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X-ray Diffraction from Close-Packed Structures with Stacking Faults. I. *hcc* Crystals

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The kinematical theory of X-ray diffraction by *hcc* crystals with growth and deformation faults is developed. The intensity distribution in reciprocal space is derived as a function of five parameters which represent three growth and two deformation fault probabilities. Only reflexions with $H-K\neq 3N$, N an integer, are affected by faulting and generally exhibit changes in integrated intensity and broadening. In addition, reflexions with $L=6M\pm 1$ and $6M\pm 2$, M an integer, exhibit profile peak shift and profile asymmetry. It is shown that nine independent combinations of the five fault probabilities can be determined from the measured profile characteristics.

Introduction

X-ray diffraction from faulted close-packed crystals with a range of influence equal to 2, *i.e.*, *h* and *c* crystals [Jagodzinski (1949*a*) configurational symbols for h.c.p. and f.c.c. crystals respectively] has been considered by several authors. Wilson (1942) and Hendricks & Teller (1942) considered the case of growth faults while Patterson (1952) and Christian (1954) have considered deformation faults. (A growth fault arises when during the layer-by-layer growth of a crystal, the stacking rule is not obeyed in adding one new layer, but is otherwise obeyed throughout the crystal, while a deformation fault arises through the process of glide of one part of the crystal with respect to the remainder.) A general treatment for *h* and *c* crystals containing growth and deformation faults simultaneously has been given by Gevers (1954). Effects of extrinsic faults for *h* and *c* crystals have been found by Lele, Anantharaman & Johnson (1967) and Johnson (1963) respectively. (For *h* and *c* crystals, an extrinsic fault arises through the insertion of a close-packed layer.) Alternative treatments for extrinsic faults in *h* crystals and for deformation and extrinsic faults in *c* crystals have been given by Holloway (1969), Warren & Warekois (1955) and Warren (1963) respectively. The work has been reviewed by Warren (1959) and Wagner (1966).

X-ray diffraction from faulted close-packed crystals with a range of influence equal to 3, *i.e.*, *hc* (d.h.c.p.) crystals has been considered by Jagodzinski (1949*b*) for two types of growth faults and by Gevers (1954) and Lele, Prasad & Anantharaman (1969) for deformation faults. Prasad & Lele (1971) have given a comprehensive treatment for a total of nine types of fault (including the above three types).

There are three close-packed crystal structures with a range of influence equal to 4, namely *hcc*, *hhc* (samarium type) and *hhcc* structures. Gevers (1954) has given a general treatment for crystals of these three types containing growth faults as also for one type of deformation fault in *hcc* crystals. The object of the present paper is to complement the work on *hcc* crystals by carrying out the calculations to a stage where the fault probabilities are directly related to the experimentally observable diffraction effects. Further, unlike Gevers, we distinguish between deformation faults occurring between an *hh*, *hc* and *cc* pair of layers as they lead to configurations which are not equivalent energetically.

The *hcc* structure can be considered as a layer structure produced by the regular stacking of close-packed layers in the sequence $ABCACB,A$ where the letters A, B and C denote the three possible positions of the close-packed layers and the comma marks the completion of the repeat period (unit cell). The geometrical structure factors for different H,K,L are given in Table 1. A different notation (Nabarro, 1967) for the growth and deformation faults, virtual processes for their forma-

tion and stacking sequences containing the faults (indicated by vertical bar) are given in Table 2. The following calculations have been made under assumptions usual in this type of work (see *e.g.*, Prasad & Lele, 1971).

Table 1. *Structure factors for hcc crystals*

			$\lvert F\rvert$		
	L	$6M$	$6M\pm1$	$6M\pm2$	$6M\pm3$
$H-K$					
$3N$		$6f$	0	0	0
$3N\pm1$		0	$\sqrt{3}f$	$3f$	$\sqrt{3}f$

