4.2. X-RAYS

Table 4.2.4.1. *Table of wavelengths and energies for the characteristic radiations used in Tables 4.2.4.2 and 4.2.4.3*

Radiation	λ (Å)	E (keV)
Ag $K\bar{\alpha}$	0.5608	22.103
$K\beta_1$	0.4970	24.942
Pd $K\bar{\alpha}$	0.5869	21.125
$K\beta_1$	0.5205	23.819
Rh $K\bar{\alpha}$	0.6147	20.169
$K\beta_1$	0.5456	22.724
Mo $K\bar{\alpha}$	0.7107	17.444
$K\beta_1$	0.6323	19.608
Zn $K\bar{\alpha}$	1.4364	8.631
$K\beta_1$	1.2952	9.572
Cu $K\bar{\alpha}$	1.5418	8.041
$K\beta_1$	1.3922	8.905
Ni $K\bar{\alpha}$	1.6591	7.472
$K\beta_1$	1.5001	8.265
Co $K\bar{\alpha}$	1.7905	6.925
$K\beta_1$	1.6208	7.629
Fe $K\bar{\alpha}$	1.9373	6.400
$K\beta_1$	1.7565	7.038
Mn $K\bar{\alpha}$	2.1031	5.895
$K\beta_1$	1.9102	6.490
Cr $K\bar{\alpha}$	2.2909	5.412
$K\beta_1$	2.0848	5.947
Ti $K\bar{\alpha}$	2.7496	4.509
$K\beta_1$	2.5138	4.932

in which an idealized plane-parallel slab of material is interposed normally into a parallel beam of monoenergetic X-rays initially of intensity I_0, attenuated by the interposed slab to a reduced intensity I.

The linear attenuation coefficient μ_l for multi-element substances may be obtained in two ways. Through the mass absorption coefficients, we have

$$\mu_l = \rho \sum_i g_i(\mu_m)_i, \qquad (4.2.4.3)$$

where g_i is the mass fraction of the element i for which the mass attenuation coefficient $(\mu_m)_i$ is in units of cm^2 g^{-1}, and ρ is the density of the material in units of g cm^{-3}. The summation is over all the constituent elements. The mass attenuation coefficient μ_m is sometimes written as (μ_l/ρ).

For a crystal with unit-cell volume V_c,

$$\mu_l = \frac{1}{V_c} \sum_i \sigma_i, \qquad (4.2.4.4)$$

where the summation is over all the atoms in the cell. If σ_i is in barns/atom and V_c is in Å^3, then μ_l is in cm^{-1}.

These tables list total interaction cross sections and mass attenuation coefficients for isolated atoms calculated for characteristic X-ray photon emissions ranging from Ti $K\alpha$ to Ag $K\beta$.

The total interaction cross section is defined by

$$\sigma = \sigma_{\mathrm{pe}} + \sigma_R + \sigma_C, \qquad (4.2.4.5)$$

where σ_{pe} is the photo-effect cross section; σ_R is the Rayleigh (unmodified, elastic) cross section; σ_C is the Compton (modified, inelastic) cross section.

The reader's attention is drawn to the fact that in the neighbourhood of an absorption edge for aggregations of atoms significant deviations may be found because of cooperative effects (XAFS and XANES). A discussion of these effects is given in Section 4.2.3.

4.2.4.2. *Sources of information*

4.2.4.2.1. *Theoretical photo-effect data: σ_{pe}*

Of the many theoretical data sets in existence, those of Storm & Israel (1970), Cromer & Liberman (1970), and Scofield (1973) have often been used as bench marks against which both experimental and theoretical data have been compared. In particular, theoretical data produced using the **S**-matrix approach have been compared with these values. See, for example, Kissel, Roy & Pratt (1980). Some indication of the extent to which agreement exists between the different theoretical data sets is given in §4.2.6.2.4 (Tables 4.2.6.3 and 4.2.6.5). These tables show that the values of $f'(\omega, 0)$, which is proportional to σ, calculated using modern relativistic quantum mechanics, agree to better than 1%. It has also been demonstrated by Creagh & Hubbell (1987, 1990) in their analysis of the results of the IUCr X-ray Attenuation Project that there appears to be no rational basis for preferring one of these data sets over the other.

These tables do not list separately photo-effect cross sections. However, should these be required, the data can be found using Table 4.2.6.8. The cross section in barns/atom is related to $f'(\omega, 0)$ expressed in electrons/atom by $\sigma = 5636\lambda f'(\omega, 0)$, where λ is expressed in ångströms.

The values for σ_{pe} used in this compilation are derived from recent tabulations based on relativistic Hartree–Fock–Dirac–Slater calculations by Creagh. The extent to which this data set differs from other theoretical and experimental data sets has been discussed by Creagh (1990).

4.2.4.2.2. *Theoretical Rayleigh scattering data: σ_R*

If each of the atoms gives rise to scattering in which momentum but not energy changes occur, and if each of the atoms can be considered to scatter as if it were an isolated atom, the cross section may be written as

$$\sigma_R = \pi r_e^2 \int_{-1}^{1} (1 + \cos^2 \varphi) f^2(q, Z) \,\mathrm{d}(\cos \varphi), \qquad (4.2.4.6)$$

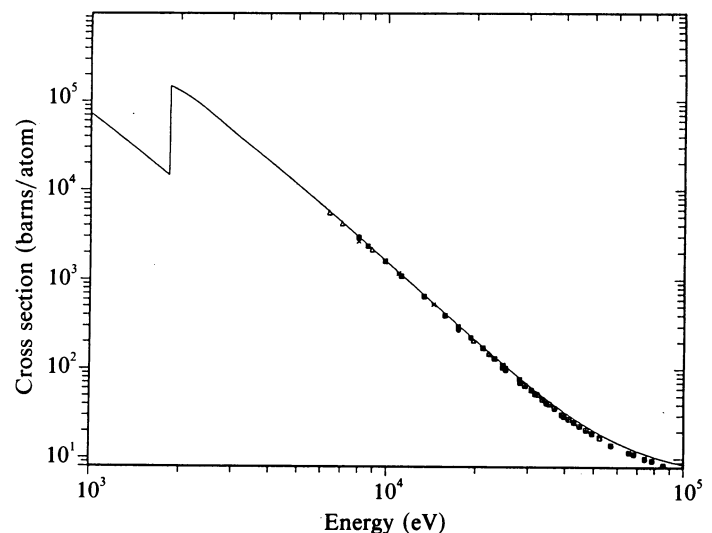where
r_e is the classical radius of the electron;

Fig. 4.2.4.2. The total cross section for silicon ($Z = 14$) compared with the unrenormalized Scofield values. The measured and theoretical attenuation coefficients show systematic differences of several percent for the photon energy range 10 to 100 keV.

221

references