International Tables for Crystallography (2010). Vol. B, Figure 2.5.3.21, p. 350.

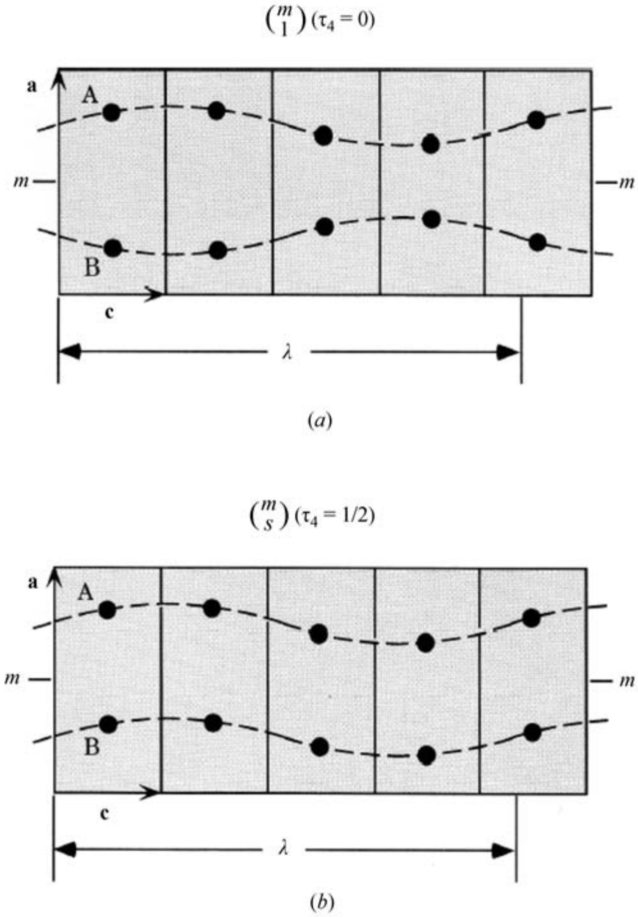

Fig. 2.5.3.20. (*a*) Mirror symmetry of modulation waves $\binom{m}{1}$ $\tau_4 = 0$. (*b*) Glide symmetry of modulation waves $\binom{m}{s}$ $\tau_4 = \frac{1}{2}$. The wave number vector of modulation is $k_3\mathbf{c}^*$.

extinction occurs for glide components *s*, *q* and *h* but does not for glide component *t*. When the average structure does not have a glide component, dynamical extinction due to a glide component τ_4 appears in odd-order incommensurate reflections. When the average structure has a glide component, dynamical extinction due to a glide component τ_4 appears in incommensurate reflections with $h_i + h_4 = 2n + 1$, where h_i and h_4 are the reflection indices for the average structure and incommensurate structure, respectively. Details are given in the paper by Terauchi *et al.* (1994).

Fig. 2.5.3.20(*a*) illustrates mirror symmetry $\binom{m}{1}$ between atom rows A and B, which is perpendicular to the *b* axis with no glide component ($\tau_4 = 0$). Here, the wave number vector of the modulation is assumed to be $\mathbf{k} = k_3\mathbf{c}^*$ following the treatment of de Wolff *et al.* (1981). Fig. 2.5.3.20(*b*) illustrates glide symmetry $\binom{m}{s}$ with a glide component $\tau_4 = \frac{1}{2}$. The structure factor $F(h_1h_2h_3h_4)$ is written for the glide plane $\binom{m}{s}$ of an infinite incommensurate crystal as

$$\begin{aligned} F(h_1h_2h_3h_4) &= \sum_{\mu=1}^{N} f_\mu \exp[2\pi i(h_1\bar{x}_1^\mu + h_2\bar{x}_2^\mu + h_3\bar{x}_3^\mu)] \\ &\quad \times \int_0^1 \exp\{2\pi i[h_1u_1^\mu + h_2u_2^\mu + (h_3 + h_4k_3)u_3^\mu + h_4\bar{x}_4^\mu]\}\, \mathrm{d}\bar{x}_4^\mu \\ &\quad + \exp(h_4\pi i)\sum_{\mu=1}^{N} f_\mu \exp[2\pi i(h_1\bar{x}_1^\mu - h_2\bar{x}_2^\mu + h_3\bar{x}_3^\mu)] \\ &\quad \times \int_0^1 \exp\{2\pi i[h_1u_1^\mu - h_2u_2^\mu + (h_3 + h_4k_3)u_3^\mu + h_4\bar{x}_4^\mu]\}\, \mathrm{d}\bar{x}_4^\mu. \end{aligned} \tag{2.5.3.10}$$

