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Acta Cryst. (1989). A**45**, 797-801

The Monte Carlo Simulation of Random Stacking Faults in Close-Packed Structures

BY B. I. NIKOLIN AND A. YU. BABKEVICH

Institute of Metal Physics, Academy of Sciences of the Ukrainian SSR, 36 Vernadsky str., 252142 Kiev 142, USSR

(*Received* 22 *February* 1989; *accepted* 23 *June* 1989)

Abstract

A new approach to the estimation of the concentration of random stacking faults in close-packed structures (and also multilayers) is presented. It is based on the Monte Carlo computer simulation of the arrangement of stacking faults in a crystal, given by an appropriate h-k sequence. Thus the corresponding intensity (structure-factor) distribution along the streaked reciprocal-lattice rows may be calculated from nearly the same expression as for a perfect multilayer structure. In particular, good agreement is observed with the computations on the basis of the intensity equations derived for several particular cases. Some peculiarities in the diffracted intensity distribution of crystals with multilayer structures containing random stacking faults of different types, or having different dimensions of the hexagonal unit cell, are pointed out.

1. Introduction

Stacking faults (SF) are frequently observed in close-packed structures. In some cases they are expected to be randomly distributed, *i.e.* the spacing between them is random. Random stacking faults (RSF) may result in one or more of the following diffraction effects: shift, broadening, asymmetry of the diffraction maxima and redistribution of the integrated intensity. Pertinent information about the types of SF as well as their concentrations in crystals can be obtained from a comparison of theoretically predicted diffraction effects with those visible on X-ray diffraction patterns. The theory of the intensity of X-ray diffuse scattering by the simplest close-packed structures such as h.c.p. ($2H$), f.c.c. ($3C$) and $4H$ containing random faults has been well developed by Wilson (1942), Paterson (1952), Christian (1954), Johnson (1963), Lele, Anantharaman & Johnson (1967) and Lele, Prasad & Anantharaman (1969). Because RSF are also observed in multilayer (long-period) polytype-like structures [see Verma & Krishna (1966), Nikolin (1984), Sebastian & Krishna (1987) and literature quoted therein], attempts have been made to construct a more general diffraction theory by Kakinoki & Komura (1965), Kakinoki (1967), Rushits & Mirzaev (1979), Kagan, Unikel' & Fadeeva (1982) and Berliner & Werner (1986). Nevertheless, the Kakinoki & Komura (1965) and Kakinoki (1967) approach, where the correlation between s neighbouring layers must be taken into account, becomes exceedingly complex even for structures with comparatively low periodicity, since 2^{s-1}-order matrices are necessary. Later, the theory was developed by Rushits & Mirzaev (1979), who studied the stacking disorder due to deformation faults only. The Kagan *et al.* (1982) method treated the problem for crystals of any symmetry group and complexity but with low defect concentrations.

In the following, we will give a technique to derive the intensity distribution of any given close-packed structure with arbitrary content of RSF of all existing types. Its distinguishing feature consists of a random arrangement of SF's by the Monte Carlo simulation computer program.

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2. Statement of the model

The initial crystal is set by an appropriate sequence of close-packed layers using the h–k notation, introduced by Belov (1947), together with the classical ABC notation. The notation 'h' or 'k' means that the layer is arranged with respect to the two preceding ones in a hexagonal or a cubic manner. The regular sequence of the layers in a perfect close-packed crystal can then generally be represented by h–k symbols, *e.g.* hkk ($9R$ structure), and this means that a regular sequence can be constructed by periodic repetition of this prescription. We shall start with such a sequence for further insertion of stacking faults and calculation of the corresponding diffraction intensity distribution.

A question arises concerning the crystal dimensions, which are commonly assumed to be infinite for analytical solutions. As a consequence of limited memory and requirement for speed of computers the size of simulated crystals is usually restricted. On the other hand, it is obvious that a decrease in the crystal dimensions results in broadening of the reflections. Thus it is necessary to investigate the influence of crystal size, R, which is expressed in terms of the number of given close-packed layers, on the diffraction maxima half-width in reciprocal space, δ. A plot of $\delta(R)$ for the reflections of an f.c.c. crystal shows (see Fig. 1) that at $R \geq 500$ layers δ depends weakly on R. However, if we take into account the actual accuracy of intensity determination from X-ray rotation or oscillation patterns and the benefits of lowering the total computation time, as well as a pronounced δ dependence from the RSF concentration (see Fig. 1), we may take the crystal size to be equal to $R = 300$–500 layers, especially when qualitative analysis is desirable. It is necessary to note that owing to additional broadening resulting from finite crystal dimensions we can determine the SF content to within 0·005. Hence, to define low SF concentrations or to evaluate this value precisely, infinite-crystal solutions are preferable for comparison with experimental results.