Diffraction from faulted crystals

Following Warren (1959), the diffracted intensity is given by

$$I(h_3)=\psi^2\sum_m\langle\exp[i\Phi_m]\rangle\exp[2\pi imh_3/6] \qquad (1)$$

where

$$\Phi_m=(2\pi/3)(H-K)q_m\,, \qquad (2)$$

q_m being a stochastic variate equal to 0, 1 or 2 respectively according as the m layer is A, B or C when the origin layer is A. Values of q_m for B and C layers at the origin can be obtained by cyclic permutation. It can be shown that

$$\langle\exp[i\Phi_m]\rangle=C\varrho^m \qquad (3)$$

where ϱ is a solution of the so-called characteristic equation and C can be obtained from the initial conditions. Characteristic equations for growth as also deformation faults have been obtained by Gevers [1954; equations (12) and (28)]. Omitting terms with squares and higher powers of the fault probabilities as also their cross products, combining the two equations and distinguishing between the two types of deformation fault, we have for the characteristic equation:

$$\varrho^6+\alpha_c\varrho^5+\alpha_h\varrho^2+\alpha_{hc}\varrho-(1-2\alpha_h-2\alpha_{hc}-2\alpha_c-6\alpha_{hcc}-3\alpha_{3h})=0 \quad \text{for} \quad \alpha\text{'s}\ll1, \qquad (4)$$

where α_x is the probability of the occurrence of faults of type x (Table 2). For convenience, the relationship to Gevers notation is given below:

$$\alpha_h\to1-\alpha_1=1-\alpha_2; \quad \alpha_{hcc}\to\beta$$
$$\alpha_{hc}\to1-\alpha_3; \quad \alpha_{3h}\to\beta$$
$$\alpha_c\to\alpha_4\,.$$

Solutions of equation (4) may be expressed in the following form:

$$\varrho_\nu=Z_\nu\exp(-2\pi i)\left(\frac{\nu}{6}+X_\nu\right) \qquad \nu=0 \text{ to } 5, \qquad (5)$$

where Z_ν and X_ν are real and are given by

$$Z_0=1-\tfrac{1}{2}\alpha_{hc}-\tfrac{1}{2}\alpha_h-\tfrac{1}{2}\alpha_c-\alpha_{hcc}-\tfrac{1}{2}\alpha_{3h}; \quad X_0=0$$
$$Z_1=1-(\tfrac{5}{12})\alpha_{hc}-\tfrac{1}{4}\alpha_h-(\tfrac{5}{12})\alpha_c-\alpha_{hcc}-\tfrac{1}{2}\alpha_{3h};$$
$$X_1=-\frac{\sqrt{3}}{24\pi}(\alpha_{hc}+\alpha_h-\alpha_c)$$
$$Z_2=1-\tfrac{1}{4}\alpha_{hc}-\tfrac{1}{4}\alpha_h-\tfrac{1}{4}\alpha_c-\alpha_{hcc}-\tfrac{1}{2}\alpha_{3h};$$
$$X_2=-\frac{\sqrt{3}}{24\pi}(\alpha_{hc}-\alpha_h-\alpha_c)$$
$$Z_3=1-(\tfrac{1}{6})\alpha_{hc}-\tfrac{1}{2}\alpha_h-(\tfrac{1}{6})\alpha_c-\alpha_{hcc}-\tfrac{1}{2}\alpha_{3h}; \quad X_3=0$$
$$Z_4=Z_2; \quad X_4=-X_2$$
$$Z_5=Z_1; \quad X_5=-X_1\,. \qquad (6)$$

As mentioned earlier the C_ν's can be found from the initial conditions. These, found by direct evaluation from all possible stacking sequences of six layers, are given below:

$$\langle\exp i\Phi_0\rangle=1$$
$$\langle\exp i\Phi_1\rangle=-\tfrac{1}{2}$$
$$\langle\exp i\Phi_2\rangle=\tfrac{1}{6}(\alpha_{hc}+2\alpha_h-\alpha_c+6\alpha_{3h})$$
$$\langle\exp i\Phi_3\rangle=-\tfrac{1}{6}(2\alpha_{hc}+\alpha_h-2\alpha_c+3\alpha_{3h})$$
$$\langle\exp i\Phi_4\rangle=\tfrac{1}{6}(4\alpha_{hc}-4\alpha_h-\alpha_c+6\alpha_{hcc})$$
$$\langle\exp i\Phi_5\rangle=-\tfrac{1}{2}(1-3\alpha_h-2\alpha_c-4\alpha_{hcc}-2\alpha_{3h}). \qquad (7)$$

Substituting from equations (5), (6) and (7) in equation (3) and solving the resultant set of six simultaneous equations for the C_ν's, we have

