1\bar{2}/2}+\frac{\sigma_3}{\sigma_2^{3/2}}S_2S_{12/2}S_{1\bar{2}/2}\\
&+\left(\frac{\sigma_4}{2\sigma_2^2}-\frac{\sigma_3^2}{\sigma_2^3}\right)S_1S_2S_{12/2}^2+\left(\frac{\sigma_4}{2\sigma_2^2}-\frac{\sigma_3^2}{\sigma_2^3}\right)S_1S_2S_{1\bar{2}/2}^2\\
&+\frac{\sigma_{3P}}{\sigma_{2P}^{1/2}\sigma_2}S_{1P}S_{12/2}S_{1\bar{2}/2}+\frac{\sigma_{3P}}{\sigma_{2P}^{1/2}\sigma_2}S_{2P}S_{12/2}S_{1\bar{2}/2}\\
&+\frac{\sigma_{4P}}{2\sigma_{2P}\sigma_2}S_{1P}S_{2P}S_{12/2}^2+\frac{\sigma_{4P}}{2\sigma_{2P}\sigma_2}S_{1P}S_{2P}S_{1\bar{2}/2}^2\Big]\Big\}.\end{aligned} \qquad (8)$$

The distribution (8) leads directly to the joint conditional probability distribution of the pair $\varphi_{\mathbf{h}}$, $\varphi_{\mathbf{k}}$, given S_{1P}, S_{2P} and the magnitudes of the four structure factors $E_{\mathbf{h}}$, $E_{\mathbf{k}}$, $E_{(\mathbf{h}+\mathbf{k})/2}$ and $E_{(\mathbf{h}-\mathbf{k})/2}$.

2.2. *The joint conditional probability distribution of the pair of phases* $\varphi_{\mathbf{h}}$, $\varphi_{\mathbf{k}}$ *given the four magnitudes* $|E_{\mathbf{h}}|$, $|E_{\mathbf{k}}|$, $|E_{(\mathbf{h}\pm\mathbf{k})/2}|$ *and the known part* $E^P_{\mathbf{h}}$, $E^P_{\mathbf{k}}$ *of the heavy-atom contribution*

Let $|E_{\mathbf{h}}|=R_1$, $|E_{\mathbf{k}}|=R_2$, $|E_{(\mathbf{h}+\mathbf{k})/2}|=R_{12/2}$, $|E_{(\mathbf{h}-\mathbf{k})/2}|=R_{1\bar{2}/2}$ be the magnitudes of the structure factors and $\varphi_{\mathbf{h}}$, $\varphi_{\mathbf{k}}$ be the phases of the normalized structure factors $E_{\mathbf{h}}$ and $E_{\mathbf{k}}$, which themselves are random variables. The joint conditional probability distribution of the two phases $\varphi_{\mathbf{h}}$ and $\varphi_{\mathbf{k}}$ given R_1, R_2, $R_{12/2}$, $R_{1\bar{2}/2}$ and S_{1P}, S_{2P} is denoted by $P(\varphi_1, \varphi_2|R_1, R_2, R_{12/2}, R_{1\bar{2}/2}, S_{1P}, S_{2P})$ and is found from (8) by fixing S_{1P}, S_{2P} and the magnitudes of S_1, S_2, $S_{12/2}$, $S_{1\bar{2}/2}$ and summing with respect to $\varphi_{12/2}$, $\varphi_{1\bar{2}/2}$ over their two possible values 0 and π, and multiplying by a suitable normalizing constant K. Thus,