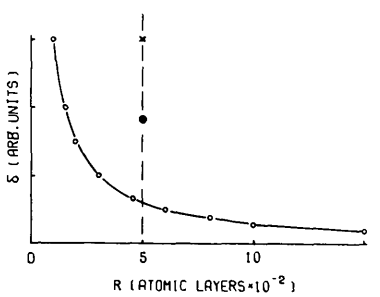

Fig. 1. Half-width of the 111($3C$) reflection, δ, as a function of crystal size, R. RSF concentration: ○ $\alpha = 0$; ● $\alpha = 0{\cdot}01$; × $\alpha = 0{\cdot}02$.

Table 1. *Stacking faults in close-packed structures*

Structure	Fault configuration in ABC and h–k notations	Fault type: Intrinsic (I) or extrinsic (E)	Fault type: Other classification
F.c.c. ($3C$)	...*ABC ABC ABC ABC*...	Free of faults	
	kk kkk kkk kk		
	...*ABC ABA BCA B*...	I	Deformation
	kk khh kkk		
	...*ABC ABA CAB C*...	E	Double deformation
	kk khk hkk		
	...*ABC ABA CBA*...	—	Growth or twin
	kk khk kk		
H.c.p. ($2H$)	...*AB AB AB AB AB*...	Free of faults	
	h hh hh hh h		
	...*AB AB AC BC BC*...	I	Deformation
	h hh kk hh h		
	...*AB AB AC BA BA B*...	E	—
	h hh kk kh hh		
	...*AB AB AC AC AC*...	I	Growth
	h hh kh hh h		

Stacking-fault configurations

A stacking fault may be defined as a break in the normal sequence of layers in a close-packed structure. As SF's destroy the stacking rule attributed to the initial structure, a definite rearrangement of the h–k symbols takes place. Table 1 lists the possible fault configurations in the $2H$ and $3C$ structures along with the different notations used to represent them. It is apparent from the table that when a growth fault occurs 'h' changes to 'k' (or *vice versa*) in one layer, and the deformation fault changes both the arrangement of the layer in which the discontinuity occurs and that of the next one ($h \rightarrow k$, $k \rightarrow h$). The extrinsic fault results in a three-layer configuration, where one k-type layer is sandwiched between the supplanted ($h \rightleftarrows k$) layers. As is readily verified, this simple rule is valid for SF's in multilayer close-packed structures as well. For phase transitions at which one multilayer structure is transformed into another, SF's of the layer displacement type are involved, where a single layer is displaced from one close-packed position (say A) to another (say B or C) by diffusion processes (Nishiyama, Kakinoki & Kajiwara, 1965; Pandey & Krishna, 1981). A certain set (group) of such single displacements is usually regarded as one elementary shift (Mirzaev & Rushits, 1976). In our designation such complex shifts may be given by a substitution of several layers in the reference sequence for an appropriate combination of h–k symbols inherent in the SF under examination. By using the accepted rules with respect to any close-packed structure, one can introduce all possible fault configurations without the limitation of SF concentration.

A random distribution of SF's is created by means of the Monte Carlo simulation computer program. As the first step, the Monte Carlo routine generates a set of pseudorandom values with uniform separation in the interval (0, 1). In the second step, this distribution is converted into a set of numbers from

1 to R. In this way we obtain a set of sites, where the SF's are to be inserted by an appropriate conversion of the h-k symbols. Since the ABC sequence can readily be obtained from the h-k notation, one can calculate the intensity (structure factor) at any position of the reciprocal lattice from nearly the same expression as for the perfect multilayer structure, *i.e.* by neglecting f^2 (f being the scattering power of a single layer of the structure):

$$I = F^2 = FF^*$$

where

$$F = \sum_p \exp[2\pi i Lp/N] + \sum_q \exp\{2\pi i[(H-K)/3 + qL/N]\} + \sum_r \exp\{2\pi i[(K-H)/3 + rL/N]\}. \quad (1)$$

Here p, q, r are the numbers of A-, B- and C-type layers, respectively; H, K, L are the hexagonal indices. It is common knowledge that only the reflections with $H-K \neq 0 \bmod 3$ are affected by faulting. We put $H=1$, $K=0$, because Verma & Krishna (1966) specified that the relative intensity calculation for the $10.L$ reciprocal-lattice row only is sufficient for comparison with the measured intensity distribution.