Table 2. *Stacking faults in hcc crystals*

Fault	Notation	Process of formation	Stacking sequence
Growth	*hc*	Removal of 1 layer + glide	*c c h c h c h* / *B A B C | B A C A*
	h	Removal of 2 layers + glide	*h c c h h c h* / *C B A B | A C B C*
	c	Insertion of 1 layer + glide	*c h c c c h c* / *A B C A | B A C B*
Deformation	*hcc*	Glide	*c c h c h c c* / *B A B C | B A C B*
	3h	Glide	*h c c h h h c* / *C B A B | A B A C*

$$C_0=0$$

$$C_1=\tfrac{1}{12}\Big\{1+\tfrac{3}{4}\alpha_h-2\alpha_{hcc}-\tfrac{1}{2}\alpha_{3h} - \frac{i}{\sqrt{3}}(\alpha_{hc}+\alpha_c+3\alpha_{hcc}-3\alpha_{3h})\Big\}$$

$$C_2=\tfrac{1}{4}\Big\{1-\tfrac{1}{3}\alpha_{hc}-\tfrac{5}{12}\alpha_h+\tfrac{1}{3}\alpha_c-\tfrac{1}{2}\alpha_{3h} - \frac{i}{4\sqrt{3}}(3\alpha_{3h}-4\alpha_{hcc}+4\alpha_{3h})\Big\}$$

$$C_3=\tfrac{1}{3}\{1+\tfrac{1}{2}\alpha_{hc}+\tfrac{1}{4}\alpha_h-\tfrac{1}{2}\alpha_c+\alpha_{hcc}+\alpha_{3h}\} \quad (8)$$

$$C_4=C_2^*$$

$$C_5=C_1^*$$

where * denotes complex conjugation.

Substituting from equations (3) and (5) in (1), we have on simplification

$$\begin{aligned}I(h_3)=\psi^2&\Big[C_{1r}\sum_m Z_1^{|m|}\cos 2\pi m\left(\frac{h_3}{6}-\tfrac{1}{6}-X_1\right)\\&-C_{1i}\sum_m Z_1^{|m|}\sin 2\pi|m|\left(\frac{h_3}{6}-\tfrac{1}{6}-X_1\right)\Big]\\&+\psi^2\Big[C_{2r}\sum_m Z_2^{|m|}\cos 2\pi m\left(\frac{h_3}{6}-\tfrac{2}{6}-X_2\right)\\&-C_{2i}\sum_m Z_2^{|m|}\sin 2\pi|m|\left(\frac{h_3}{6}-\tfrac{2}{6}-X_2\right)\Big]\\&+\psi^2\Big[C_3\sum_m Z_3^{|m|}\cos 2\pi m\left(\frac{h_3}{6}-\tfrac{3}{6}\right)\Big]\\&+\psi^2\Big[C_{2r}\sum_m Z_2^{|m|}\cos 2\pi m\left(\frac{h_3}{6}-\tfrac{4}{6}+X_2\right)\\&+C_{2i}\sum_m Z_2^{|m|}\sin 2\pi|m|\left(\frac{h_3}{6}-\tfrac{4}{6}+X_2\right)\Big]\\&+\psi^2\Big[C_{1r}\sum_m Z_1^{|m|}\cos 2\pi m\left(\frac{h_3}{6}-\tfrac{5}{6}+X_1\right)\\&+C_{1i}\sum_m Z_1^{|m|}\sin 2\pi|m|\left(\frac{h_3}{6}-\tfrac{5}{6}+X_1\right)\Big] \quad (9)\end{aligned}$$

where C_{vr} and C_{vi} are the real and imaginary parts of C_v and are given by

$$C_{vr}=\tfrac{1}{2}(C_v+C_v^*);\quad C_{vi}=\frac{1}{2i}(C_v-C_v^*)\quad v=1,2. \quad (10)$$

