

4.3. ELECTRON DIFFRACTION

$$\frac{d^2\sigma}{d\Omega d(\Delta E)} = \frac{4\gamma^2 R}{\Delta E k^2} \frac{1}{\theta^2 + \theta_E^2} \frac{df(0, \Delta E)}{d(\Delta E)}. \quad (4.3.4.44)$$

The major angular dependence is contained, as in the low-loss domain, in the Lorentzian factor $(\theta^2 + \theta_E^2)^{-1}$, with the characteristic inelastic angle θ_E being again equal to $\Delta E/\gamma m_0 v^2$. Over this reduced scattering-angle domain, known as the dipole region, the GOS is approximately constant and the inner-shell EELS spectrum is directly proportional to the photoabsorption cross section σ_{opt} , whose data can be used to test the results of single-atom calculations. For larger scattering angles, Fig. 4.3.4.24 exhibits two distinct behaviours for energy losses just above the edge ($df/d\Delta E$ drops regularly to zero), and for energy losses much greater than the core-edge threshold. In the latter case, the oscillator strength is mostly concentrated in the Bethe ridge, the maximum of which occurs for:

$$\left. \begin{aligned} (qa_0)^2 &= \frac{\Delta E}{R} \quad (\text{non-relativistic formula}), \\ (qa_0)^2 &= \frac{\Delta E (\Delta E)^2}{R 2m_0 c^2 R} \quad (\text{relativistic formula}). \end{aligned} \right\} \quad (4.3.4.45)$$

This contribution at large scattering angles is equivalent to direct knock-on collisions of free electrons, *i.e.* to the curve $\Delta E = \hbar^2 q^2/2m_0$ lying in the middle of the valence-electron-hole excitations continuum (see Fig. 4.3.4.13). The non-zero width of the Bethe ridge can be used as an electron Compton profile to analyse the momentum distribution of the atomic electrons [see also §4.3.4.4.4(c)].

The energy dependence of the cross section, responsible for the various edge shapes discussed in §4.3.4.4.1, is governed by

$$\frac{1}{\Delta E} \frac{df(\mathbf{q}, \Delta E)}{d(\Delta E)},$$

i.e. it corresponds to sections through the Bethe surface at constant \mathbf{q} . Within the general theory described above, various models have been developed for practical calculations of energy differential cross sections.

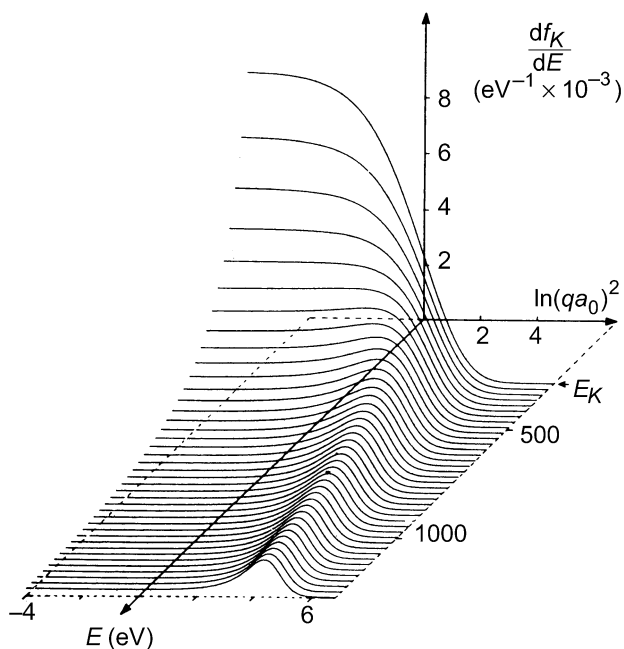


Fig. 4.3.4.24. Bethe surface for K -shell ionization, calculated using a hydrogenic model. The generalized oscillator strength is zero for energy loss E below the threshold E_K . The horizontal coordinate is related to scattering angle through q [from Egerton (1979)].

The hydrogenic model due to Egerton (1979) is an extension of the quantum-mechanical calculations for a hydrogen atom to inner-shell electron excitations in an atom Z by introduction of some useful parametrization (effective nuclear charge, effective threshold energy). It is applied in practice for K and $L_{2,3}$ shells.

In the Hartree–Slater (or Dirac–Slater) description, one calculates the final continuum-state wavefunction in a self-consistent central field atomic potential (Leapman, Rez & Mayers, 1980; Rez, 1989). The radial dependence of these wavefunctions is given by the solution of a Schrödinger equation with an effective potential:

$$V_{\text{eff}}(r) = V(r) + \frac{l'(l' + 1)\hbar^2}{2m_0 r^2}, \quad (4.3.4.46)$$

where $[l'(l' + 1)\hbar^2]/2m_0 r^2$ is the centrifugal potential, which is important for explaining the occurrence of delayed maxima in spectra involving final states of higher l' . This approach is now useful for any major $K, L_{2,3}, M_{4,5}, \dots$ edge, as illustrated by Ahn & Rez (1985) and more specifically in rare-earth elements by Manoubi, Rez & Colliex (1989).

These differential cross sections can be integrated over the relevant angular and energy domains to provide data comparable with experimental measurements. In practice, one records the energy spectral distribution of electrons scattered into all angles up to the acceptance value β of the collection aperture. The integration has therefore to be made from $q_{\text{min}} \simeq k\theta_E$ for the zero scattering-angle limit, up to $q_{\text{max}} \simeq k\beta$. Fig. 4.3.4.25 shows how such calculated profiles can be used for fitting experimental data.

Setting $\beta = \pi$ [or equal to an effective upper limit $\theta_{\text{max}} \simeq (\Delta E/E_0)^{1/2}$ corresponding to the criterion $q_{\text{max}} r \simeq 1$], the integral cross section is the total cross section for the excitation of a given core level. These ionization cross sections are required for quantification in all analytical techniques using core-level excitations and de-excitations, such as EELS, Auger electron spectroscopy, and X-ray microanalysis (see Powell, 1976, 1984). A convenient way of comparing total cross sections is to rewrite the Bethe asymptotic cross section as

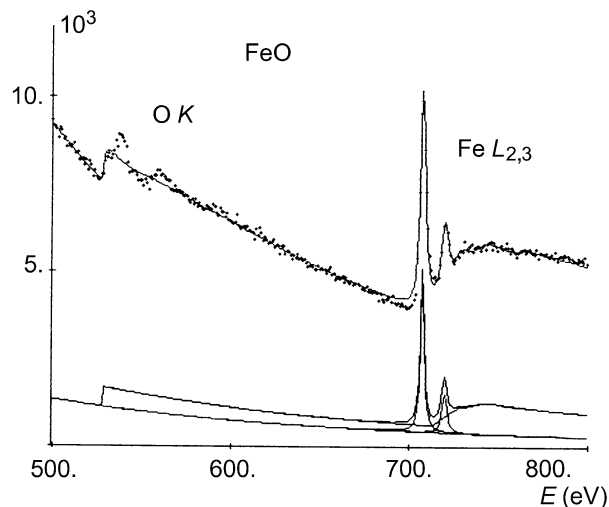


Fig. 4.3.4.25. A novel technique for simulating an energy-loss spectrum with two distinct edges as a superposition of theoretical contributions (hydrogenic saw-tooth for $O K$, Lorentzian white lines and delayed continuum for $Fe L_{2,3}$ calculated with the Hartree–Slater description). The best fit between the experimental and the simulated spectra is shown; it can be used to evaluate the relative concentration of the two elements [see Manoubi *et al.* (1990)].