$$\begin{aligned}\mathcal{P}&(\varphi_1, \varphi_2|R_1, R_2, R_{12/2}, R_{1\bar{2}/2}, S_{1P}, S_{2P})\\
&=\frac{1}{K}\exp\left[\left(\frac{\sigma_4}{2\sigma_2^2}-\frac{\sigma_3^2}{\sigma_2^3}\right)R_1R_2\right.\\
&\qquad\left.\times\cos(\varphi_1+\varphi_2)(R_{12/2}^2+R_{1\bar{2}/2}^2)\right]\\
&\quad\times\cosh\left[\frac{\sigma_3}{\sigma_2^{3/2}}R_{12/2}R_{1\bar{2}/2}(R_1\cos\varphi_1+R_2\cos\varphi_2)\right]\\
&\quad\times\exp\left[\frac{\sigma_{4P}}{2\sigma_{2P}\sigma_2}S_{1P}S_{2P}(R_{12/2}^2+R_{1\bar{2}/2}^2)\right]\\
&\quad\times\cosh\left[\frac{\sigma_{3P}}{\sigma_{2P}^{1/2}\sigma_2}R_{12/2}R_{1\bar{2}/2}(S_{1P}+S_{1P})\right],\end{aligned} \qquad (9)$$

where K is a suitable normalizing constant independent of φ_1 and φ_2.

2.3. *The conditional probability distribution of the structure seminvariant* $\psi=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}$, *given the four magnitudes* $|E_{\mathbf{h}}|$, $|E_{\mathbf{k}}|$, $|E_{(\mathbf{h}+\mathbf{k})/2}|$, $|E_{(\mathbf{h}-\mathbf{k})/2}|$ *and the known part* S_{1P}, S_{2P} *of the heavy-atom contribution*

The structure seminvariant $\psi=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}$ is a random variable whose conditional probability distribution is found from (9). Thus,

$$\begin{aligned}\mathcal{P}&(\psi|R_1, R_2, R_{12/2}, R_{1\bar{2}/2}, S_{1P}, S_{2P})\\
&=\frac{1}{M}\exp\left[\left(\frac{\sigma_4}{2\sigma_2^2}-\frac{\sigma_3^2}{\sigma_2^3}\right)\right.\\
&\qquad\left.\times R_1, R_2\cos\psi(R_{12/2}^2+R_{1\bar{2}/2}^2)\right]\\
&\quad\times\cosh\left[\frac{\sigma_3}{\sigma_2^{3/2}}R_{12/2}R_{1\bar{2}/2}(R_1+R_2\cos\psi)\right]\\
&\quad\times\exp\left[\frac{\sigma_{4P}}{2\sigma_{2P}\sigma_2}S_{1P}S_{2P}(R_{12/2}^2+R_{1\bar{2}/2}^2)\right]\\
&\quad\times\cosh\left[\frac{\sigma_{3P}}{\sigma_{2P}^{1/2}\sigma_2}R_{12/2}R_{1\bar{2}/2}(S_{1P}+S_{2P})\right],\end{aligned} \qquad (10)$$

where

$$\begin{aligned}M&=\exp\left[\left(\frac{\sigma_4}{2\sigma_2^2}-\frac{\sigma_3^2}{\sigma_2^3}\right)R_1R_2(R_{12/2}^2+R_{1\bar{2}/2}^2)\right]\\
&\quad\times\cosh\left[\frac{\sigma_3}{\sigma_2^{3/2}}R_{12/2}R_{1\bar{2}/2}(R_1+R_2)\right]\\
&\quad\times\exp\left[\frac{\sigma_{4P}}{2\sigma_{2P}\sigma_2}|S_{1P}||S_{2P}|(R_{12/2}^2+R_{1\bar{2}/2}^2)\right]\\
&\quad\times\cosh\left[\frac{\sigma_{3P}}{\sigma_{2P}^{1/2}\sigma_2}R_{12/2}R_{1\bar{2}/2}(|S_{1P}|+|S_{2P}|)\right]\\
&\quad+\exp\left[-\left(\frac{\sigma_4}{2\sigma_2^2}-\frac{\sigma_3^2}{\sigma_2^3}\right)R_1R_2(R_{12/2}^2+R_{1\bar{2}/2}^2)\right]\end{aligned}$$

$$\times\cosh\left[\frac{\sigma_3}{\sigma_2^{3/2}}R_{12/2}R_{1\bar{2}/2}(R_1-R_2)\right]$$
$$\times\exp\left[-\frac{\sigma_{4P}}{2\sigma_{2P}\sigma_2}|S_{1P}||S_{2P}|(R^2_{12/2}+R^2_{1\bar{2}/2})\right]$$
$$\times\cosh\left[\frac{\sigma_{3P}}{\sigma_{2P}^{1/2}\sigma_2}R_{12/2}R_{1\bar{2}/2}(|S_{1P}|+|S_{2P}|)\right]. \qquad (11)$$

