International Tables for Crystallography (2006). Vol. C, Table 9.2.1.3, p. 758.

Jahnke, 1970; Farkas-Jahnke & Dornberger-Schiff, 1969) and have been reviewed by Farkas-Jahnke (1983). These have been used to derive the structures of ZnS, SiC, and $TiS_{1.7}$ polytypes. These methods are extremely sensitive to experimental errors in the intensities.

9.2.1.8. *Stacking faults in close-packed structures*

The two alternative positions for the stacking of successive close-packed layers give rise to the possibility of occurrence of faults where the stacking rule is broken without violating the law of close packing. Such faults are frequently observed in crystals of polytypic materials as well as close-packed martensites of cobalt, noble-metal-based and certain iron-based alloys (Andrade, Chandrasekaran & Delaey 1984; Kabra, Pandey & Lele, 1988*a*; Nishiyama, 1978; Pandey, 1988).

The classical method of classifying stacking faults in 2*H* and 3*C* structures as growth and deformation types, depending on whether the fault has resulted as an accident during growth or by shear through the vector **s**, leads to considerable ambiguities since the same fault configuration can result from more than one physical process. For a detailed account of the limitations of the notations based on the process of formation, the reader is referred to the articles by Pandey (1984*a*) and Pandey & Krishna (1982*b*).

Frank (1951) has classified stacking faults as intrinsic or extrinsic purely on geometrical considerations. In intrinsic faults, the perfect stacking sequence on each side of the fault extends right up to the contact plane of the two crystal halves while in extrinsic faults the contact plane does not belong to the stacking sequence on either side of it. In intrinsic faults, the contact plane may be an atomic or non-atomic plane whereas in extrinsic faults the contact plane is always an atomic plane. Instead of contact plane, one can use the concept of fault plane defined with respect to the initial stacking sequence. This system of classification is preferable to that based on the process of formation. However, the terms intrinsic and extrinsic have been used in the literature in a very restricted sense by associating these with the precipitation of vacancies and interstitials, respectively (see, for example, Weertman & Weertman, 1984). While the precipitation of vacancies may lead to intrinsic fault configuration, this is by no means the only process by which intrinsic faults can result. For example, there are geometrically 18 possible intrinsic fault configurations in the 6*H* (33) structure (Pandey & Krishna, 1975) but only two of these can result from the precipitation of vacancies. Similarly, layer-displacement faults involved in SiC transformations are extrinsic type but do not result from the precipitation of interstitials (see Pandey, Lele & Krishna, 1980*a*,*b*,*c*; Kabra, Pandey & Lele, 1986). It is therefore desirable not to associate the geometrical notation of Frank with any particular process of formation.

The intrinsic–extrinsic scheme of classification of faults when used in conjunction with the concept of assigning subscripts to different close-packed layers (Prasad & Lele, 1971; Pandey & Krishna, 1976*b*) can provide a very compact and unique way of representing intrinsic fault configurations even in long-period structures (Pandey, 1984*b*). We shall briefly explain this notation in relation to one hexagonal (6*H*) and one rhombohedral (9*R*) structure.

Table 9.2.1.3. *Intrinsic fault configurations in the 6H* (*$A_0B_1C_2A_3C_4B_5$, …*) *structure*

Fault configuration *ABC* sequence	Subscript notation
$\ldots A\,B\,C\,A\,C\,B\,A_0 \mid C_0\,A\,B\,C\,B\,A\,C \ldots$	$I_{0,0}$
$\ldots A\,B\,C\,A\,C\,B\,A_0 \mid C_1\,A\,B\,A\,C\,B\,C \ldots$	$I_{0,1}$
$\ldots A\,B\,C\,A\,C\,B\,A_0 \mid C_2\,A\,C\,B\,A\,B\,C \ldots$	$I_{0,2}$
$\ldots A\,B\,C\,A\,C\,B\,A_0 \mid C_3\,B\,A\,C\,A\,B\,C \ldots$	$I_{0,3}$
$\ldots A\,B\,C\,A\,C\,B\,A_0 \mid C_4\,B\,A\,B\,C\,A\,C \ldots$	$I_{0,4}$
$\ldots A\,B\,C\,A\,C\,B\,A_0 \mid C_5\,B\,C\,A\,B\,A\,C \ldots$	$I_{0,5}$
$\ldots A\,B\,C\,A\,C\,B\,A\,B_1 \mid A_0\,B\,C\,A\,C\,B\,A \ldots$	$I_{1,0}$
$\ldots A\,B\,C\,A\,C\,B\,A\,B_1 \mid A_1\,B\,C\,B\,A\,C\,A \ldots$	$I_{1,1}$
$\ldots A\,B\,C\,A\,C\,B\,A\,B_1 \mid A_2\,B\,A\,C\,B\,C\,A \ldots$	$I_{1,2}$
$\ldots A\,B\,C\,A\,C\,B\,A\,B_1 \mid A_3\,C\,B\,A\,B\,C\,A \ldots$	$I_{1,3}$
$\ldots A\,B\,C\,A\,C\,B\,A\,B_1 \mid A_4\,C\,B\,C\,A\,B\,A \ldots$	$I_{1,4}$
$\ldots A\,B\,C\,A\,C\,B\,A\,B_1 \mid A_5\,C\,A\,B\,C\,B\,A \ldots$	$I_{1,5}$
$\ldots A\,B\,C\,A\,C\,B\,A\,B\,C_2 \mid B_0\,C\,A\,B\,A\,C\,B \ldots$	$I_{2,0}$
$\ldots A\,B\,C\,A\,C\,B\,A\,B\,C_2 \mid B_1\,C\,A\,C\,B\,A\,B \ldots$	$I_{2,1}$
$\ldots A\,B\,C\,A\,C\,B\,A\,B\,C_2 \mid B_2\,C\,B\,A\,C\,A\,B \ldots$	$I_{2,2}$
$\ldots A\,B\,C\,A\,C\,B\,A\,B\,C_2 \mid B_3\,A\,C\,B\,C\,A\,B \ldots$	$I_{2,3}$
$\ldots A\,B\,C\,A\,C\,B\,A\,B\,C_2 \mid B_4\,A\,C\,A\,B\,C\,B \ldots$	$I_{2,4}$
$\ldots A\,B\,C\,A\,C\,B\,A\,B\,C_2 \mid B_5\,A\,B\,C\,A\,C\,B \ldots$	$I_{2,5}$

