

## 4. PRODUCTION AND PROPERTIES OF RADIATIONS

variance with the predictions of Wagenfeld's (1975) non-relativistic model.

4.2.6.2.4. *Intercomparison of theories*

A discussion of the validity of the non-relativistic dipole approximation for the calculation of forward Rayleigh scattering amplitudes has been given by Roy & Pratt (1982). They compared their relativistic multipole calculations with the relativistic dipole approximation and with the non-relativistic dipole approximation for two elements, silver and lead. They concluded that a relativistic correction to the form factor of order  $(Z\alpha)^2$  persists in the high-energy limit, and that this constant correction accounts for much of the deviation from the non-relativistic dipole approximation at all energies above threshold. In addition, their results illustrate that cancelling occurs amongst the relativistic, retardation, and higher multipole contributions to the scattering amplitude. This implies that care must be taken in assessing where to terminate the series that describes the multipolarity of the scattering process.

In a later paper, Roy, Kissel & Pratt (1983) discussed the elastic photon scattering for small momentum transfers and the validity of the form-factor theories. In this paper, which compares the relativistic modified form factor with experimental results for lead and a relativistic form factor and the tabulation by Hubbell, Veigele, Briggs, Brown, Cromer & Howerton (1975), it is shown that the modified relativistic form-factor approach gives better agreement with experiment for high momentum transfers ( $< 104 \text{ \AA}^{-1}$ ) than the non-relativistic, form-factor theories.

Kissel *et al.* (1980) used the  $S$ -matrix technique to calculate the real part of the forward-scattering amplitude  $f'(\omega, 0)$  for the inert gases at the wavelength of Mo  $K\alpha_1$ . These values are compared with the predictions of the relativistic dipole theory (RDP) and the relativistic multipole theory (RMP) in Table 4.2.6.2(a). In most cases, the agreement between the  $S$  matrix and the RMP theory is excellent, considering the differences in the methodology of the two sets of calculations. Table 4.2.6.2(b) shows comparisons of the real part of the forward-scattering amplitude  $f'(\omega, 0)$  calculated for the atoms aluminium, silicon, zinc, germanium, silver, samarium, tantalum and lead using the approach of Kissel *et al.* (1980) with that of Cromer & Liberman (1970, 1981), with tabulations by Wagenfeld (1975), and with values taken from the tables in this section. Although reasonably satisfactory agreement exists between the relativistic values, large differences exist between the non-relativistic value (Wagenfeld, 1975) and the relativistic values. The major difference between the relativistic values occurs because of differences in estimation of the self-consistent-field term, which is proportional to  $E_{\text{tot}}/mc^2$ . The Cromer & Liberman (1970) relativistic dipole value is  $+\frac{5}{3}(E_{\text{tot}}/mc^2)$ , whereas the tabulation in this section uses the relativistic multipole value of  $(+E_{\text{tot}}/mc^2)$ . This causes a vertical shift of the curve, but does not alter its shape. Should better estimates of the self-energy term be found, the correction is simply that of adding a constant to each value of  $f'(\omega, 0)$  for each atomic species. There is a significant discrepancy between the Kissel *et al.* (1980) result for  $^{62}\text{Sm}$  and the other theoretical values. This is the only major point of difference, however, and the results are better in accord with the relativistic multipole approach than with the relativistic dipole approach. Note that the relativistic multipole approach does not include the Stibius-Jensen correction, which alters the shape of the curve.

In §4.2.6.3.3, some examples are given to illustrate the extent to which predictions of these theories agree with experimental data for  $f''(\omega, 0)$ .

That there is little to choose between the different theoretical approaches where the calculation of  $f''(\omega, 0)$  is concerned is illustrated in Table 4.2.6.3. In most cases, the agreement between the scattering matrix, relativistic dipole, and relativistic multipole values is within 1%. In contrast, there are some significant differences between the relativistic and the non-relativistic values of  $f''(\omega, 0)$ . The extent of the discrepancies is greater the higher the atomic number, as one might expect from the assumptions made in the formulation of the non-relativistic model. Some detailed comparisons of theoretical and experimental data for linear attenuation coefficients [proportional to  $f''(\omega, 0)$ ] have been given by Creagh & Hubbell (1987) for silicon, and for copper and carbon by Gerward (1982, 1983). These tend to confirm the assertion that, at the 1% level of accuracy, there is little to choose between the various relativistic models for computing scattering cross sections.

Further discussion of this is given in §4.2.6.3.3.

4.2.6.3. *Modern experimental techniques*

The atomic scattering factor enters directly into expressions for such macroscopic material properties as the *refractive index*,  $n$ , and the *linear attenuation coefficient*,  $\mu_1$ . The refractive index depends on the dielectric susceptibility  $\chi$  through

$$n = (1 + \chi)^{1/2}, \quad (4.2.6.35)$$

where

$$\chi = -\frac{r_e \lambda^2}{\pi} \sum_j N_j f_j(\omega, \Delta) \quad (4.2.6.36)$$

and  $N_j$  is the number density of atoms of type  $j$ .

The imaginary part of the dispersion correction  $f''(\omega, \Delta)$  for the case where  $\Delta = 0$  is related to the atomic scattering cross section through equation (4.2.6.23).

Experimental techniques that measure refractive indices or X-ray attenuation coefficients to determine the dispersion corrections involve measurements for which the scattering vector,  $\Delta$ , is zero or close to it. Data from these experiments may be compared *directly* with data sets such as Cromer & Liberman (1970, 1981).

Other techniques measure the intensities of Bragg reflections from crystalline materials or the variation of intensities within one particular Laue reflection (*Pendellösung*). For these cases,  $\Delta = g_{hkl}$ , the reciprocal-lattice vector for the reflection or reflections measured. These techniques can be compared only indirectly with existing relativistic tabulations, since these have been developed for the  $\Delta = 0$  case. Data are available for elements having atomic numbers less than 20 in the non-relativistic case (Wagenfeld, 1975).

The following sections will discuss some modern techniques for the measurement of dispersion corrections, and an inter-comparison will be made between experimental data and theoretical calculations for a representative selection of atoms and at two extremes of photon energies: near to and remote from an absorption edge of those atoms.

4.2.6.3.1. *Determination of the real part of the dispersion correction:  $f'(\omega, 0)$* 

*X-ray interferometer techniques* are now used extensively for the measurement of the refractive index of materials and hence