Table 2.5.3.13. *Wavevectors, point- and space-group symbols and CBED symmetries of one-dimensionally modulated crystals*

Wavevector transformation	Point-group symbol	Symmetry of incommensurate reflection	Space-group symbol	Dynamical extinction lines
$\mathbf{k} \rightarrow \mathbf{k}$	1	Same symmetry as average structure	1, s (1/2), t ($\pm$1/3), q ($\pm$1/4), h ($\pm$1/6)	Yes for s, q and h
$\mathbf{k} \rightarrow -\mathbf{k}$	$\bar{1}$	No symmetry	$\bar{1}$	No

reflections ought to show the symmetry of the average structure, while the incommensurate reflections lose the symmetry.

The problem of the finite size of the illuminated area is discussed using equations (2.5.3.7) and (2.5.3.8) in a paper by Terauchi & Tanaka (1993) and in the book by Tanaka *et al.* (1994, pp. 156–205). The results are as follows: Even if the size and position of an illuminated specimen area are changed, the intensity distribution in a CBED pattern changes but the symmetry of the pattern does not. To obtain the symmetries of incommensurate crystals, it is not necessary to take CBED patterns from an area whose diameter is larger than the period of the modulated structure. The symmetries of the modulated structure can appear when more than one unit cell of the average structure is illuminated for displacive modulations. For substitutional modulations, a specimen volume that produces the average atom form factor is needed, namely a volume of about 1 nm diameter area and 50 nm thick.

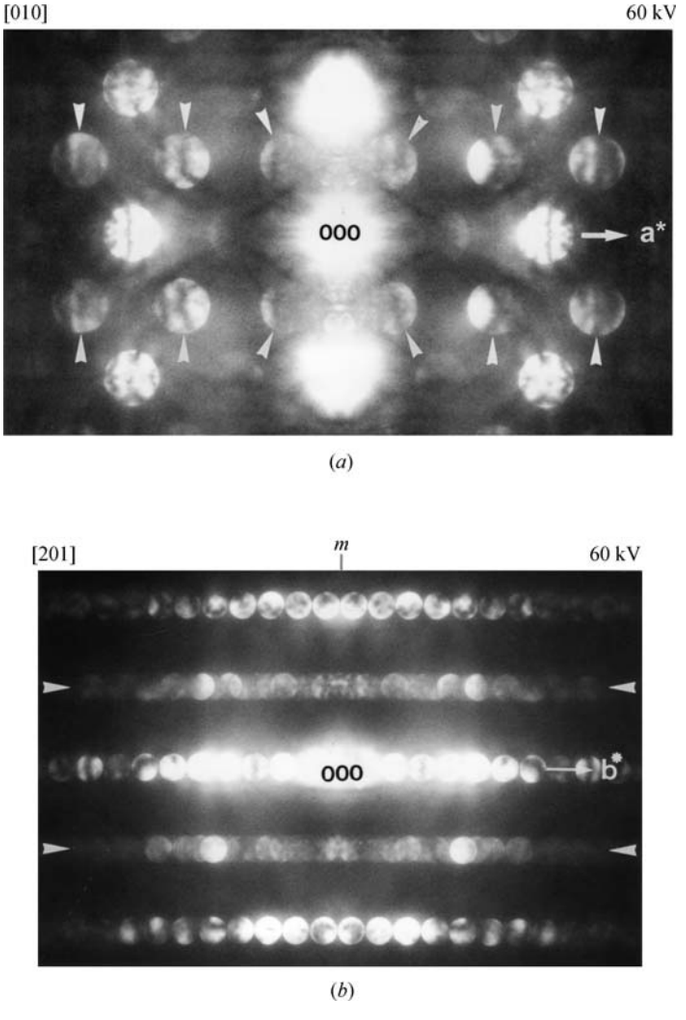

Fig. 2.5.3.19. CBED patterns of the incommensurate phase of $Sr_2Nb_2O_7$ taken at 60 kV. (*a*) [010] incidence: fundamental reflections show a mirror symmetry perpendicular to the a^* axis but incommensurate reflections do not [symmetry ($^m_1$)]. (*b*) [201] incidence: incommensurate reflections show mirror symmetry perpendicular to the b^* axis [symmetry ($^m_1$)]. The wave number vector of the modulation is $\mathbf{k} = (\frac{1}{2} - \delta)\mathbf{a}^*$.

