Table 9.2.1.4. *Intrinsic fault configurations in the 9R* ($A_0B_1A_2C_0A_1C_2B_0C_1B_2, \ldots$) *structure*

Fault configuration *ABC* sequence	Subscript notation
$\ldots A\ B\ A\ C\ A\ C\ B\ C\ B\ A_0 \mid C_0\ A\ C\ B\ C\ B\ A\ B\ A \ldots$	$I_{0,0}$
$\ldots A\ B\ A\ C\ A\ C\ B\ C\ B\ A_0 \mid C_1\ B\ A\ B\ A\ C\ A\ C\ B \ldots$	$I_{0,1}$
$\ldots A\ B\ A\ C\ A\ C\ B\ C\ B\ A_0 \mid C_2\ B\ C\ B\ A\ B\ A\ C\ A \ldots$	$I_{0,2}$
$\ldots A\ B\ A\ C\ A\ C\ B\ C\ B\ A_0 \mid C_{\bar{0}}\ B\ C\ A\ C\ A\ B\ A\ B \ldots$	$I_{0,\bar{0}}$
$\ldots A\ B\ A\ C\ A\ C\ B\ C\ B\ A_0 \mid C_{\bar{1}}\ A\ B\ A\ B\ C\ B\ C\ A \ldots$	$I_{0,\bar{1}}$
$\ldots A\ B\ A\ C\ A\ C\ B\ C\ B\ A_0 \mid C_{\bar{2}}\ A\ C\ A\ B\ A\ B\ C\ B \ldots$	$I_{0,\bar{2}}$
$\ldots A\ B\ A\ C\ A\ C\ B\ C\ B\ A\ B_1 \mid C_0\ A\ C\ B\ C\ B\ A\ B\ A \ldots$	$I_{1,0}$
$\ldots A\ B\ A\ C\ A\ C\ B\ C\ B\ A\ B_1 \mid C_1\ B\ A\ B\ A\ C\ A\ C\ B \ldots$	$I_{1,1}$
$\ldots A\ B\ A\ C\ A\ C\ B\ C\ B\ A\ B_1 \mid C_2\ B\ C\ B\ A\ B\ A\ C\ A \ldots$	$I_{1,2}$
$\ldots A\ B\ A\ C\ A\ C\ B\ C\ B\ A\ B_1 \mid C_{\bar{0}}\ B\ C\ A\ C\ A\ B\ A\ B \ldots$	$I_{1,\bar{0}}$
$\ldots A\ B\ A\ C\ A\ C\ B\ C\ B\ A\ B_1 \mid C_{\bar{1}}\ A\ B\ A\ B\ C\ B\ C\ A \ldots$	$I_{1,\bar{1}}$
$\ldots A\ B\ A\ C\ A\ C\ B\ C\ B\ A\ B_1 \mid C_{\bar{2}}\ A\ C\ A\ B\ A\ B\ C\ B \ldots$	$I_{1,\bar{2}}$
$\ldots A\ B\ A\ C\ A\ C\ B\ C\ B\ A\ B\ A_2 \mid B_0\ C\ B\ A\ B\ A\ C\ A\ C \ldots$	$I_{2,0}$
$\ldots A\ B\ A\ C\ A\ C\ B\ C\ B\ A\ B\ A_2 \mid B_1\ A\ C\ A\ C\ B\ C\ B\ A \ldots$	$I_{2,1}$
$\ldots A\ B\ A\ C\ A\ C\ B\ C\ B\ A\ B\ A_2 \mid B_2\ A\ B\ A\ C\ A\ C\ B\ C \ldots$	$I_{2,2}$
$\ldots A\ B\ A\ C\ A\ C\ B\ C\ B\ A\ B\ A_2 \mid B_{\bar{0}}\ A\ B\ C\ B\ C\ A\ C\ A \ldots$	$I_{2,\bar{0}}$
$\ldots A\ B\ A\ C\ A\ C\ B\ C\ B\ A\ B\ A_2 \mid B_{\bar{1}}\ C\ A\ C\ A\ B\ A\ B\ C \ldots$	$I_{2,\bar{1}}$
$\ldots A\ B\ A\ C\ A\ C\ B\ C\ B\ A\ B\ A_2 \mid B_{\bar{2}}\ C\ B\ C\ A\ C\ A\ B\ A \ldots$	$I_{2,\bar{2}}$

Note: $I_{0,\bar{0}}$ and $I_{1,\bar{1}}$, $I_{0,\bar{1}}$ and $I_{1,\bar{2}}$, $I_{0,\bar{2}}$ and $I_{2,\bar{1}}$, and $I_{1,2}$ and $I_{2,0}$ are crystallographically equivalent.