If $\mathscr{P}_+(\mathscr{P}_-)$ denotes the conditional probability that

$$\cos\psi=+1(-1), \qquad (12)$$

then (10) is replaced by

$$\mathscr{P}_\pm=\frac{1}{M}\exp\left[\pm\left(\frac{\sigma_4}{2\sigma_2^2}-\frac{\sigma_3^2}{\sigma_2^3}\right)R_1R_2(R^2_{12/2}+R^2_{1\bar{2}/2})\right]$$
$$\times\cosh\left[\frac{\sigma_3}{\sigma_2^{3/2}}R_{12/2}R_{1\bar{2}/2}(R_1\pm R_2)\right]$$
$$\times\exp\left[\frac{\sigma_{4P}}{2\sigma_{2P}\sigma_2}S_{1P}S_{2P}(R^2_{12/2}+R^2_{1\bar{2}/1})\right]$$
$$\times\cosh\left[\frac{\sigma_{3P}}{\sigma_{2P}^{1/2}\sigma_2}R_{12/2}R_{1\bar{2}/2}(S_{1P}+S_{2P})\right], \qquad (13)$$

where upper (lower) signs go together. If $R_{12/2}R_{1\bar{2}/2}\simeq 0$, then

$$\mathscr{P}_\pm=\frac{1}{M}\exp\left[\pm\left(\frac{\sigma_4}{2\sigma_2^2}-\frac{\sigma_3^2}{\sigma_2^3}\right)R_1R_2(R^2_{12/2}+R^2_{1\bar{2}/2})\right]$$
$$\times\exp\left[\frac{\sigma_{4P}}{2\sigma_{2P}\sigma_2}S_{1P}S_{2P}(R^2_{12/2}+R^2_{1\bar{2}/2})\right] \qquad (14)$$

and

$$M=\exp\left[\left(\frac{\sigma_4}{2\sigma_2^2}-\frac{\sigma_3^2}{\sigma_2^3}\right)R_1R_2(R^2_{12/2}+R^2_{1\bar{2}/2})\right]$$
$$\times\exp\left[\frac{\sigma_{4P}}{2\sigma_{2P}\sigma_2}|S_{1P}||S_{2P}|(R^2_{12/2}+R^2_{1\bar{2}/2})\right]$$
$$+\exp\left[-\left(\frac{\sigma_4}{2\sigma_2^2}-\frac{\sigma_3^2}{\sigma_2^3}\right)R_1R_2(R^2_{12/2}+R^2_{1\bar{2}/2})\right]$$
$$\times\exp\left[-\frac{\sigma_{4P}}{2\sigma_{2P}\sigma_2}|S_{1P}||S_{2P}|(R^2_{12/2}+R^2_{1\bar{2}/2})\right]. \qquad (15)$$

If $R_{12/2}R_{1\bar{2}/2}\simeq 0$, (14) implies that when $S_{1P}S_{2P}=0$, $\mathscr{P}_+<1/2$, which is well known. When $S_{1P}S_{2P}\ll 0$, $\mathscr{P}_+$ is still further reduced, as anticipated.

3. Application and discussion

The result obtained here is applied to the known structure of a derivative of β-lactam ($C_{18}H_{15}ClN_2O_5$) (Nigam, Ghosh & Mitra, 1982). As the structure belongs to the centrosymmetric space group $P2_1/a$, the results obtained are equally applicable in this case also. It is assumed that the coordinates of the chlorine atom are known; its contribution to the structure factors is calculated. Using $|E|$ values greater than 2, the pairs $\mathbf{h}$, $\mathbf{k}$ satisfying $\mathbf{h}+\mathbf{k}=0 \pmod{\boldsymbol{\omega}}$ are found. The values of $\mathscr{P}_+$ for these pairs are calculated from (13).

