

X-ray Diffraction by Close-Packed Crystals with 'Growth Stacking Faults' Assuming an 'n-Layer Influence'

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The X-ray intensity diffracted by close-packed crystals with 'growth stacking faults' is calculated in the case of a general 'n-layer influence'.

1. Introduction

It has been proved (Jagodzinski, 1949) that the X-ray intensity diffracted by close-packed crystals with 'growth stacking faults' is

$$I = |F|^2 \frac{\sin^2 \frac{1}{2} N_1 A_1}{\sin^2 \frac{1}{2} A_1} \cdot \frac{\sin^2 \frac{1}{2} N_2 A_2}{\sin^2 \frac{1}{2} A_2} \left[\frac{1+2Q}{3} \cdot \frac{\sin^2 \frac{1}{2} N_3 A_3}{\sin^2 \frac{1}{2} A_3} + (1-Q) \sum_r \frac{C_r N_3 (1-x_r^2)}{1-2x_r \cos A_3 + x_r^2} \right], \quad (1)$$

where the x_r 's are the roots of a characteristic equation and where the C_r 's are the solution of the system

$$\sum_r C_r x_r^m = P_m - \frac{1}{3}. \quad (2)$$

In this article we shall calculate the characteristic equation in the general case of an 'n-layer influence'.

n layers can occur in $s = 2^{n-2} = 4l$ ($l = 2^{n-4}$) arrangements a_i . The assumption of an 'n-layer influence' means that the way [hexagonal (h) or cubic (k)] in which a new layer continues the sequence of n layers will depend on the arrangement of these n preceding layers. We have then to introduce s transition probabilities α_i , so that we have

$$a_i \begin{cases} \rightarrow h \text{ prob. } (1-\alpha_i), & (3a) \\ \rightarrow k \text{ prob. } \alpha_i. & (3b) \end{cases}$$

Let W_i be the probability that a given layer is in an a_i -arrangement with its $(n-1)$ predecessors and P_m the occurrence probability that two layers, m layers apart, are in the relationship $A(B, C) \dots A(B, C)$, while $p_m^{(i)}$ will be the partial probability that the last of these two layers (layer 0 and layer m) is in the arrangement a_i . Then we have

$$\sum_{i=1}^s W_i = 1 \quad \text{and} \quad P_m = \sum_{i=1}^s p_m^{(i)}. \quad (4a, 4b)$$

Let us now consider the scheme of Fig. 1. On the first line (layer 1, 2, 3) is noted the arrangement h or k of the first three layers, while on the following lines is indicated the way, h or k , in which the sequence of the layers is continued. Each series of symbols h and k joined by straight lines constitutes one of the possible arrangements a_i and no other arrangement can possibly exist. They can then be numbered easily as shown in the figure.

Suppose we add a new layer [layer $(n+1)$] to the sequences I and consider then the new sequences II of the last n layers. For these we then obtain the scheme

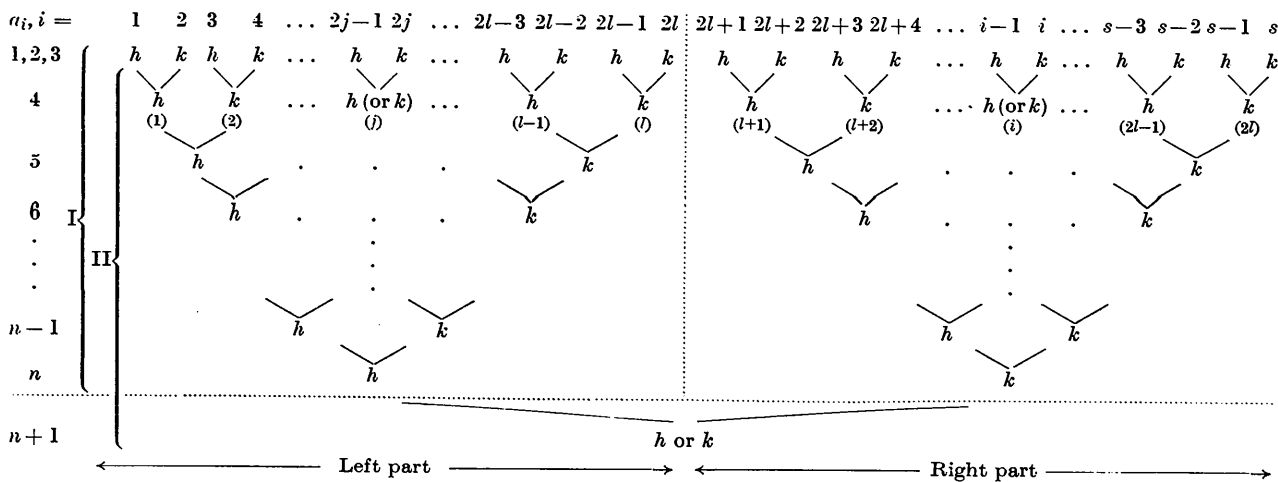


Fig. 1.

which starts on the second line and ends with an h (or a k), depending on the way in which the new layer is added. This new scheme is equivalent to the left (or right) part of the original one.