Notes:

(1) Dotted vertical lines represent the location of the fault plane with respect to the initial stacking sequence on the left-hand side.

(2) $I_{0,1}$ and $I_{2,3}$, $I_{0,2}$ and $I_{1,3}$, $I_{1,1}$ and $I_{2,2}$, and $I_{1,4}$ and $I_{2,5}$ are crystallographically equivalent.

In the 6*H* (*ABCACB*, … or *hkkhkk*) structure, six kinds of layers that can be assigned subscripts 0, 1, 2, 3, 4, and 5 need to be distinguished (Pandey, 1984*b*). Choosing the 0-type layer in '*h*' configuration such that the layer next to it is related through the shift vector +**s** (which causes cyclic $A \rightarrow B \rightarrow C \rightarrow A$ shift), the perfect 6*H* structure can be written as

$$\begin{array}{ccccccccccccc} & h & k & k & h & k & k & h & k & k & h & k & k \\ \ldots & A_0 & B_1 & C_2 & A_3 & C_4 & B_5 & A_0 & B_1 & C_2 & A_3 & C_4 & B_5 \ldots . \\ & & +\mathbf{s} & +\mathbf{s} & +\mathbf{s} & -\mathbf{s} & -\mathbf{s} & -\mathbf{s} & +\mathbf{s} & +\mathbf{s} & +\mathbf{s} & -\mathbf{s} & -\mathbf{s} \end{array}$$

There are six crystallographically equivalent ways of writing this structure with the first layer in position *A*: (i) $A_0B_1C_2A_3C_4B_5$; (ii) $A_1B_2C_3B_4A_5C_0$; (iii) $A_2B_3A_4C_5B_0C_1$; (iv) $A_3C_4B_5A_0B_1C_2$; (v) $A_4C_5B_0C_1A_2B_3$; and (vi) $A_5C_0A_1B_2C_3B_4$. Similarly, there are six ways of writing the 6*H* structure with the starting layer in position *B* or *C*. Since an intrinsic fault marks the beginning of a fresh 6*H* sequence, there can be 36 possible intrinsic fault configurations in the 6*H* (*ABCACB*, …) structure. All these intrinsic fault configurations can be described by symbols like $I_{r,s}$, where *r* and *s* stand for the subscript of the layer on the left- and right-hand sides of the fault plane while *I* represents intrinsic. Knowing the two symbols (*r* and *s*), one can write down the complete *ABC* stacking sequence. It may be noted that, of the 36 possible intrinsic fault configurations, only 14 are crystallographically indistinguishable (for details, see Pandey, 1984*b*). This notation can be used for any hexagonal polytype and requires only the identification of various layer types in the structure. For rhombohedral polytypes, one must consider the layer types in both the obverse and the reverse settings. For example, six layer types need to be distinguished in the 9*R* (*hhk*) structure:

Obverse:

$$\begin{array}{cccccccccc} & h & h & k & h & h & k & h & h & k \\ \ldots & A_0 & B_1 & A_2 & C_0 & A_1 & C_2 & B_0 & C_1 & B_2 \ldots ; \\ & & +\mathbf{s} & -\mathbf{s} & -\mathbf{s} & +\mathbf{s} & -\mathbf{s} & -\mathbf{s} & +\mathbf{s} & -\mathbf{s} \end{array}$$