Performing the summations in equation (9), we have

$$\begin{aligned}I(h_3)=\psi^2&C_{1r}\times\frac{1-Z_1^2-2(C_{1i}/C_{1r})Z_1\sin 2\pi\left(\frac{h_3}{6}-\tfrac{1}{6}-X_1\right)}{1+Z_1^2-2Z_1\cos 2\pi\left(\frac{h_3}{6}-\tfrac{1}{6}-X_1\right)}\\&+\psi^2C_{2r}\times\frac{1-Z_2^2-2(C_{2i}/C_{2r})Z_2\sin 2\pi\left(\frac{h_3}{6}-\tfrac{2}{6}-X_2\right)}{1+Z_2^2-2Z_2\cos 2\pi\left(\frac{h_3}{6}-\tfrac{2}{6}-X_2\right)}\\&+\psi^2C_3\cdot\frac{1-Z_3^2}{1+Z_3^2-2Z_3\cos 2\pi\left(\frac{h_3}{6}-\tfrac{3}{6}\right)}\\&+\psi^2C_{2r}\times\frac{1-Z_2^2+2(C_{2i}/C_{2r})Z_2\sin 2\pi\left(\frac{h_3}{6}-\tfrac{4}{6}+X_2\right)}{1+Z_2^2-2Z_2\cos 2\pi\left(\frac{h_3}{6}-\tfrac{4}{6}+X_2\right)}\\&+\psi^2C_{1r}\times\frac{1-Z_1^2+2(C_{1i}/C_{1r})Z_1\sin 2\pi\left(\frac{h_3}{6}-\tfrac{5}{6}+X_1\right)}{1+Z_1^2-2Z_1\cos 2\pi\left(\frac{h_3}{6}-\tfrac{5}{6}+X_1\right)}.\end{aligned} \quad (11)$$

Description of diffraction effects

Reflexions with $H-K=3N$, $L=6M$, M and N integers, remain sharp. For reflexions with $H-K=3N\pm1$, the first, second, third, fourth and fifth terms on the right-hand side of equation (11) give rise to broadened peaks corresponding to $L=6M+1$, $6M+2$, $6M+3$, $6M+4$ and $6M+5$ respectively. In general, there are changes in integrated intensity and profile broadening for all reflexions. Further, except for reflexions with $L=6M\pm3$, all reflexions show profile peak shift and profile asymmetry. These effects can be utilized for estimating fault probabilities. Quantitative expressions for these profile characteristic are given below.

Profile integrated intensity

The integrated intensities T_1, T_2 and T_3 in reciprocal space for reflexions with $L=6M\pm1$, $6M\pm2$ and $6M\pm3$ respectively can be obtained by integrating separately the terms on the right-hand side of equation (11). The fractional changes in the ratios R_{21} and R_{31} of the integrated intensities T_2, T_1 and T_3, T_1 are given by

$$\Delta R_{21}/R_{21}=-\tfrac{1}{6}(2\alpha_{hc}+7\alpha_h-2\alpha_c-12\alpha_{hcc}) \quad (12)$$

$$\Delta R_{31}/R_{31}=\tfrac{1}{2}(\alpha_{hc}-\alpha_h-\alpha_c+6\alpha_{hcc}+3\alpha_{3h}). \quad (13)$$

By experimental measurement of the quantities $\Delta R_{21}/R_{21}$ and $\Delta R_{31}/R_{31}$ one obtains two different compound fault probabilities, that is, combinations of the fault probabilities.

Profile peak shift

For reflexions with $L=6M\pm1$ and $6M\pm2$, the peak shifts after conversion to $2\theta^\circ$ coordinates are given respectively by

$$\Delta(2\theta_m)_1^0=\pm\frac{90\sqrt{3}}{\pi^2}\cdot\frac{|L|d^2}{c^2}\cdot\tan\theta(\alpha_{hc}+\alpha_h-\alpha_c) \quad \text{for } L=6M\pm1 \quad (14)$$

$$\Delta(2\theta_m)_2^0 = \pm \frac{90\sqrt{3}}{\pi^2} \cdot \frac{|L|d^2}{c^2} \cdot \tan\theta(\alpha_{hc} - \alpha_h - \alpha_c) \quad \text{for } L = 6M \pm 2 \ . \quad (15)$$

Profile peak shift measurements thus lead to estimates of two more compound fault probabilities.