If we note that each number j on the second line is associated with the numbers $2j-1$ and $2j$ on the first line, we can state that if a sequence of n layers in an a_{2j-1} or an a_{2j} arrangement is continued by an h - (or a k -) arranged layer, we obtain a_j (or a_{j+2l}) as the arrangement of the last n layers. We express this symbolically in the following way:

$$a_{2j-\lambda}+h \rightarrow a_j \quad \text{and} \\ a_{2j-\lambda}+k \rightarrow a_{j+2l} \quad (j:1, 2, \dots, 2l) (\lambda = 0, 1). \quad (5a, 5b)$$

From (5) we obtain the following rules:

$$(a_{4j-\varepsilon}+h)+h \rightarrow a_{2j-\nu}+h \rightarrow a_j, \quad (6a)$$

$$(a_{4j-\varepsilon}+k)+h \rightarrow a_{2j+2l-\nu}+h \rightarrow a_{j+l}, \quad (6b)$$

$$(a_{4j-\varepsilon}+h)+k \rightarrow a_{2j-\nu}+k \rightarrow a_{j+2l}, \quad (6c)$$

$$(a_{4j-\varepsilon}+k)+k \rightarrow a_{2j+2l-\nu}+k \rightarrow a_{j+3l}, \quad (6d)$$

$$a_{2j-\lambda}+k \rightarrow a_{j+2l}, \quad a_{2j+2l-\lambda}+k \rightarrow a_{j+3l}. \quad (6e), (6f)$$

$$(\varepsilon = 0, 1, 2, 3;$$

$$\nu = \begin{cases} 0 & \text{if } \varepsilon = 0, 1; \\ 1 & \text{if } \varepsilon = 2, 3; \end{cases} \lambda = 0, 1, j = 1, \dots, l).$$

With the aid of (5) and (3) we obtain:

$$W_j = \sum_{\lambda=0}^1 W_{2j-\lambda} (1-\alpha_{2j+\lambda}) \quad \text{and}$$

$$W_{j+2l} = \sum_{\lambda=0}^1 W_{2j-\lambda} \alpha_{2j-\lambda} \quad (j = 1, 2, \dots, 2l) (\lambda = 0, 1). \quad (7a, 7b)$$

The expressions (7) and (4a) form a system which enables us to calculate

$$W_i (i = 1, \dots, 4l).$$

2. Calculation of P_m

The layer m can be the last in any one of the following arrangements:

(1) a_j (or a_{j+l}) which terminate as $\dots hh$ (or kh). Layer m will (like the zero layer) be an A -layer if layer $(m-2)$ is also A , layer $(m-1)$ is arranged either h or k , and layer m is arranged h only. For this we have, if we take (3) and (6a) (or (3) and (6b)) into account:

$$p_m^{(j)} = \sum_{\varepsilon=0}^3 p_{m-2}^{(4j-\varepsilon)} (1-\alpha_{4j-\varepsilon}) (1-\alpha_{2j-\nu}) \quad (8a)$$

and

$$p_m^{(j+l)} = \sum_{\varepsilon=0}^3 p_{m-2}^{(4j-\varepsilon)} \alpha_{4j-\varepsilon} (1-\alpha_{2j+2l-\nu}) \quad (8b)$$

$$(j = 1, \dots, l) \left(\nu = \begin{cases} 0 & \text{if } \varepsilon = 0, 1 \\ 1 & \text{if } \varepsilon = 2, 3 \end{cases} \right).$$

(2) a_{j+2l} (or a_{j+3l}) which terminate as $\dots hk$ (or kk). For these the probabilities W_{j+2l} (or W_{j+3l}) depend on the following possibilities:

(a) the layer m is an A -layer,

(b) layer $(m-1)$ is an A -layer arranged as $a_{2j-\lambda}$ (or $a_{2j+2l-\lambda}$) [see (6e) (or (6f))] and followed by a k -arranged layer m , or

(c) layer $(m-2)$ is an A -layer arranged as $a_{4j-\varepsilon}$ (or $a_{4j-\varepsilon}$) [see (6c) (or (6d))], followed by an h - or k -arranged layer $(m-1)$, and by a k -arranged layer m . If we take this into account, and also (3) and (6c) (or (6d)), we have:

$$W_{j+2l} = p_m^{(j+2l)} + \sum_{\lambda=0}^1 p_{m-1}^{(2j-\lambda)} \alpha_{2j-\lambda} + \sum_{\varepsilon=0}^3 p_{m-2}^{(4j-\varepsilon)} (1-\alpha_{4j-\varepsilon}) \alpha_{2j-\nu} \quad (9a)$$

$$W_{j+3l} = p_m^{(j+3l)} + \sum_{\lambda=0}^1 p_{m-1}^{(2j+2l-\lambda)} \alpha_{2j+2l-\lambda} + \sum_{\varepsilon=0}^3 p_{m-2}^{(4j-\varepsilon)} \alpha_{4j-\varepsilon} \alpha_{2j+2l-\nu} \quad (9b)$$

$$(j = 1, \dots, l) \left(\nu = \begin{cases} 0 & \text{if } \varepsilon = 0, 1 \\ 1 & \text{if } \varepsilon = 2, 3 \end{cases} \right).$$

The expressions (4b), (8) and (9) form a linear system which has a solution of the form

$$p_m^{(i)} = c_0^{(i)} + \sum_r c_r^{(i)} x_r^m, \quad P_m = C_0 + \sum_r C_r x_r^m, \quad (10)$$

where x_r are the roots of a characteristic equation. This equation can be found in the usual way (Gevers, 1952, 1954) by substituting the formulae (10) in the system.