It is obvious that if the crystal contains m SF's, there are C_R^m possible nonregular arrangements among R close-packed layers of this crystal. Therefore, the resulting intensity distribution along the $10.L$ reciprocal-lattice row may be thought of as a superposition of intensities calculated for all different variants of SF arrangement. But even for a SF content $\alpha = 0{\cdot}01$ and $R = 300$ layers, it is rather cumbersome to calculate the intensity for all the existing $C_{300}^3 \simeq 1{\cdot}5 \times 10^4$ combinations. Trial computations showed that satisfactory results may be achieved when 100 to 200 variants are averaged.

3. Applications

The accuracy of this method was verified by comparing the results of diffracted intensity calculations for f.c.c. ($3C$), h.c.p. ($2H$) and $9R$ lattices with growth, deformation and extrinsic SF's both obtained with the help of the Monte Carlo computer simulation technique and with the aid of the intensity expressions derived by Wilson (1942), Paterson (1952), Christian (1954), Johnson (1963), Lele *et al.* (1967), Rushits & Mirzaev (1979). In all cases the X-ray diffraction spectra profiles obtained by different methods are in good agreement (*e.g.* Figs. 2, 3, 4*a*). Moreover, we calculate the diffracted intensity distribution for f.c.c. crystals with deformation SF's and compare the difference in angular peak position of 111 and 200 reflections for $\alpha = 0$ and $\alpha = 0{\cdot}024$. Thus we obtain

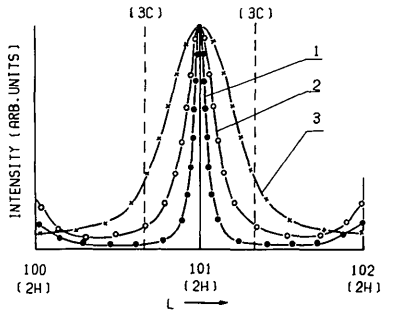

Fig. 2. Calculated variation of the intensity distribution along the $10.L$ reciprocal-lattice row of a $2H$ crystal containing a random distribution of growth (1), deformation (2), extrinsic (3) stacking faults ($\alpha = \beta = \gamma = 0{\cdot}2$). The present data (——) are compared with line profiles calculated from the Wilson (●), Christian (○) and Lele, Anantharaman & Johnson (×) expressions, respectively.

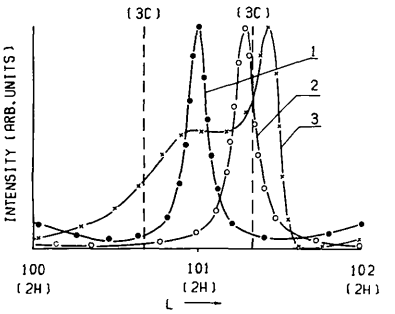

Fig. 3. Calculated variation of the intensity distribution along the $10.L$ reciprocal-lattice row of a $3C$ crystal containing a random distribution of growth ($\beta = 0{\cdot}7$) (1), deformation ($\alpha = 0{\cdot}15$) (2), extrinsic ($\gamma = 0{\cdot}25$) (3) stacking faults. The present data (——) are compared with line profiles calculated from the Paterson (○, ●) and Johnson (×) expressions, respectively.

