International Tables for Crystallography (2006). Vol. C, Figure 4.3.4.2, p. 392.

powerful technique for the low-energy range ($\lesssim 0.1$ eV). On the other hand, inelastic X-ray scattering is well suited for the study of high momentum and large energy transfers because the energy resolution is limited to ~ 1 eV and the cross section increases with momentum transfer. In the intermediate range, inelastic electron scattering [or electron energy-loss spectroscopy (EELS)] is the most useful technique. For recent reviews on different aspects of the subject, the reader may consult the texts by Schnatterly (1979), Raether (1980), Colliex (1984), Egerton (1986), and Spence (1988).

4.3.4.1.2. *Parameters involved in the description of a single inelastic scattering event*

The importance of inelastic scattering as a function of energy and momentum transfer is governed by a double differential cross section:

$$\frac{d^2\sigma}{d\Omega\, d(\Delta E)}, \qquad (4.3.4.1)$$

where $d\Omega$ corresponds to the solid angle of acceptance of the detector and $d(\Delta E)$ to the energy window transmitted by the spectrometer. The experimental conditions must therefore be defined before any interpretation of the data is possible. Integrations of the cross section over the relevant angular and energy-loss domains correspond to partial or total cross sections, depending on the feature measured. For instance, the total inelastic cross section (σ_i) corresponds to the probability of suffering any energy loss while being scattered into all solid angles. The discrimination between elastic and inelastic signal is generally defined by the energy resolution of the spectrometer, that is the minimum energy loss that can be unambiguously distinguished from the zero-loss peak; it is therefore very dependent on the instrumentation used.

The kinematics of a single inelastic event can be described as shown in Fig. 4.3.4.2. In contrast to the elastic case, there is no simple relation between the scattering angle θ and the transfer of momentum $\hbar\mathbf{q}$. One has also to take into account the energy loss ΔE. Combining both equations of conservation of momentum and energy,

$$\frac{\hbar^2 k'^2}{2m_0} + \Delta E = \frac{\hbar^2 k^2}{2m_0}, \qquad (4.3.4.2)$$

and

$$q^2 = k^2 + k'^2 - 2kk' \cos\theta, \qquad (4.3.4.3)$$

one obtains

$$(qa_0)^2 = \frac{2E_0}{R}\left[1 - \left(1 - \frac{\Delta E}{E_0}\right)^{1/2} \cos\theta\right] - \frac{\Delta E}{R}, \qquad (4.3.4.4)$$

where the fundamental units $a_0 = \hbar^2/m_0 e^2$ = Bohr radius and $R = m_0 e^4/2\hbar^2$ = Rydberg energy are used to introduce dimensionless quantities. In this kinematical description, one deals only with factors concerning the primary or the scattered particle, without considering specifically the information on the ejected electron. For a core-electron excitation of an atom, one distinguishes $\mathbf{q}$ (the momentum exchanged by the incident particle) and χ (the momentum gained by the excited electron), the difference being absorbed by the recoil of the target nucleus (Maslen & Rossouw, 1983).

4.3.4.1.3. *Problems associated with multiple scattering*

The strong coupling potential between the primary electron and the solid target is responsible for the occurrence of multiple inelastic events (and of mixed inelastic–elastic events) for thick specimens. To describe the interaction of a primary particle with an assembly of randomly distributed scattering centres (with a density N per unit volume), a useful concept is the mean free path defined as

$$\Lambda = 1/N\sigma \qquad (4.3.4.5)$$

for the cross section σ. The ratio t/Λ measures the probability of occurrence of the event associated with the cross section σ when the incident particle travels a given length t through the material. This is true in the single scattering case, that is when $t/\Lambda \ll 1$.

For increased thicknesses, one must take into account all multiple scattering events and this contribution begins to be non-negligible for $t \gtrsim$ a few tens of nanometres. Multiple scattering is responsible for a broadening of the angular distribution of the

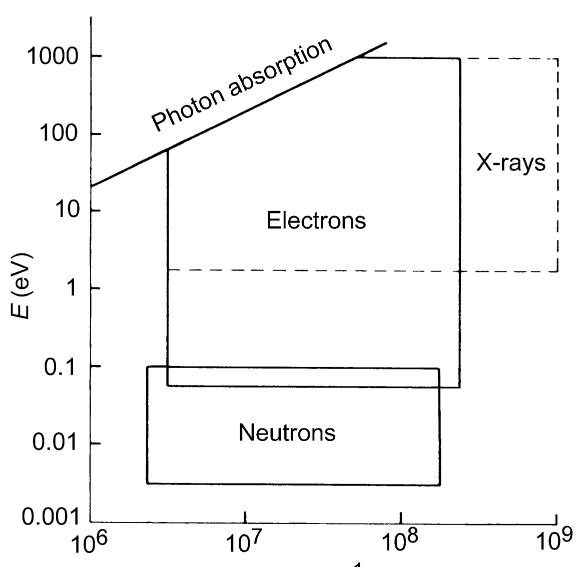

Fig. 4.3.4.1. Definition of the regions in (E, q) space that can be investigated with the different primary sources of particles available at present [courtesy of Schnatterly (1979)].

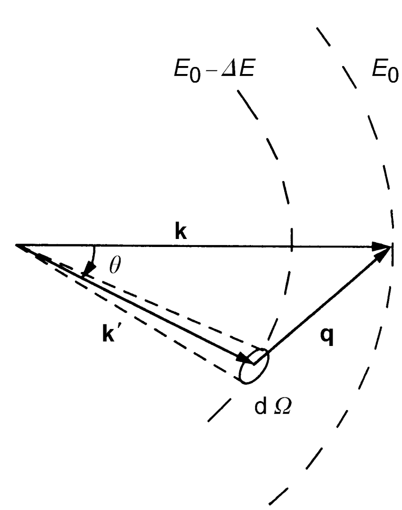

Fig. 4.3.4.2. A primary electron of energy E_0 and wavevector $\mathbf{k}$ is inelastically scattered into a state of energy $E_0 - \Delta E$ and wavevector $\mathbf{k}'$. The energy loss is ΔE and the momentum change is $\hbar\mathbf{q}$. The scattering angle is θ and the scattered electron is collected within an aperture of solid angle $d\Omega$.

references