International Tables for Crystallography (2010). Vol. B, Figure 2.5.3.13, p. 344.

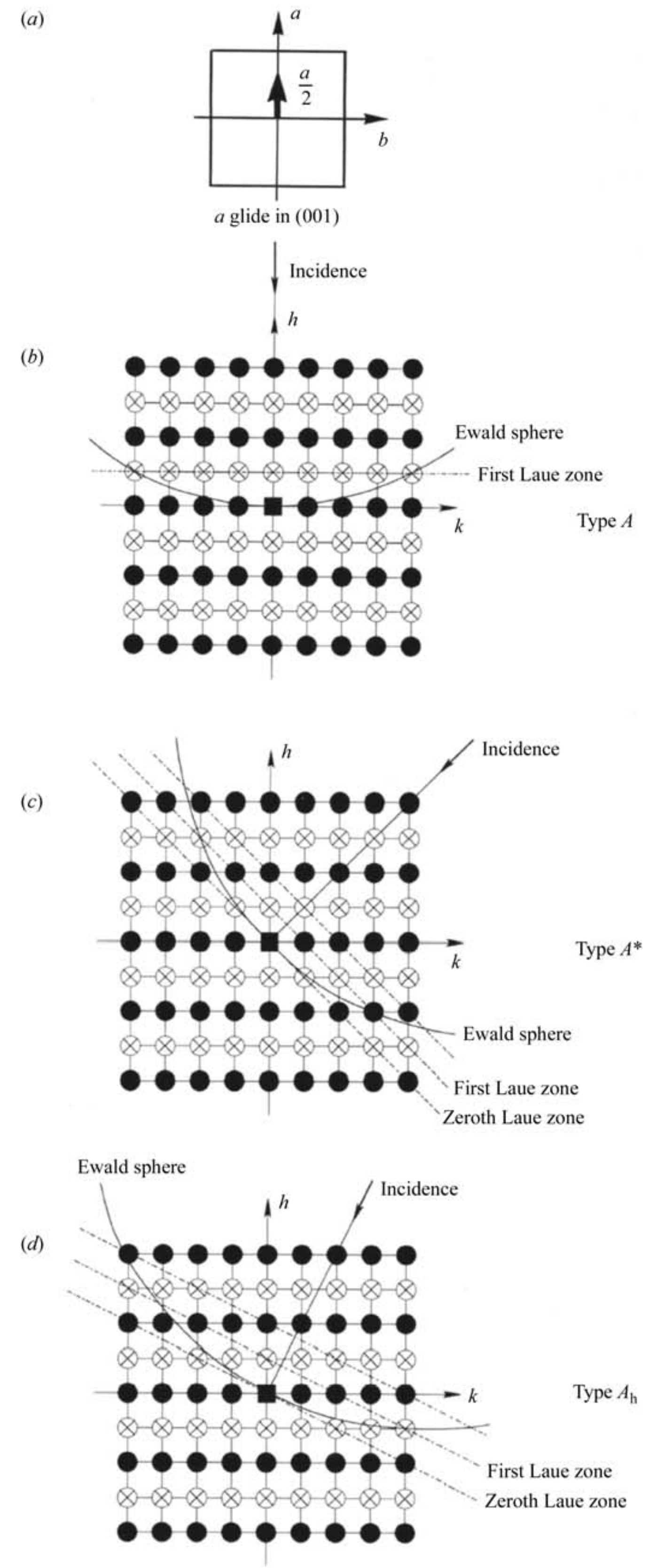

Fig. 2.5.3.13. Illustration of dynamical extinction lines appearing in HOLZ reflections due to glide planes. Black circles and circled crosses show kinematically allowed and kinematically forbidden reflections, respectively. (*a*) *a* glide in the (001) plane. (*b*) [100] incidence: dynamical extinction lines are formed in HOLZ reflections on both sides of the incident beam (type *A*). (*c*) [110] incidence: an extinction line is formed at a HOLZ reflection on one side of the incident beam because on the other side the Ewald sphere intersects an allowed HOLZ reflection (type *A**). (*d*) An incidence between [100] and [110]: an extinction line is formed at a HOLZ reflection on one side of the incident beam because on the other side the Ewald sphere does not intersect a HOLZ reflection (type A_h).