We obtain then the equation of degree $2s$ $\det. C=0$, where the matrix C is

$$C = x^2 E + xG + (G-H)(G+H), \quad (11)$$

where E is the unit matrix of order s ,

$$G = \begin{pmatrix} 0 & 0 & 0 & 0 & \dots & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & & & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \dots & \dots & 0 & 0 \\ \alpha_1 & \alpha_2 & 0 & 0 & \dots & \dots & 0 & 0 \\ 0 & 0 & \alpha_3 & \alpha_4 & \dots & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & & & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \dots & \dots & \alpha_{s-1} & \alpha_s \end{pmatrix}$$

and

$$H = \begin{pmatrix} 1-\alpha_1 & 1-\alpha_2 & 0 & 0 & \dots & \dots & 0 & 0 \\ 0 & 0 & 1-\alpha_3 & 1-\alpha_4 & \dots & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & & & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \dots & \dots & 1-\alpha_{s-1} & 1-\alpha_s \\ 0 & 0 & 0 & 0 & \dots & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & & & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \dots & \dots & 0 & 0 \end{pmatrix}.$$

It can be proved that this equation is equivalent to the one given by Kakinoki & Komura (1952), and that the formulae given by Wilson (1942), Jagodzinski (1949) and Gevers (1952, 1954) are special cases of (11).

With the aid of (4a) and (7) it can be proved that $C_0 = \frac{1}{3}$ and the C_r 's can be calculated by solving the system (2). The values of P_m ($m = 0, 1, \dots, 2s-1$) may indeed be calculated directly with the aid of (8), (9) and (4b), if we take into account that

$$p_0^{(i)} = W_i \quad \text{and} \quad p_1^{(i)} = 0 \quad (i = 1, \dots, s).$$

It has already been demonstrated (Gevers 1953, 1954) how the expression

$$\sum_r \frac{C_r(1-x_r^2)}{1-2x_r \cos A_3 + x_r^2}$$

of formula (1) can be calculated without solving the

characteristic equation (11) and the system (2), and how an equivalent numerical equation can be calculated from measurements of the diffuse X-ray intensity.

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The Determination of the Crystal Structure of $\text{Ni}_4\text{Mn}_{11}\text{Al}_{60}$

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The crystal structure of the intermetallic compound $\text{Ni}_4\text{Mn}_{11}\text{Al}_{60}$ has been determined using image-seeking functions on Patterson projections and sections. By choosing appropriate sections parallel to densely packed planes of atoms it has been possible to obtain in this way a trial structure which subsequent refinement has shown to be very accurate.

Introduction

The purpose of this paper is first to give a preliminary account of the structure of an intermetallic compound having the composition $\text{Ni}_4\text{Mn}_{11}\text{Al}_{60}$, and secondly to indicate a method of analysis which seems likely to be successful with *layered* structures, even though they may be very complicated. This method uses minimum image-seeking functions, as described by Buerger (1950, 1951), to analyse selected sections of the three-dimensional Patterson synthesis.

If a structure shows marked layering of atoms perpendicular to one particular direction, the Patterson synthesis, $P(U, V, W)$, must have a corresponding layered nature, so that it may be possible to include most of the important features of the full Patterson synthesis in a few sections lying parallel to the densely packed atomic planes. Analysis of such sections may be performed most conveniently by scanning with a plane, or nearly plane, image-seeking function. A suitable function might well be found by examination

of the origin region of the Patterson if one of the selected sections passes through the origin, or, if not, by exam-

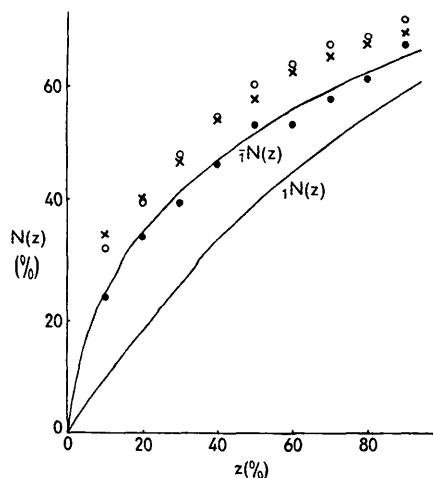


Fig. 1. Intensity distribution in the $(hk0)$, $(h0l)$ and $(hk4)$ sets, represented by crosses, open circles and full circles respectively; $N(z)$ is the fraction of intensities less than $z\%$ of the mean intensity.

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