

2.5. ELECTRON DIFFRACTION AND ELECTRON MICROSCOPY IN STRUCTURE DETERMINATION

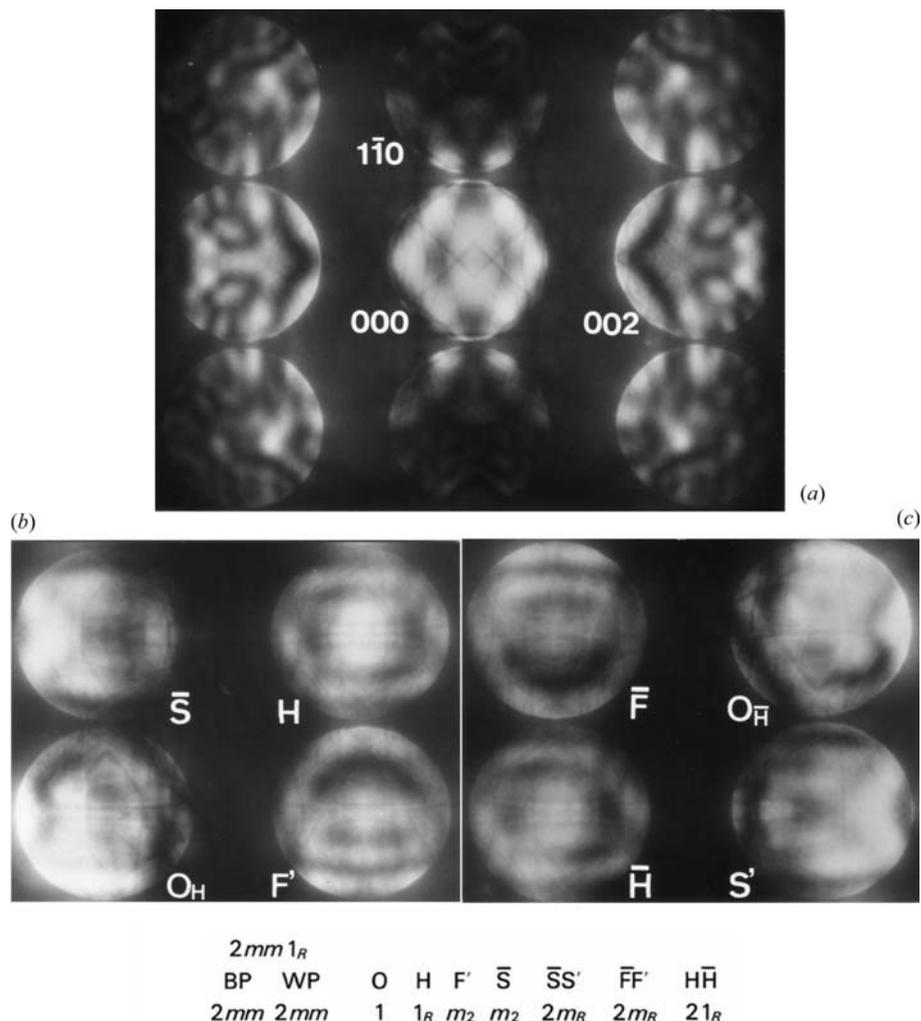


Fig. 2.5.3.9. CBED patterns of V_3Si taken with the $[110]$ incidence. (a) Zone-axis pattern, (b) rectangular four-beam pattern with excitation of reflections H , \bar{S} and F , (c) rectangular four-beam pattern with excitation of reflections \bar{H} , S and \bar{F} .

the 010 vector having the same excitation errors. The following equation holds:

$$\begin{aligned}
 &F(h_1, k_1)F(h_2, k_2) \dots F(h_n, k_n) \quad \text{for path } a \\
 &= -F(\bar{h}_n, k_n)F(\bar{h}_{n-1}, k_{n-1}) \dots F(\bar{h}_1, k_1) \quad \text{for path } c.
 \end{aligned}
 \tag{2.5.3.3}$$

Since the waves passing through these paths have the same amplitude but opposite signs, these waves are superposed on the 010 discs and cancel out, resulting in dark line B in this disc, as shown in Fig. 2.5.3.10(b). Line B appears perpendicular to line A at the exact Bragg positions. When *Umweganregung* paths are present only in the zeroth-order Laue zone, the glide plane and screw axis produce the same dynamical extinction lines A and B . We call these lines A_2 and B_2 lines, subscript 2 indicating that the *Umweganregung* paths lie in the zeroth-order Laue zone.

The dynamical extinction effect is analogous to interference phenomena in the Michelson interferometer. That is, the incident beam is split into two beams by Bragg reflections in a crystal. These beams take different paths, in which they suffer a relative phase shift of π and are finally superposed on a kinematically forbidden reflection to cancel out.

When the paths include higher-order Laue zones, the glide plane produces only extinction lines A but the screw axis causes only extinction lines B . These facts are attributed to the different relations between structure factors for a 2_1 screw axis and a glide plane,

$$F(hkl) = (-1)^k F(\bar{h}k\bar{l}) \quad \text{for a } 2_1 \text{ screw axis in the } [010] \text{ direction,}
 \tag{2.5.3.4}$$

$$F(hkl) = (-1)^k F(\bar{h}\bar{k}l) \quad \text{for a } b \text{ glide in the } (100) \text{ plane.}
 \tag{2.5.3.5}$$

In the case of the glide plane, extinction lines A are still formed because two waves passing through paths a and b have opposite signs to each other according to equation (2.5.3.5), but extinction lines B are not produced because equation (2.5.3.4) holds only for the 2_1 screw axis. In the case of the 2_1 screw axis, only the waves passing through paths a and c have opposite signs according to equation (2.5.3.4), forming extinction lines B only. We call these lines A_3 and B_3 dynamical extinction lines, suffix 3 indicating the *Umweganregung* paths being *via* higher-order Laue zones.

It was predicted by Gjønnes & Moodie (1965) that a horizontal glide plane g' gives a dark spot at the crossing point between extinction lines A and B (Fig. 2.5.3.10b) due to the cancellation between the waves passing through paths b and c . Tanaka, Terauchi & Sekii (1987) observed this dynamical extinction, though it appeared in a slightly different manner to that predicted by Gjønnes & Moodie (1965). Table 2.5.3.8 summarizes the appearance of the dynamical extinction lines for the glide planes g and g' and the 2_1 screw axis. The three space-group symmetry elements can be identified from the observed extinctions because these three symmetry elements produce different kinds of dynamical extinctions.