the centre of the perfect crystal (*A–B–A* stacking) is replaced by an inversion centre at the midpoint of the single rhombohedral cell *A–B–C*; the projected symmetry is also reduced from hexagonal to trigonal: both whole pattern and central beam then have the symmetry of $3m1$. The $2H$ polytype of TaS_2 ($P6_3/mmc$) (Tanaka & Terauchi, 1985) gives a second clear example. (*b*) In the case of a [111] gold crystal, sectioning the f.c.c. structure parallel to [111] preparatory to producing the twin already reduces the finite crystal symmetry to $R\bar{3}m$, *i.e.* a trigonal space group for which the central beam, and the HOLZ reflections in particular, exhibit the trigonal symmetry of $31m$ (rather than the $3m1$ of trigonal graphite). A central-plane twin boundary with no associated translation introduces a central horizontal mirror plane into the crystal. For the zone-axis pattern the only symmetry change will be in the central beam, which will become centrosymmetric, increasing its symmetry to $6mm$. Using diffraction-group terminology these cases are seen to be relative inverses. Unfaulted graphite has the BESR group $6mm1_R$ (central beam and whole pattern hexagonal); central-plane faulting results in a change to the group 6_Rmm_R. Unfaulted [111] gold correspondingly has the BESR group symmetry 6_Rmm_R; central-plane twinning results in the addition of the element 1_R (for a central mirror plane), leading to the group $6mm1_R$.

(iv) Finally, no present-day discussion of electron-crystallographic investigations of symmetry could be complete without reference to two aspects of non-classical symmetries widely discussed in the literature in recent years. The recent discovery of noncrystallographic point symmetries in certain alloys (Shechtman *et al.*, 1984) has led to the study of quasi-crystallinity. An excellent record of the experimental side of this subject may be found in the book *Convergent-beam electron diffraction III* by Tanaka *et al.* (1994), while the appropriate space-group theory has been developed by Mermin (1992). It would be inappropriate to comment further on this new subject here other than to state that this is clearly an area of study where combined HREM, CBED and selected-area diffraction (SAD) evidence is vital to structural elucidation.

The other relatively new topic is that of modulated structures. From experimental evidence, two distinct structural phenomena can be distinguished for structures exhibiting incommensurate superlattice reflections. Firstly, there are 'Vernier' phases, which exist within certain composition ranges of solid solutions and are composed of two extensive substructures, for which the superspace-group nomenclature developed by de Wolff *et al.* (1981) is structurally valid (*e.g.* Withers *et al.*, 1993). Secondly, there are structures essentially composed of random mixtures of two or more substructures existing as microdomains within the whole crystal (*e.g.* Grzinic, 1985). Here the SAD patterns will contain superlattice reflections with characteristic profiles and/or irregularities of spacings. A well illustrated review of incommensurate-structure analysis in general is given in the book by Tanaka *et al.* (1994), while specific discussions of this topic are given by Goodman *et al.* (1992), and Goodman & Miller (1993).

2.5.3.7. *Present limitations and general conclusions*

The list of examples given here must necessarily be regarded as unsatisfactory considering the vastness of the subject, although some attempt has been made to choose a diverse range of problems which will illustrate the principles involved. Some particular aspects, however, need further mention.

One of these concerns the problem of examining large-unit-cell materials with a high diffraction-pattern density. This limits the possible convergence angle, if overlap is to be avoided, and leaves numerous but featureless discs [for example Goodman (1984*b*)]. Technical advances which have been made to overcome this problem include the beam-rocking technique (Eades, 1980) and LACBED (Tanaka *et al.*, 1980), both of which are reviewed by Tanaka & Terauchi (1985) and Eades *et al.* (1983). The disadvantage of these latter methods is that they both require a significantly larger area of specimen than does the conventional technique, and it may be that more sophisticated methods of handling the crowded conventional patterns are still needed.

Next, the matter of accuracy must be considered. There are two aspects of the subject where this is of concern. Firstly, there is a very definite limit to the sensitivity with which symmetry can be detected. In a simple structure of medium-light atoms, displacements of say 0.1 Å or less from a pseudomirror plane could easily be overlooked. An important aspect of CBED analysis, not mentioned above, is the *N*-beam computation of patterns which is required when something approaching a refinement (in the context of electron diffraction) is being attempted. Although this quantitative aspect has a long history [for example see Johnson (1972)], it has only recently been incorporated into symmetry studies as a routine (Creek & Spargo, 1985; Tanaka, 1994). Multi-slice programs which have been developed to produce computer-simulated pattern output are available (Section 2.5.3.8).

Next there is concern as to the allocation of a space group to structures which microscopically have a much lower symmetry (Goodman *et al.*, 1984). This arises because the volume sampled by the electron probe necessarily contains a large number of unit cells. Reliable microscopic interpretation of certain nonstoichiometric materials requires that investigations be accompanied by high-resolution microscopy. Frequently (especially in mineralogical samples), nonstoichiometry implies that a space group exists only on average, and that the concept of absolute symmetry elements is inapplicable.

From earlier and concluding remarks it will be clear that combined X-ray/CBED and CBED/electron-microscopy studies of inorganic materials represents the standard ideal approach to space-group analysis at present; given this approach, all the space-group problems of classical crystallography appear soluble. As has been noted earlier, it is important that HREM be considered jointly with CBED in determining space group by electron crystallography, and that only by this joint study can the so-called 'phase problem' be completely overcome. The example of the space-group pairs $I222/I2_12_12_1$ and $I23/I2_13$ has already been cited. Using CBED, it might be expected that FOLZ lines would show a break from twofold symmetry with the incident beam aligned with a 2_1 axis. However, a direct distinction should be made apparent from high-resolution electron micrographs. Other less clear-cut cases occur where the HREM images allow a space-group distinction to be made between possible space groups of the same arithmetic class, especially when only one morphology is readily obtained (*e.g.* $P222_1$, $P22_12_1$, $P2_12_12_1$).

The slightly more subtle problem of distinguishing enantiomorphic space-group pairs can be solved by one of two approaches: either the crystal must be rotated around an axis by a known amount to obtain two projections, or the required three-dimensional phase information can be deduced from specific three-beam-interaction data. This problem is part of the more general problem of solving handedness in an asymmetric structure, and is discussed in detail by Johnson & Preston (1994).

2.5.3.8. *Computer programs available*

(1) A FORTRAN source listing of program *TCBED* for simulating three-dimensional convergent-beam patterns with absorption by the Bloch-wave method: Zuo *et al.* (1989) [see also *Electron microdiffraction* (Spence & Zuo, 1992) for other useful programs and worked examples for the analysis of these diffraction

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references