

## 2. RECIPROCAL SPACE IN CRYSTAL-STRUCTURE DETERMINATION

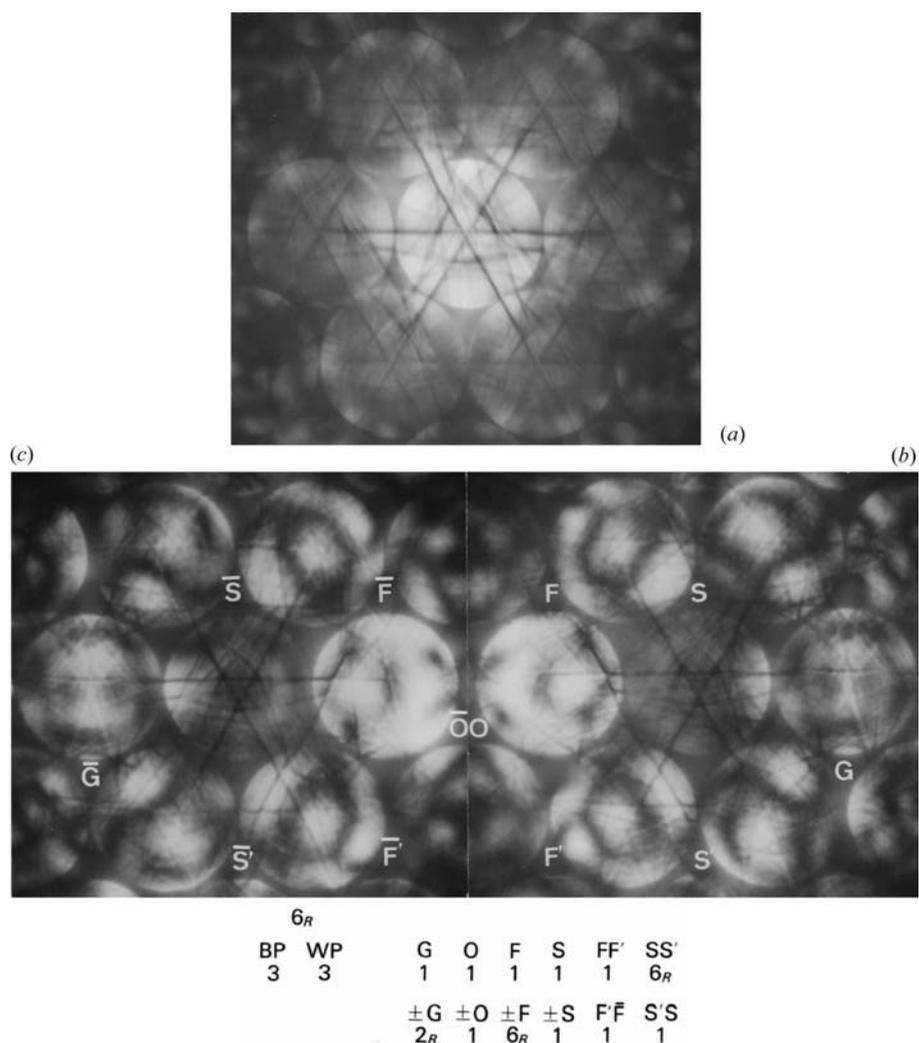


Fig. 2.5.3.8. CBED patterns of FeS<sub>2</sub> taken with the [111] incidence. (a) Zone-axis pattern, (b) hexagonal six-beam pattern with excitation of reflection +G, (c) hexagonal six-beam pattern with excitation of reflection -G. Symmetry 6<sub>R</sub> is noted between discs S and S' and discs F̄ and F̄'.

(1965) discussed the dynamical extinction in a more general way considering not only ZOLZ reflections but also HOLZ reflections. They completely clarified the dynamical extinction rules by considering the exact cancellation which may occur along certain symmetry-related multiple-scattering paths. Based on the results of Gjønnes & Moodie (1965), Tanaka, Sekii & Nagasawa (1983) tabulated the dynamical extinctions expected at all the possible crystal orientations for all the space groups. These were later tabulated in a better form on pages 162 to 172 of the book by Tanaka & Terauchi (1985).

Fig. 2.5.3.10(a) illustrates *Umweganregung* paths to a kinematically forbidden reflection. The 0k0 (*k* = odd) reflections are kinematically forbidden because a *b*-glide plane exists perpendicular to the *a* axis and/or a 2<sub>1</sub> screw axis exists in the *b* direction. Let us consider an *Umweganregung* path *a* in the zeroth-order Laue zone to the 010 forbidden reflection and path *b* which is symmetric to path *a* with respect to axis *k*. Owing to the translation of one half of the lattice parameter *b* caused by the glide plane and/or the 2<sub>1</sub> screw axis, the following relations hold between the crystal structure factors:

$$\begin{aligned} F(h, k) &= F(\bar{h}, k) \quad \text{for } k = 2n, \\ F(h, k) &= -F(\bar{h}, k) \quad \text{for } k = 2n + 1. \end{aligned} \quad (2.5.3.1)$$

That is, the structure factors of reflections *hk*0 and  $\bar{h}k$ 0 have the same phase for even *k* but have opposite phases for odd *k*.

Since an *Umweganregung* path to the kinematically forbidden reflection 0k0 contains an odd number of reflections with odd *k*, the following relations hold:

$$\begin{aligned} &F(h_1, k_1)F(h_2, k_2) \dots F(h_n, k_n) \quad \text{for path } a \\ &= -F(\bar{h}_1, k_1)F(\bar{h}_2, k_2) \dots F(\bar{h}_n, k_n) \quad \text{for path } b, \end{aligned} \quad (2.5.3.2)$$

where

$$\sum_{i=1}^n h_i = 0, \quad \sum_{i=1}^n k_i = k \quad (k = \text{odd})$$

and the functions including the excitation errors are omitted because only the cases in which the functions are the same for all the paths are considered. The excitation errors for paths *a* and *b* become the same when the projection of the Laue point along the zone axis concerned, *L*, lies on axis *k*. Since the two waves passing through paths *a* and *b* have the same amplitude but opposite signs, these waves are superposed on the 0k0 discs (*k* = odd) and cancel out, resulting in dark lines *A* in the forbidden discs, as shown in Fig. 2.5.3.10(b). The line *A* runs parallel to axis *k* passing through the projection point of the zone axis.

In path *c*, the reflections are arranged in the reverse order to those in path *b*. When the 010 reflection is exactly excited, two paths *a* and *c* are symmetric with respect to the bisector *m'*-*m'* of