

## 4.3. DIFFUSE SCATTERING IN ELECTRON DIFFRACTION

and their variation with composition, treatment *etc.* Many features in the scattering which pass unrecognized in extensive X-ray or neutron investigations will be observed readily with electrons, frequently inviting other ways of interpretation.

Most such studies have been concerned with substitutional disorder, but the extensive investigations of thermal streaks by Honjo and co-workers should be mentioned (Honjo *et al.*, 1964). Diffuse spots and streaks from disorder have been observed from a wide range of substances. The most frequent may be streaks due to planar faults, one of the most common objects studied by electron microscopy. Diffraction patterns are usually sufficient to determine the orientation and the fault vector; the positions and distribution of faults are more easily seen by dark-field microscopy, whereas the detailed atomic arrangement is best studied by high-resolution imaging of the structure [Section 4.3.8 in *IT C* (2004)].

This combination of diffraction and different imaging techniques cannot be applied in the same way to the study of the essentially three-dimensional substitutional local order. Considerable effort has therefore been made to interpret the details of diffuse scattering, leaving the determination of the short-range-order (SRO) parameters usually to X-ray or neutron studies.

Frequently, characteristic shapes or splitting of the diffuse spots from *e.g.* binary alloys are observed. They reflect order extending over many atomic distances, and have been assumed to arise from forces other than the near-neighbour pair forces invoked in the theory of local order. A relationship between the diffuse-scattering distribution and the Fourier transform of the effective atom-pair-interaction potential is given by the ordering theory of Clapp & Moss (1968). An interpretation in terms of long-range forces carried by the conduction electrons was proposed by Krivoglaz (1969). Extensive studies of alloy systems (Ohshima & Watanabe, 1973) show that the separations,  $m$ , observed in split diffuse spots from many alloys follow the predicted variation with the electron/atom ratio  $e/a$ :

$$m = \left[ \frac{12}{\pi} (e/a) \right]^{1/3} t - \sqrt{2},$$

where  $m$  is measured along the [110] direction in units of  $2a^*$  and  $t$  is a truncation factor for the Fermi surface.

A similarity between the location of diffuse maxima and the shape of the Fermi surface has been noted also for other structures, notably some defect rock-salt-type structures. Although this may offer a clue to the forces involved in the ordering, it entails no description of the local structure. Several attempts have been made to formulate principles for building the disordered structure, from small ordered domains embedded in less ordered regions (Hashimoto, 1974), by a network of antiphase boundaries, or by building the structure from clusters with the average composition and coordination (De Ridder *et al.*, 1976). Evidence for such models may be sought by computer simulations, in the details of the SRO scattering as seen in electron diffraction, or in images.

The cluster model is most directly tied to the location of diffuse scattering, noting that a relation between order parameters derived from clusters consistent with the ordered state can be used to predict the position of diffuse scattering in the form of surfaces in reciprocal space, *e.g.* the relation  $\cos h + \cos k + \cos l = 0$  for ordering of octahedral clusters in the rock-salt-type structure (Sauvage & Parthé, 1974).

Some of the models imply local fluctuations in order which may be observable either by diffraction from very small regions or by imaging. Microdiffraction studies (Tanaka & Cowley, 1985) do indeed show that spots from 1–1.5 nm regions in disordered LiFeO<sub>2</sub> appear on the locus of diffuse maxima observed in diffraction from larger areas.

Imaging of local variations in the SRO structure has been pursued with different techniques (De Ridder *et al.*, 1976; Tanaka & Cowley, 1985; De Meulenaere *et al.*, 1998), *viz.*: dark field using diffuse spots only; bright field with the central spot *plus* diffuse spots; lattice image. With domains of about 3 nm or more, high-resolution images seem to give clear indication of their presence and form. For smaller ordered regions, the interpretation becomes increasingly complex: Since the domains will then usually not extend through the thickness of the foil, they cannot be imaged separately. Since image-contrast calculations essentially demand complete specification of the local structure, a model beyond the statistical description must be constructed in order to be compared with observations. On the other hand, these models of the local structure should be consistent with the statistics derived from diffraction patterns collected from a larger volume.

## References

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#### 4. DIFFUSE SCATTERING AND RELATED TOPICS

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