Green & Hauptman (1976) derived the probability distribution of the structure seminvariant $\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}$ for equal atoms. For unequal atoms, their results are generalized by means of

$$\mathscr{Q}_\pm\simeq\frac{1}{L}\exp\left[\pm\left(\frac{\sigma_4}{2\sigma_2^2}-\frac{\sigma_3^2}{\sigma_2^3}\right)R_1R_2(R^2_{12/2}+R^2_{1\bar{2}/2})\right]$$
$$\times\cosh\left[\frac{\sigma_3}{\sigma_2^{3/2}}R_{12/2}R_{1\bar{2}/2}(R_1\pm R_2)\right].$$

Table 1 shows values of $\mathscr{P}_+$ and $\mathscr{Q}_+$ for 25 pairs of structure seminvariants; comparison of $\mathscr{P}_+$ and $\mathscr{Q}_+$ is made under different conditions, as discussed here. The entries in rows 1 to 11 show that when $S_{1P}S_{2P}>0$ and $\mathscr{Q}_+>1/2$ then $\mathscr{P}_+>\mathscr{Q}_+$. In row 12, $S_{1P}\simeq 0$, the contribution of $S_{1P}S_{2P}$ is small and $\mathscr{P}_+=\mathscr{Q}_+$. Rows 13, 15 and 16 show that when $S_{1P}S_{2P}<0$ then $\mathscr{P}_+<\mathscr{Q}_+$, and the actual sign of $E_{\mathbf{h}}E_{\mathbf{k}}$ is positive. In rows 18, 20, 21, 23 and 25 the probability that $E_{\mathbf{h}}E_{\mathbf{k}}$ be negative can be predicted with greater reliability but not conclusively since $\mathscr{P}_+<\mathscr{Q}_+$. In row 23, particularly, $\mathscr{Q}_+>1/2$ so that $E_{\mathbf{h}}E_{\mathbf{k}}$ is probably positive ($R_{12/2}R_{1\bar{2}/2}$ is large) if one ignores the contribution from the heavy atom, but when the contribution of $S_{1P}S_{2P}$ is taken into account, one obtains $\mathscr{P}_+<1/2$, the correct probability. In row 22, $\mathscr{P}_+=\mathscr{Q}_+$, since $S_{1P}S_{2P}$ is small. Again, in row 17, $\mathscr{P}_+>\mathscr{Q}_+$ since $S_{1P}S_{2P}>0$ although in this case the sign of $E_{\mathbf{h}}E_{\mathbf{k}}$ is negative.

Thus, it is clear from the above discussion that when phase information from the known part is available the seminvariant phases can be determined with greater reliability. If the heavy-atom contribution, or part of a structure, is known by Patterson or other methods, the contribution of the known part to the total structure factors can be calculated. This information together with the information from 'neighbors' will be of great value in estimating the structure seminvariants in order to find the solution for the rest of the structure. As is clear from Table 1, it is then possible to estimate reliably a greater number of structure seminvariants, and negative indications will also be more definitive. This will be of help in the process of finding new signs of other reflections. In the present derivations terms up to the order of $1/N$ have been retained. Inclusion of higher-order terms will, however, lead to better probability estimations. Also, for more complex structures it may be necessary

Table 1. 25 *Values of* $\mathscr{P}_+$ *and* $\mathscr{Q}_+$ *for a derivative of* β-*lactam*

Signs in parentheses are the true signs of the main reflections.