Profile integral breadth

The integral breadth is defined as the ratio of the profile integrated intensity and the profile maximum. Considering each of the terms in equation (11) separately and converting to $2\theta^\circ$ coordinates we have

$$(\beta_f)_1^0 = \frac{90}{\pi} \cdot \frac{|L|d^2}{c^2} \cdot \tan\theta(5\alpha_{hc} + 3\alpha_h + 5\alpha_c + 12\alpha_{hcc} + 6\alpha_{3h}) \quad \text{for } L = 6M \pm 1 \quad (16)$$

$$(\beta_f)_2^0 = \frac{90}{\pi} \cdot \frac{|L|d^2}{c^2} \cdot \tan\theta(3\alpha_{hc} + 3\alpha_h + 3\alpha_c + 12\alpha_{hcc} + 6\alpha_{3h}) \quad \text{for } L = 6M \pm 2 \quad (17)$$

$$(\beta_f)_3^0 = \frac{90}{\pi} \cdot \frac{|L|d^2}{c^2} \cdot \tan\theta(2\alpha_{hc} + 6\alpha_h + 2\alpha_c + 12\alpha_{hcc} + 6\alpha_{3h}) \quad \text{for } L = 6M \pm 3 \ . \quad (18)$$

Three additional compound fault parameters can, therefore, be obtained from measurements of $(\beta_f)_1^0$, $(\beta_f)_2^0$ and $(\beta_f)_3^0$.

Profile asymmetry

A simple measure of profile asymmetry is the shift of the centroid of a profile from its peak position. Following Cohen & Wagner (1962), we have from equation (9):

$$\Delta(2\theta_{c-m})_1^0 = \pm \frac{30\sqrt{3}\ln 2}{\pi^2} \cdot \tan\theta \cdot (4\alpha_{hc} + 4\alpha_c + 12\alpha_{hcc} - 12\alpha_{3h}) \quad \text{for } L = 6M \pm 1 \quad (19)$$

$$\Delta(2\theta_{c-m})_2^0 = \pm \frac{30\sqrt{3}\ln 2}{\pi^2} \cdot \tan\theta(3\alpha_{3h} - 4\alpha_{hcc} + 4\alpha_{3h}) \quad \text{for } L = 6M \pm 2 \ . \quad (20)$$

Thus, measurement of asymmetry leads to estimates of two more compound fault parameters.

Discussion

Independent estimates of a total of nine compound fault parameters can be obtained from measurements of the profile characteristics mentioned above. Since there are only five fault probabilities, we have an overdetermined set of equations and, in principle, all five fault probabilities can be found. In practice, small domains and distortions may be present within the specimen in addition to stacking faults. In principle, the effects of distortions can be eliminated by the multiple-order technique of Warren and Averbach (Warren, 1959) while the effects of domain size may be separated by considering reflexions of the type $H-K=3N$ which are not affected by faults (see, *e.g.*, Anantharaman, Rama Rao & Lele, 1972). However, second-order reflexions are, in general, too weak for reliable measurements. Further, for powder photographs, the reflexions 0006 and $11\bar{2}0$ (*i.e.* with $H-K=3N$) are superimposed on the reflexions $10\bar{1}2$ and $10\bar{1}8$ (*i.e.* with $H-K\neq 3N$) respectively. In view of the above limitations in the available data, separation of strain and domain-size effects cannot be accomplished by rigorous methods for this structure. We outline below a method based on the assumption of isotropy of domain size and strain which may be utilized for separating the three effects. At the outset, we may mention that the further development is made on the basis of data being available for the reasonably intense reflexions $10\bar{1}3$, $10\bar{1}4$, $10\bar{1}5$ and $10\bar{1}7$ which are well separated both from each other and from other reflexions. The broadening due to domain size (D) and strain (ε) may be expressed as (Anantharaman *et al.*, 1972)

$$\beta_d^0 = \frac{360}{\pi} \cdot \frac{d\tan\theta}{D} \quad (21)$$

$$\beta_s^0 = \frac{720}{\pi} \cdot \varepsilon\tan\theta \ . \quad (22)$$

Following Halder & Wagner (1966), we may write for the total broadening β as follows

$$\beta_d + \beta_f = \beta - \frac{\beta_s^2}{\beta} \ . \quad (23)$$

Substituting from equations (21) and (22) in the above and dividing both sides by $(360/\pi)\, d\tan\theta$, we have

$$\frac{1}{D} + F_v(\alpha) = \frac{\pi}{360} \cdot \frac{\beta}{d\tan\theta} - \frac{4\varepsilon^2/d^2}{\frac{\pi}{360} \cdot \frac{\beta}{d\tan\theta}} \quad (24)$$