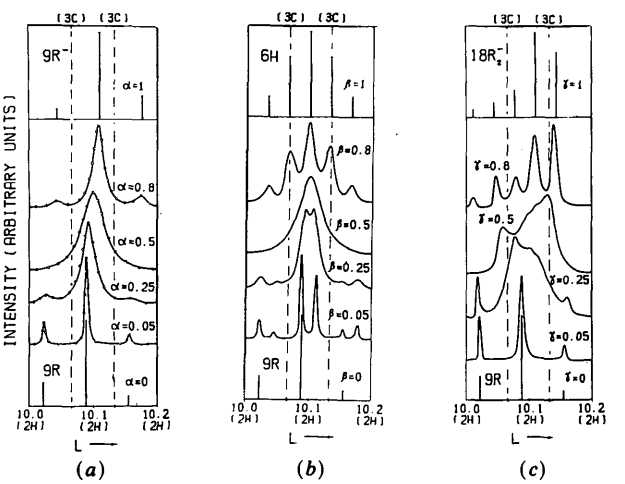

Fig. 4. Calculated variation of the intensity distribution along the $10.L$ reciprocal-lattice row of a $9R$ crystal containing a random distribution of deformation (a), growth (b) and extrinsic (c) stacking faults. The Mirzaev & Rushits results are plotted as ○. The calculated curves have been shifted vertically for different values of SF concentration for clarity.

a value for Co $K\alpha$ radiation of 0·18° [which is close to the 0·15° value given by Warren (1969)] corresponding to $\alpha = 0{\cdot}029$ derived from Warren's (1969) relation. This allows us to assume that the method proposed is suitable for an X-ray diffraction study of RSF's in close-packed structures, and for multilayers as well.

In order to distinguish the effect of the presence of various types of RSF in long-period structures, we have calculated the intensity distribution along the 10.L reciprocal-lattice row in a few cases of random faulting of 9R and 19T crystals. Fig. 4 shows the results of the diffracted intensity calculation for a 9R structure with different content of deformation, growth and extrinsic RSF's. As is readily verified, the calculated diffraction pattern corresponding to each kind of SF has its distinctive features. The increase in deformation SF concentration (α) results in equal shift and symmetrical broadening of the 9R reflections. When $\alpha = 0{\cdot}5$ the intensity distribution has the only very broadened maxima which coincide with the position 101(2H). As the concentration of deformation RSF's increases, the reflections from the 9R structure with the reverse 9R stacking sequence appear and become sharper when they gradually approach the $9R^-$ positions (see Fig. 4a).

If the 9R structure contains growth RSF's, reflections from the twin orientation ($9R^-$) arise as soon as a single growth fault is introduced (see Fig. 4b). As their concentration (β) increases, the reflections from both the 9R and $9R^-$ structures broaden and their most intense maxima move closer together. For $\beta = 0{\cdot}5$ the intensity distribution is the same as for $\alpha = 0{\cdot}5$ and has a single peak at the position 101(2H). As $\beta \rightarrow 1$ the crystalline structure approaches the perfect 6H lattice with the stacking order of the close-packed planes $(hkk)_2$ or (22).

It may be noted from Fig. 4(c) that the intensity redistribution due to the extrinsic faults appears to be more complex. If this type of RSF is introduced into a perfect 9R structure, the intensity distribution gradually transforms to the diffraction pattern attributed to the $18R_2$ structure with a layer sequence $(kkkhkh)_3$ or $(42)_3$. In this case the most intense maxima of the initial 9R structure show a considerably sharper increase in breadth than in the previous examples and shift towards the f.c.c. reflection position. This allows us to distinguish the stacking disorder due to deformation and extrinsic RSF's when the concentration of faults is small.

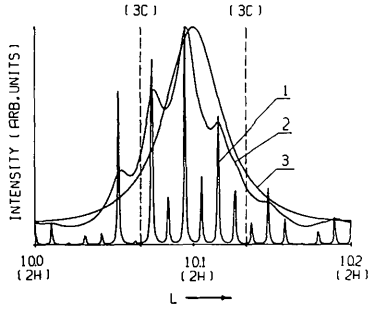

Fig. 5. Calculated variation of the intensity distribution along the 10.L reciprocal-lattice row of a 19T (11112445) structure containing a random distribution of deformation faults: (1) $\alpha = 0{\cdot}01$; (2) $\alpha = 0{\cdot}15$; (3) $\alpha = 0{\cdot}5$. The intensity equation of Rushits & Mirzaev is used.

4. Concluding remarks

The present investigations of the multilayer close-packed structures with random stacking faults allow one to make the following conclusions:

(1) The intensity distributions for the 2H, 3C and 9R lattices disordered by RSF's are the same as those obtained on the basis of the well known theories of Wilson (1942), Paterson (1952), Christian (1954), Lele *et al.* (1967), Rushits & Mirzaev (1979) and Johnson (1963).

