

#### 4. PRODUCTION AND PROPERTIES OF RADIATIONS

Scattering of X-rays from the electron spins in anti-ferromagnetically ordered materials can also be described by imposing a tensor description on the form factor (Blume, 1994). The tensor in this case is a fourth-rank tensor, and the strength of the interaction, even for the favourable case of resonance scattering, is several orders of magnitude lower in intensity than the polarization effects. Nevertheless, studies have been made on holmium and uranium arsenide, and significant magnetic Bragg scattering has been observed.

All the cases cited above represent exciting, state-of-the-art, scientific studies. However, none of the work will assist in the solution of crystal structures directly. Researchers should avoid the temptation, in the first instance, to ascribe anything but a scalar value to the form factor.

##### 4.2.6.3.3.5. Summary

For the imaginary part of the dispersion correction  $f''(\omega, \Delta)$ , the following observations can be made.

(i) Measurements of the linear absorption coefficient  $\mu_l$  from which  $f'(\omega, 0)$  is deduced should follow the recommendations set out in Subsection 4.2.3.2.

(ii) There is no rational basis for preferring one set of relativistic calculations of atomic scattering cross sections over another, as Creagh & Hubbell (1987, 1990) and Kissel *et al.* (1980) have shown.

(iii) The total scattering cross section for an ensemble of atoms is not simply the sum of the individual scattering cross sections in the neighbourhood of an absorption edge and therefore  $f'(\omega, 0)$  will fluctuate as  $\omega \rightarrow \omega_\kappa$ .

(iv) There is no dependence of  $f''(\omega, \Delta)$  and  $\Delta$ .

For the real part of the dispersion correction  $f'(\omega, \Delta)$ , the following observations can be made.

(i) The relativistic multipole values listed here tend to accord better with experiment than the non-relativistic and relativistic dipole values.

(ii) There is no dependence of  $f'(\omega, \Delta)$  on  $\Delta$ .

(iii) The theoretical tables are calculated for averaged polarizations.

(iv) Experimentalists wishing to compare their data with theoretical predictions should take account of the energy bandpass of their system when determining the appropriate theoretical value. They should also be aware of the fact that the position of the absorption edge depends on the oxidation state of the scattering atom, and that there is an inaccuracy in the tables of  $f'(\omega, 0)$  of either  $+0.20(E_{\text{tot}}/mc^2)$  or  $-0.10(E_{\text{tot}}/mc^2)$ .

##### 4.2.6.4. Table of wavelengths, energies, and linewidths used in compiling the tables of the dispersion corrections

Table 4.2.6.7 lists the characteristic emission wavelengths that are commonly used by crystallographers in their experiments. Also included are the emission energies (since many systems use energy rather than wavelength discrimination) and the line widths (full width at half-maximum) of these lines (Agarwal, 1979; Stearns, 1984; Deutsch & Hart, 1984*a,b*).

##### 4.2.6.5. Tables of the dispersion corrections for forward scattering, averaged polarization using the relativistic multipole approach

See Subsection 4.2.6.3 for comments on the accuracy of these tables. Note also that in the neighbourhood of absorption edges the values for condensed matter may be significantly different from the values in the tables due to XAFS and XANES effects. The values in Table 4.2.6.8 are for scattering by isolated atoms.