Table 2.5.3.13 shows the point-group symmetries (third column) of the incommensurate reflections for the two point-group subsymbols. For symmetry subsymbol 1, both the fundamental and incommensurate reflections show the symmetries of the average structure. For symmetry subsymbol $\bar{1}$, the fundamental reflections show the symmetries of the average structure but the incommensurate reflections do not have any symmetry. These facts imply that the symmetries of the incommensurate reflections are determined by the point group of the average structure and the modulation wavevector **k**. In other words, observation of the symmetries of the incommensurate reflections is not necessary for the determination of the point groups, although it can ascertain the point groups of the modulated crystals.

An example of point-group determination is shown for the incommensurate phase of $Sr_2Nb_2O_7$. Many materials of the $A_2B_2O_7$ family undergo phase transformations from space group $Cmcm$ to $Cmc2_1$ and further to $P2_1$ with decreasing temperature. An incommensurate phase appears between the $Cmc2_1$ phase and the $P2_1$ phase. $Sr_2Nb_2O_7$ transforms at 488 K from the $Cmc2_1$ phase into the incommensurate phase with a modulation wavevector $\mathbf{k} = (\frac{1}{2} - \delta)\mathbf{a}^*$ (δ = 0.009–0.023) but does not transform into the $P2_1$ phase. The space group of $Sr_2Nb_2O_7$ was reported as $P^{C\,mc2_1}_{\bar{1}s\bar{1}}$ (Yamamoto, 1988). (Since the space-group notation $Cmc2_1$ is broadly accepted, the direction of the modulation is taken as the a axis.) The point group of the phase is $^{mm2}_{1\,1\,\bar{1}}$. The modulation wavevector **k** is transformed to $-\mathbf{k}$ by the mirror symmetry operation perpendicular to the a axis ($^m_1$) and by the twofold rotation symmetry operation about the c axis ($^2_1$). The wavevector is transformed into itself by the mirror symmetry operation perpendicular to the b axis ($^m_1$).

Fig. 2.5.3.19(*a*) shows a CBED pattern of the incommensurate phase of $Sr_2Nb_2O_7$ taken with the [010] incidence at an accelerating voltage of 60 kV. The reflections indicated by arrowheads are the incommensurate reflections. Other reflections are the fundamental reflections. Since the pattern is produced by the interaction of the reflections in the zeroth-order Laue zone, symmetry operations ($^m_1$) and ($^2_1$) act the same. These symmetries are confirmed by the fact that the fundamental reflections show mirror symmetry perpendicular to the a^* axis (twofold rotation symmetry about the c^* axis) but the incommensurate reflections do not. Fig. 2.5.3.19(*b*) shows a CBED pattern of the incommensurate phase of $Sr_2Nb_2O_7$ taken with the [201] incidence at 60 kV. The reflections in the two rows indicated by arrowheads are the incommensurate reflections and the others are the fundamental reflections. Symmetry symbol ($^m_1$) implies that both the fundamental and incommensurate reflections display mirror symmetry perpendicular to the b^* axis. Fig. 2.5.3.19(*b*) exactly exhibits the symmetry.

2.5.3.4.3. Space-group determination

Table 2.5.3.13 shows the space-group symbols (fourth column) of the modulated crystals. When a glide (screw) component τ_4 between the modulation waves of two atom rows is 0, 1/2, $\pm$1/3, $\pm$1/4 or $\pm$1/6, symbol 1, s, t, q or h is given, respectively (de Wolff *et al.*, 1981). Such glide components are allowed for point-group symmetry 1 but are not for point-group symmetry $\bar{1}$. Dynamical