

4.3. Diffuse scattering in electron diffraction

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4.3.1. Introduction

The origins of diffuse scattering in electron-diffraction patterns are the same as in the X-ray case: inelastic scattering due to electronic excitations, thermal diffuse scattering (TDS) from atomic motions, scattering from crystal defects or disorder. For diffraction by crystals, the diffuse scattering can formally be described in terms of a nonperiodic deviation $\Delta\varphi$ from the periodic, average crystal potential, $\bar{\varphi}$:

$$\varphi(\mathbf{r}, t) = \bar{\varphi}(\mathbf{r}) + \Delta\varphi(\mathbf{r}, t), \quad (4.3.1.1)$$

where $\Delta\varphi$ may have a static component from disorder in addition to time-dependent fluctuations of the electron distribution or atomic positions.

In the kinematical case, the diffuse scattering can be treated separately. The intensity I_d as a function of the scattering variable \mathbf{u} ($|\mathbf{u}| = 2 \sin \theta / \lambda$) and energy transfer $h\nu$ is then given by the Fourier transform \mathcal{F} of $\Delta\varphi$

$$I(\mathbf{u}, \nu) = |\Delta\Phi(\mathbf{u}\nu)|^2 = |\mathcal{F}\{\Delta\varphi(\mathbf{r}, t)\}|^2 = \mathcal{F}\{P_d(\mathbf{r}, \nu)\} \quad (4.3.1.2)$$

and may also be written as the Fourier transform of a correlation function P_d representing fluctuations in space and time (see Cowley, 1981). When the energy transfers are small – as with TDS – and hence not measured, the observed intensity corresponds to an integral over ν :

$$\begin{aligned} I(\mathbf{u}) &= I_d(\mathbf{u}) + I_{av}(\mathbf{u}) \\ I_d(\mathbf{u}) &= \int I_d(\mathbf{u}, \nu) d\nu = \mathcal{F}\{P_d(\mathbf{r}, 0)\} \end{aligned}$$

and also

$$I_d(\mathbf{u}) = \langle |\Phi(\mathbf{u})|^2 \rangle - |\langle \Phi(\mathbf{u}) \rangle|^2, \quad (4.3.1.3)$$

where the brackets may indicate a time average, an expectation value, or a spatial average over the periodicity of the lattice in the case of static deviations from a periodic structure.

The considerations of TDS and static defects and disorder of Chapters 4.1 and 4.2 thus may be applied directly to electron diffraction in the kinematical approximation when the differences in experimental conditions and diffraction geometry are taken into account.

The most prominent contribution to the diffuse background in electron diffraction, however, is the inelastic scattering at low angles arising mainly from the excitation of outer electrons. This is quite different from the X-ray case where the inelastic ('incoherent') scattering, $S(\mathbf{u})$, goes to zero at small angles and increases to a value proportional to Z for high values of $|\mathbf{u}|$. The difference is due to the Coulomb nature of electron scattering, which leads to the kinematical intensity expression S/u^4 , emphasizing the small-angle region. At high angles, the inelastic scattering from an atom is then proportional to Z/u^4 , which is considerably less than the corresponding elastic scattering $(Z - f)^2/u^4$ which approaches Z^2/u^4 (Section 2.5.2) (see Fig. 4.3.1.1).

The kinematical description can be used for electron scattering only when the crystal is very thin (10 nm or less) and composed of light atoms. For heavy atoms such as Au or Pb, crystals of thickness 1 nm or more in principal orientations show strong deviations from kinematical behaviour. With increasing thickness, dynamical scattering effects first modify the sharp Bragg reflections and then have increasingly significant effects on the diffuse scattering. Bragg scattering of the diffuse scattering produces Kikuchi lines and other effects. Multiple diffuse scattering broadens the distribution and smears out detail. As the thickness increases further, the diffuse

scattering increases and the Bragg beams are reduced in intensity until there is only a diffuse 'channelling pattern' where the features depend in only a very indirect way on the incident-beam direction or on the sources of the diffuse scattering (Uyeda & Nonoyama, 1968).

The multiple-scattering effects make the quantitative interpretation of diffuse scattering more difficult and complicate the extraction of particular components, *e.g.* disorder scattering. Much of the multiple scattering involves inelastic scattering processes. However, electrons that have lost energy of the order of 1 eV or more can be subtracted experimentally by use of electron energy filters (Krahl *et al.*, 1990; Krivanek *et al.*, 1992) which are commercially available. Measurement can be made also of the complete scattering function $I(\mathbf{u}, \nu)$, but such studies have been rare. Another significant improvement to quantitative measurement of diffuse electron scattering is offered by new recording devices: slow-scan charge-couple-device cameras (Krivanek & Mooney, 1993) and imaging plates (Mori *et al.*, 1990).

There are some advantages in the use of electrons which make it uniquely valuable for particular applications.

(1) Diffuse-scattering distributions can be recorded from very small specimen regions, a few nm in diameter and a few nm thick. The diameter of the specimen area may be varied readily up to several μm .

(2) Diffraction information on defects or disorder may be correlated with high-resolution electron-microscope imaging of the same specimen area [see Section 4.3.8 in *IT C* (1999)].

(3) The electron-diffraction pattern approximates to a planar section of reciprocal space, so that complicated configurations of diffuse scattering may be readily visualized (see Fig. 4.3.1.2).

(4) Dynamical effects may be exploited to obtain information about localization of sources of the diffuse scattering within the unit cell.

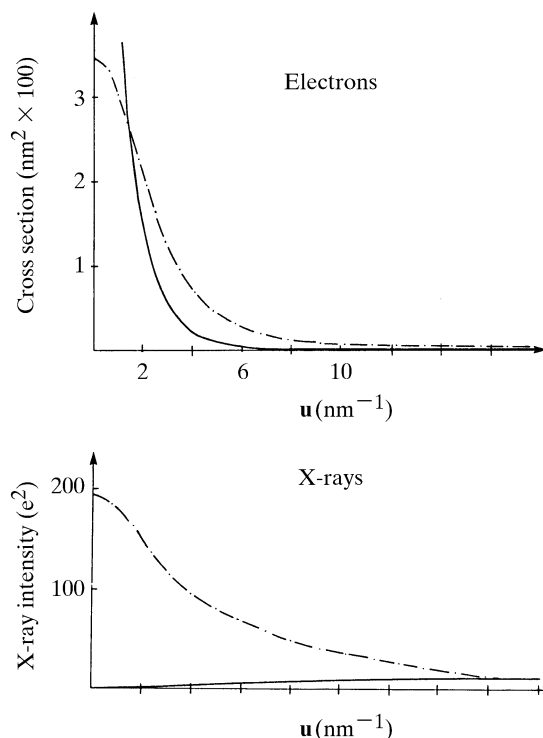


Fig. 4.3.1.1. Comparison between the kinematical inelastic scattering (full line) and elastic scattering (broken) for electrons and X-rays. Values for silicon [Freeman (1960) and *IT C* (1999)].