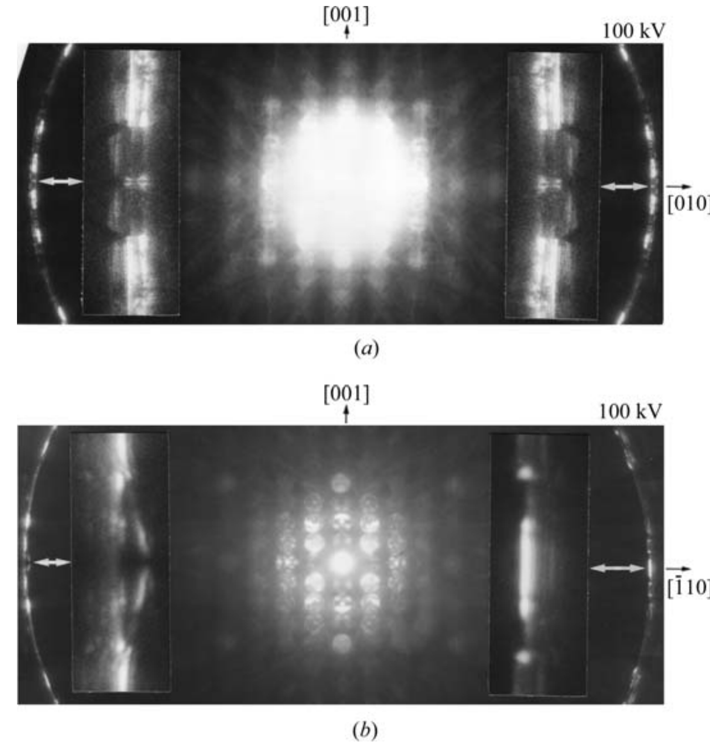

Fig. 2.5.3.14. HOLZ CBED pattern of FeS_2. (*a*) [100] incidence: type *A* dynamical extinction lines are seen clearly in the enlarged insets. (*b*) [110] incidence: a type *A** dynamical extinction line is seen clearly in the enlarged insets.

which satisfies the results obtained at the two crystal orientations is $\bar{4}3m$.

Fig. 2.5.3.16(*e*) shows an ordinary diffraction pattern taken with the [100] incidence at 80 kV. With the help of the lattice parameters and the camera length, the indices of the reflections are given as shown in the figure. The reflections $0kl$ ($k + l = 2n + 1$) are found to be kinematically forbidden. Thus, the lattice type is determined to be *I*.

The space groups having point group $\bar{4}3m$ and lattice type *I* are $I\bar{4}3m$ and $I\bar{4}3d$ from Table 2.5.3.9. Fig. 2.5.3.16(*d*) shows dynamical extinction lines A_2 in the 033 disc and equivalent discs (also broad lines A_2 in the 011 discs). Since the former space group does not give any dynamical extinction lines, the space group is determined to be $I\bar{4}3d$. For confirmation, a CBED pattern which contains the second-order-Laue-zone reflections was taken (Fig. 2.5.3.16*f*). Dynamical extinction lines *A* are seen in the 2,22,22 disc and the equivalent discs. This result also identifies the space group to be not $I\bar{4}3m$ but $I\bar{4}3d$ with the aid of Table 2.5.3.12.

2.5.3.4. Symmetry determination of incommensurate crystals

2.5.3.4.1. General remarks

Incommensurately modulated crystals do not have three-dimensional lattice periodicity. The crystals, however, recover lattice periodicity in a space higher than three dimensions. de Wolff (1974, 1977) showed that one-dimensional displacive and substitutionally modulated crystals can be described as a three-dimensional section of a (3 + 1)-dimensional periodic crystal. Janner & Janssen (1980*a*,*b*) developed a more general approach for describing a modulated crystal with *n* modulations as $(3 + n)$-dimensional periodic crystals ($n = 1, 2, \ldots$). Yamamoto (1982) derived a general structure-factor formula for *n*-dimensionally modulated crystals ($n = 1, 2, \ldots$), which holds for both displacive and substitutionally modulated crystals. Tables of the (3 + 1)-dimensional space groups for one-dimensional incommensurately modulated crystals were given by de Wolff *et al.* (1981), where the wavevector of the modulation was assumed to lie in the