

2. RECIPROCAL SPACE IN CRYSTAL-STRUCTURE DETERMINATION

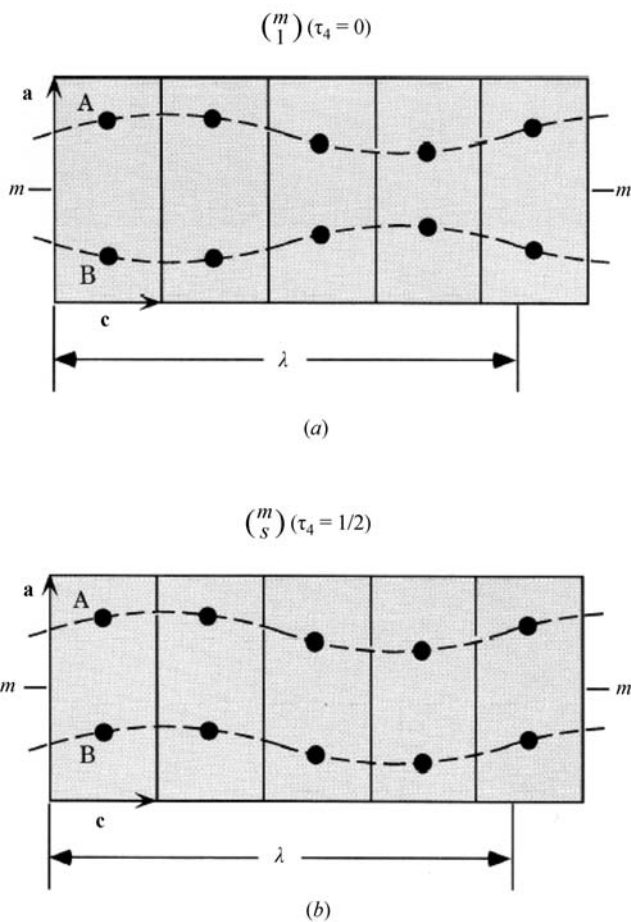


Fig. 2.5.3.20. (a) Mirror symmetry of modulation waves ( $m_1$ )  $\tau_4 = 0$ . (b) Glide symmetry of modulation waves ( $m_s$ )  $\tau_4 = \frac{1}{2}$ . The wave number vector of modulation is  $k_3c^*$ .

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  $\tau_4$  appears in odd-order incommensurate reflections. When the average structure has a glide component, dynamical extinction due to a glide component  $\tau_4$  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 ( $m_1$ ) 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  $\mathbf{k} = k_3c^*$  following the treatment of de Wolff *et al.* (1981). Fig. 2.5.3.20(b) illustrates glide symmetry ( $m_s$ ) with a glide component  $\tau_4 = \frac{1}{2}$ . The structure factor  $F(h_1h_2h_3h_4)$  is written for the glide plane ( $m_s$ ) of an infinite incommensurate crystal as

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

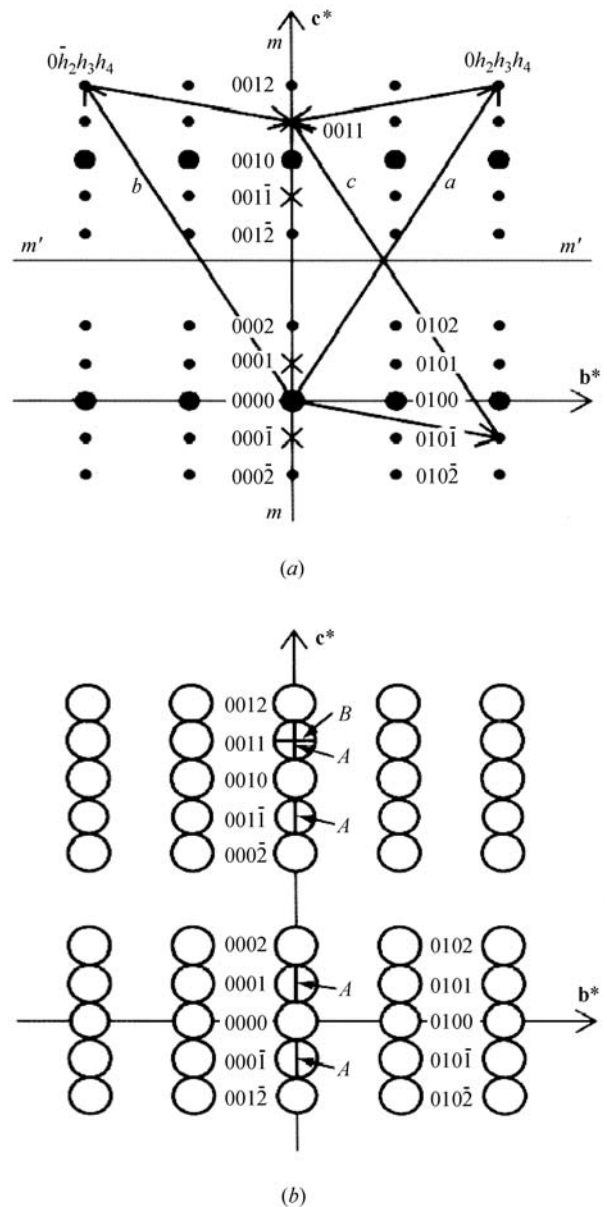


Fig. 2.5.3.21. (a) Umweganregung paths  $a$ ,  $b$  and  $c$  to the 0011 forbidden reflection. (b) Expected dynamical extinction lines are shown, the 0011 reflection being excited. The wave number vector of modulation is  $k_3c^*$ .

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  $\mathbf{k}$ . 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  $P_{1s1}^{P2mm}$  ( $\mathbf{k} = k_3c^*$ ) 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  $00h_3h_4$  ( $h_4 = \text{odd}$ ) reflections