Reverse:

$$\begin{array}{cccccccccc} & h & h & k & h & h & k & h & h & k & \\ \ldots & A_{\bar{0}} & C_{\bar{1}} & A_{\bar{2}} & B_{\bar{0}} & A_{\bar{1}} & B_{\bar{2}} & C_{\bar{0}} & B_{\bar{1}} & C_{\bar{2}} & \ldots. \\ & -\mathbf{s} & +\mathbf{s} & +\mathbf{s} & -\mathbf{s} & +\mathbf{s} & +\mathbf{s} & -\mathbf{s} & +\mathbf{s} & & \end{array}$$

In the obverse setting, we choose the origin layer (0 type) in the *h* configuration such that the next layer is cyclically shifted whereas in the reverse setting the origin layer ($\bar{0}$ type) in the *h* configuration is related to the next layer through an anticyclic shift. Tables 9.2.1.3 and 9.2.1.4 list the crystallographically unique intrinsic fault configurations in the 6*H* and 9*R* structures.

9.2.1.8.1. *Structure determination of one-dimensionally disordered crystals*

Statistical distribution of stacking faults in close-packed structures introduces disorder along the stacking axis of the close-packed layers. As a result, one observes on a single-crystal diffraction pattern not only normal Bragg scattering near the nodes of the reciprocal lattice of the average structure but also continuous diffuse scattering between the nodes owing to the incomplete destructive interference of scattered rays. Just like the extra polytype reflections, the diffuse streaks are also confined to only those rows for which $h - k \neq 0 \bmod 3$. A complete description of the real structure of such one-dimensionally disordered polytypes requires knowledge of the average structure as well as a statistical specification of the fluctuations due to stacking faults in the electron-density distribution of the average structure. This cannot be accomplished by the usual consideration of the normal Bragg reflections alone but requires a careful analysis of the diffuse intensity distribution as well (Pandey, Kabra & Lele, 1986).

The first step in the structure determination of one-dimensionally disordered structures is the specification of the geometry of stacking faults and their distribution, both of which require postulation of the physical processes responsible for their formation. An entirely random distribution of faults may result during the layer-by-layer growth of a crystal (Wilson, 1942) or during plastic deformation (Paterson, 1952). On the other hand, when faults bring about the change in the stacking sequence of layers during solid-state transformations, their distribution is non-random (Pandey, Lele & Krishna, 1980*a*,*b*,*c*; Pandey & Lele, 1986*a*,*b*; Kabra, Pandey & Lele, 1986). Unlike growth faults, which are accidentally introduced in a sequential fashion from one end of the stack of layers to the other during the actual crystal growth, stacking faults involved in solid-state transformations are introduced in a random space and time sequence (Kabra, Pandey & Lele, 1988*b*). Since the pioneering work of Wilson (1942), several different techniques have been advanced for the calculation of intensity distributions along diffuse streaks making use of Markovian chains, random walk, stochastic matrices, and the Paterson function for random and non-random distributions of stacking faults on the assumption that these are introduced in a sequential fashion (Hendricks & Teller, 1942; Jagodzinski 1949*a*,*b*; Kakinoki & Komura, 1954; Johnson, 1963; Prasad & Lele, 1971; Cowley, 1976; Pandey, Lele & Krishna, 1980*a*,*b*). The limitations of these methods for situations where non-randomly distributed faults are introduced in the random space and time sequence have led to the use of Monte Carlo techniques for the numerical calculation of pair correlations whose Fourier transforms directly yield the intensity distributions (Kabra & Pandey, 1988).

The correctness of the proposed model for disorder can be verified by comparing the theoretically calculated intensity distributions with those experimentally observed. This step is in principle analogous to the comparison of the observed Bragg intensities with those calculated for a proposed structure in the structure determination of regularly ordered layer stackings. This comparison cannot, however, be performed in a straightforward manner for one-dimensionally disordered crystals due to special problems in the measurement of diffuse intensities using a single-crystal diffractometer, stemming from incident-beam divergence, finite size of the detector slit, and multiple scattering. The problems due to incident-beam divergence in the measurement of the diffuse intensity distributions were first

 references