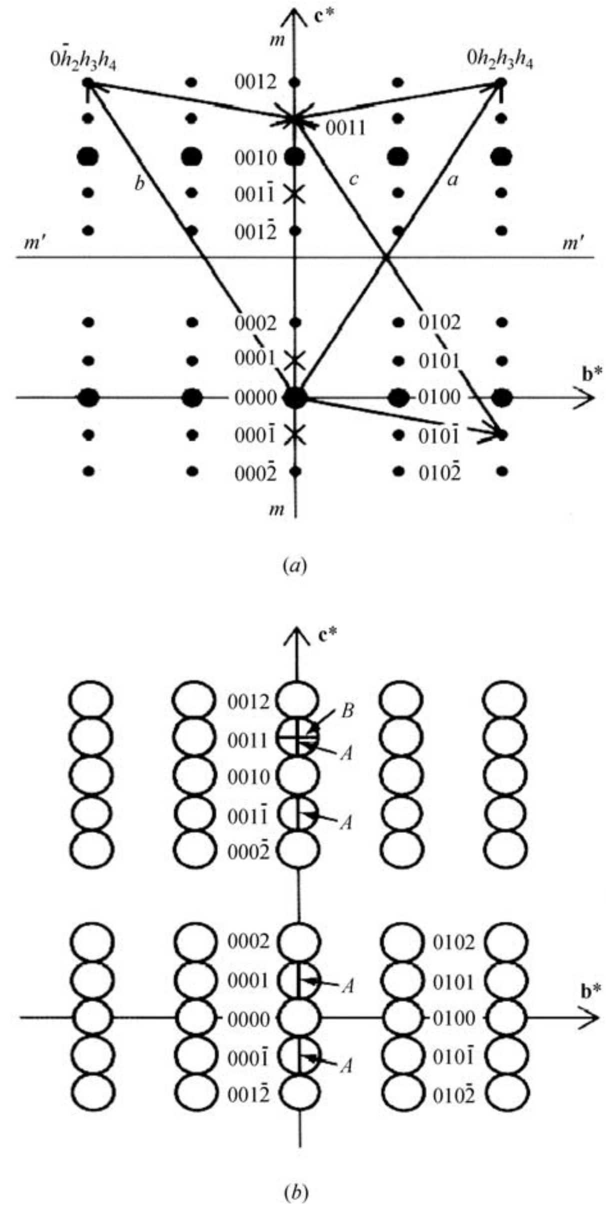

Fig. 2.5.3.21. (*a*) *Umweganregung* paths *a*, *b* and *c* to the 0011 forbidden reflection. (*b*) Expected dynamical extinction lines are shown, the 0011 reflection being excited. The wave number vector of modulation is $k_3\mathbf{c}^*$.

Thus, the following phase relations are obtained between the two structure factors:

$$\begin{aligned} F(h_1h_2h_3h_4) &= F(h_1\bar{h}_2h_3h_4) \quad \text{for } h_4 \text{ even}, \\ F(h_1h_2h_3h_4) &= -F(h_1\bar{h}_2h_3h_4) \quad \text{for } h_4 \text{ odd}. \end{aligned} \tag{2.5.3.11}$$

These relations are analogous to the phase relations between the two structure factors for an ordinary three-dimensional crystal with a glide plane. The relations imply that dynamical extinction occurs for the glide planes and screw axes of the (3 + 1)-dimensional crystal with an infinite dimension along the direction of the incommensurate modulation wavevector **k**. Terauchi *et al.* (1994) showed that approximate dynamical extinction occurs for an incommensurate crystal of finite dimension.

Fig. 2.5.3.21(*a*) and (*b*) illustrate a spot diffraction pattern and a CBED pattern, respectively, expected from a modulated crystal with a (3 + 1)-dimensional space group $P^{P2mm}_{\bar{1}s\bar{1}}$ ($\mathbf{k} = k_3\mathbf{c}^*$) at the [100] incidence. The large and small spots in Fig. 2.5.3.21(*a*) designate the fundamental ($h_4 = 0$) and incommensurate reflections ($h_4 \neq 0$), respectively. The $00h_3h_4$ (h_4 = odd) reflections

  references