where $F_v(\alpha)$ takes the values $F_1(\alpha)$, $F_2(\alpha)$ and $F_3(\alpha)$ for reflexions with $L = 6M \pm 1$, $6M \pm 2$ and $6M \pm 3$ respectively. The $F_v(\alpha)$'s are functions of the fault probabilities whose values may be found from equations (16) to (18). Introducing

$$\beta^* = \frac{\pi}{360} \cdot \frac{\beta}{d\tan\theta} \quad (25)$$

and rewritting equation (24) explicitly for each of the reflexions $10\bar{1}3$, $10\bar{1}4$, $10\bar{1}5$ and $10\bar{1}7$ which we designate by the suffices 1, 2, 3 and 4 respectively, we obtain

$$\frac{1}{D} + F_3(\alpha) = \beta_1^* - \frac{4\varepsilon^2/d_1^2}{\beta_1^*} \quad (26)$$

$$\frac{1}{D} + F_2(\alpha) = \beta_2^* - \frac{4\varepsilon^2/d_2^2}{\beta_2^*} \quad (27)$$

$$\frac{1}{D} + F_1(\alpha) = \beta_3^* - \frac{4\varepsilon^2/d_3^2}{\beta_3^*} \quad (28)$$

$$\frac{1}{D} + F_1(\alpha) = \beta_4^* - \frac{4\varepsilon^2/d_4^2}{\beta_4^*} \ . \quad (29)$$

We first solve equations (28) and (29) for ε and $(1/D)+F_1(\alpha)$. The value of ε is then substituted in equations (26) and (27) to yield estimates of $(1/D)+F_3(\alpha)$ and $(1/D)+F_2(\alpha)$. Eliminating $(1/D)$ from each of the two pairs of equations, we can evaluate two independent combinations of $F_1(\alpha)$, $F_2(\alpha)$ and $F_3(\alpha)$, say $F_1(\alpha)-F_2(\alpha)$ and $F_2(\alpha)-F_3(\alpha)$. These could then be utilized along with estimates of three other compound fault parameters obtained from other measurements, say profile peak shift and profile asymmetry for the $10\bar{1}4$, $10\bar{1}5$ and $10\bar{1}7$ reflexions to enable a complete evaluation of the fault probabilities to be made.

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A Method of Determining the Distortion of Coordination Polyhedra

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The distortion of an observed coordination polyhedron can be evaluated from a comparison of this polyhedron with the least-squares best-fit polyhedron with optimum location, orientation, size parameters and prescribed symmetry. A set of atoms at positions, $\mathbf{x}(1), \ldots \mathbf{x}(n)$, may be fitted to the set $\mathbf{y}(1), \ldots \mathbf{y}(n)$ by rearranging the matrix equations:

$$\mathbf{y}(i)=\mathbf{t}+R\lambda(i)\mathbf{x}(i) \quad (i=1,n)$$

and solving for the unknown parameters of the translation vector, $\mathbf{t}$, the rotation matrix, R, and the (diagonal) dilation matrices, $\lambda(i)$, which optimize the fit between the two sets. The elements of the (one or more) dilation matrices may be constrained to fix the fitted set to the desired symmetry. The solution is effected by means of a two-stage iterative least-squares technique employing the so-called 'small-angle' rotation matrix. The average distance between corresponding atoms of the two sets, which is a minimum at the point of optimum fit, provides a unique one-parameter characterization of the degree of distortion between the two configurations. The magnitudes of the operations needed to produce the best fit are also recoverable from the least-squares solution.

Introduction

Coordination polyhedra observed in crystal structures are, more often than not, distorted to some degree from their ideal configurations. The extent of this distortion is a significant crystal chemical parameter. It is, however, difficult to determine quantitatively. Several methods of characterizing such distortion have been suggested (see, *e.g.*, Robinson, Gibbs & Ribbe, 1971) and, in general, are measures of the spread of interatomic distances or angles about their means or ideal values. Undoubtedly such variation in bond length and angles does increase from undistorted to more distorted polyhedra. It is, however, not uncommon to encounter real polyhedra, which are distorted from some ideal configuration, but yet have all bond lengths equal or all bond angles equal to those of the ideal configuration. Furthermore, it may be desirable to know the degree of distortion relative to a lower symmetry subgroup of the ideal configuration,