Number	Indices of main terms: h			Indices of main terms: k			Observed magnitudes, $\lvert E\rvert$				Heavy-atom contribution E^P		$\mathscr{P}_+$	$\mathscr{Q}_+$
							h	**k**	$\frac{1}{2}(\mathbf{h}+\mathbf{k})$	$\frac{1}{2}(\mathbf{h}-\mathbf{k})$	**h**	**k**		
1	4	8	9	2	0	11	2·46(−)	2·81(−)	3·49	2·34	−1·91	−1·04	0·99	0·95
2	2	13	3	0	1	3	2·35(−)	2·06(−)	2·79	2·60	−0·58	−1·86	0·98	0·91
3	9	4	4	5	4	12	2·61(+)	2·05(+)	2·04	1·89	1·86	1·99	0·97	0·73
4	9	4	4	3	12	6	2·61(+)	2·12(+)	2·11	2·06	1·86	1·65	0·97	0·78
5	2	11	7	2	9	1	2·50(+)	2·54(+)	2·36	2·06	1·06	1·87	0·97	0·83
6	8	9	2	2	11	0	2·21(+)	2·63(+)	2·36	0·84	1·59	1·86	0·97	0·75
7	4	17	0	2	7	0	2·56(+)	2·10(+)	2·33	2·04	1·98	1·20	0·97	0·80
8	7	13	1	3	13	9	2·70(+)	2·50(+)	2·38	1·56	1·96	1·57	0·96	0·74
9	4	10	3	4	8	9	2·03(−)	2·46(−)	1·88	2·06	−1·60	−1·91	0·95	0·73
10	6	2	10	2	2	6	2·06(+)	2·05(+)	2·23	1·95	1·46	0·92	0·89	0·75
11	3	14	2	1	6	0	2·31(+)	2·60(+)	1·88	2·34	1·34	0·56	0·88	0·79
12	4	11	3	0	1	3	2·01(+)	2·06(−)	1·92	3·14	0·01	−1·86	0·86	0·86
13	5	7	5	5	3	1	2·20(+)	3·00(+)	2·26	2·59	−0·09	1·37	0·83	0·89
14	2	10	4	0	2	2	2·36(−)	2·59(−)	1·43	2·34	−1·59	−0·67	0·82	0·69
15	3	5	8	3	11	2	2·85(+)	2·00(+)	3·05	2·59	1·89	−0·48	0·76	0·93
16	6	14	2	2	4	12	2·57(−)	2·38(−)	1·85	2·08	−0·42	0·11	0·74	0·75
17	8	8	4	2	2	6	2·25(−)	2·05(+)	0·88	2·61	0·93	0·92	0·63	0·53
18	5	5	7	3	13	9	2·14(−)	2·50(+)	1·50	2·34	−0·69	1·57	0·53	0·69
19	9	5	3	1	7	11	2·06(−)	2·12(+)	1·99	0·53	−0·35	−0·77	0·50	0·49
20	3	5	8	3	3	10	2·85(+)	3·05(−)	1·78	1·11	1·89	−0·66	0·50	0·59
21	6	14	2	2	2	6	2·57(−)	2·05(+)	1·80	0·16	−0·42	0·92	0·48	0·49
22	4	11	3	2	1	11	2·01(+)	2·69(−)	1·99	0·54	0·01	−1·58	0·48	0·48
23	4	16	2	2	2	6	2·00(−)	2·05(+)	2·89	2·26	−1·66	0·92	0·46	0·87
24	3	14	2	3	6	0	2·30(+)	2·16(−)	2·06	2·07	1·34	−1·39	0·43	0·76
25	5	5	3	1	7	11	2·26(−)	2·12(+)	1·99	0·74	1·85	−0·81	0·41	0·51

to employ the higher neighborhoods for the better estimation of structure invariants and seminvariants.

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The Dynamic Theory of X-ray Diffraction by the One-dimensional Ideal Superlattice. I. Diffraction by the Arbitrary Superlattice

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Abstract

The theory of X-ray two-beam dynamic diffraction by the one-dimensional ideal superlattice (SL) in the Laue and Bragg cases is developed. The reflection and transmission amplitudes of the SL are expressed by those for one period of the SL. General expressions revealing the behavior of the diffraction pattern, irrespective of the particular model, are obtained. A detailed analysis is carried out for the most important case: $z_0 \ll \bar{\Lambda}$ (z_0 and $\bar{\Lambda}$ being the SL period and the mean extinction length of the crystal, respectively).

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