(2) The deformation RSF's cannot transform one multilayer structure into another. Such transitions are possible when growth or extrinsic RSF's of high density are introduced into the initial multilayer structure.

(3) For the same concentration of RSF's, the more streaked reflections correspond to the structures of greater N. For instance, the weakest reflections of the 9R structure vanish when the density of SF's is greater than 0·25. As regards the 19T structure mentioned above, the majority of reflections disappear when the density of deformation faults is $\alpha = 0{\cdot}15$, and with $\alpha = 0{\cdot}2$ there are only single broadened reflections on the intensity distribution (see Figs. 4a, 5).

Consequently, if most of the permitted reflections from a multilayer close-packed structure with large N ($\sim 10^2$) are on the X-ray diffraction pattern, the RSF concentration of any type in this structure is not greater than 0·1.

(4) The broadening of the most intense diffraction maxima of the initial close-packed structure is proportional to the number of layers in a SF configuration. Therefore, the other conditions being the same, the broadening due to the growth SF is the lowest, the middle broadening corresponds to the deformation SF and the largest to the extrinsic SF (see Figs. 2, 4).

The authors thank Mrs T. V. Bilenko for her technical assistance.

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SHORT COMMUNICATIONS

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Acta Cryst. (1989). A**45**, 801-802

The coset and double coset decomposition of the 32 crystallographic point groups.

By V. JANOVEC and E. DVORAKOVA, *Institute of Physics, Czechoslovak Academy of Sciences, POB* 24, *Na Slovance* 2, 18040 *Prague* 8, *Czechoslovakia* and T. R. WIKE* and D. B. LITVIN, *Department of Physics, The Pennsylvania State University, The Berks Campus, PO Box* 7009, *Reading, PA* 19610-6009, *USA*

(*Received* 3 *March* 1989; *accepted* 11 *July* 1989)

Abstract

The coset and double coset decompositions of the 32 crystallographic point groups with respect to each of their subgroups are tabulated.

I. Introduction

The mathematical concept of the coset decomposition of a group with respect to one of its subgroups has wide applications in crystallography and solid-state physics. The points of any crystallographic orbit are in a one-to-one correspondence with the cosets of the coset decomposition of the crystallographic group with respect to the site symmetry group of one of its points (Wondratschek, 1983). Coset decompositions have been applied in the analysis of domains of ferroic crystals using coset decompositions of point groups (Aizu, 1970; Janovec, 1972) and of space groups (Aizu, 1974; Janovec, 1972, 1976). This concept has also been used in the derivation of twin laws for (pseudo-)merohedry (Flack, 1987).

The mathematical concept of the double coset decomposition of a group is less well known and has been used in applications to a lesser extent than the coset decomposition [see Ruch & Klein (1987) and references therein]. The double coset decomposition has been used in a tensorial classification of domain pairs in the case where each domain is characterized by a unique form of a physical property tensor (Janovec, 1972) and in the case where more than a single domain is characterized by a specific form of a physical property tensor (Litvin & Wike, 1989).

In § II we briefly review the definitions of coset and double coset decompositions. Tables of the coset and double coset decompositions of the 32 crystallographic point groups with respect to each of their subgroups are given in § III.

II. Coset and double coset decompositions

For a given group G and subgroup H one writes the left coset decomposition of G with respect to H symbolically as

$$G = H + g_2H + g_3H + \ldots + g_nH$$

where g_iH denotes the subset of elements of G obtained by multiplying each element of the subgroup H from the left by the element g_i of G (Hall, 1959). Each subset of elements g_iH, $i = 1, 2, \ldots, n$, is called a left coset of G with respect to H, and the elements g_i, $i = 1, 2, \ldots, n$, of G are called the left coset representatives of the left coset decomposition of G with respect to H.

The subset of elements of G in each coset of the left coset decomposition of G with respect to H is unique, but the coset representatives are not unique. A coset representative g_i can be replaced by the element g_ih, where h is an arbitrary element of the subgroup H.

For a given group G and subgroup H, one writes the double coset decomposition of G with respect to H symbolically as

$$G = H + Hg_2^{dc}H + Hg_3^{dc}H + \ldots + Hg_m^{dc}H$$

where $Hg_j^{dc}H$ denotes the subset of *distinct* elements of G

* Present address: General Electric Aerospace, PO Box 8048, Philadelphia, PA 19101, USA.

0108-7673/89/110801-02$03.00