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X-RAY ATTENUATION COEFFICIENTS: CURRENT STATE OF KNOWLEDGE AND AVAILABILITY

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Abstract—The current state of knowledge of X-ray attenuation coefficients in the photon energy range 1–100 keV is presented. Recent sources of experimental and theoretical data are given as well as compilations, tables and other useful tools for calculation of X-ray attenuation in matter.

1. INTRODUCTION

Accurate X-ray attenuation coefficients are required in a variety of applications. Consider for example X-ray diffraction (XRD) for the investigation of the fine structure of matter. Absorption takes place in the specimen itself and affects the intensities of the diffracted rays. This is taken into account by the absorption factor which depends on the specimen shape and the diffraction geometry (Cullity, 1978).

X-ray fluoroescence analysis (XRF) is a non-destructive method of chemical analysis. The intensity of a fluoroescent line is not in general proportional to the concentration of the element considered. This is, among other things, due to matrix absorption. There are changes both in the absorption of the primary beam travelling into the sample and the absorption of the fluoroescence radiation travelling out (Jenkins, 1974).

Analytical electron microscopy and electron microprobe analysis are other powerful methods of chemical analysis, particularly in conjunction with the energy dispersive spectrometer (EDS). The Cliff–Lorimer factor, k_{AB}, relating the weight fraction of elements A/B to their X-ray intensity is independent of specimen composition and thickness in the thin film approximation. In practice, however, the k-factors have to be corrected for X-ray absorption in the specimen (Williams, 1984). Proton-induced X-ray emission (PIXE) analysis is an alternative method, where X-rays are generated in the sample by proton bombardment. X-ray attenuation coefficients play a more important role in thick target PIXE than in the analogous technique of electron microprobe analysis, due to the greater ion ranges (Campbell *et al.*, 1983).

Radiography, finally, relies directly on the recording of the absorption power in the specimen under investigation. The ideal image represents a 3-dimensional function $\mu_1(x, y, z)$ which describes the distribution of the linear attenuation coefficient in the object. Tomography is concerned with the display of this 3-dimensional information through the formation of images of thin slices. The most well known application is the medical X-ray scanner, but computer assisted or film-based tomography can also be applied to imaging of industrial and archaeological objects in a nondestructive way (D'Amico *et al.*, 1992; Lindegaard-Andersen *et al.*, 1990).

This list of applications, which by no means is exhaustive, clearly indicates the importance of having access to accurate X-ray attenuation coefficients. A widespread discontent with the quality of compiled data caused the International Union of Crystallography (IUCr) to inaugurate a project aimed at improving the techniques for the measurement of attenuation coefficients and for producing better sets of tables for experimenters. Some results of the project have been published (Creagh and Hubbell, 1987, 1990). Experiences from the project have been useful in producing the new tables of X-ray attenuation coefficients in the *International Tables for Crystallography, Vol. C* (Creagh and Hubbell, 1992).

The status of photon cross section data was summarized by Hubbell (1982a) at the 2nd International Symposium on Radiation Physics (ISRP-2) in Penang, Malaysia. The purpose of the present work is not to give a complete coverage of the subject. Rather, the intention has been to review some of the developments during the last decade and to point out recent experimental and theoretical work as well as compilations, tables and other useful tools for calculation of X-ray attenuation coefficients. Furthermore, the need for further work in the field is stressed. The discussion has been limited mainly to the photon energy range from 1 to 100 keV. Mass energy-transfer and mass energy-absorption coefficients, important for dosimetric applications, are not discussed in the present work. The reader is referred to a recent review and tabulation by Higgins *et al.* (1992).

DEFINITIONS

The linear attenuation coefficient, μ_l, describes the fractional reduction of the beam intensity, $-dI/I$, in a thin layer of thickness dx in an absorbing medium:

$$-\frac{dI}{I} = \mu_l \, dx. \tag{1}$$

For a homogeneous medium, equation (1) is readily integrated to give the well known Beer–Lambert law:

$$I = I_0 e^{-\mu_l x} \tag{2}$$

where x is the thickness of a plane parallel layer which has surfaces normal to the beam direction, I_0 is the intensity of the incident beam and I is the intensity of the emergent beam.

The mass attenuation coefficient, $\mu_m = \mu_l/\rho$, where ρ is the absorber density, is proportional to the total photon interaction cross section, σ, through the relation

$$\mu_m = \sigma \frac{N_A}{M} \tag{3}$$

where N_A is Avogadro's number and M is the atomic weight of the absorber material. In the energy range considered here, the total photon interaction cross section is generally given by

$$\sigma = \sigma_{pe} + \sigma_R + \sigma_C \tag{4}$$

where σ_{pe} is the photoeffect cross section, σ_R the Rayleigh (coherent) scattering cross section and σ_C the Compton (incoherent) scattering cross section. Coherence in this context implies a fixed phase relationship between the incident and scattered waves for a single atom. Rayleigh scattering assumes an assembly of independent scattering atoms.

For a large perfect crystal, e.g. a silicon single crystal, the coherent scattering is more complicated because of the cooperative solid-state effects of Laue–Bragg scattering (diffraction). The coherent scattering then consists of radiation channelled into directions given by Bragg's law as well as diffuse scattering due to the thermal vibration of the atoms. In this case, the total photon interaction cross section can be written

$$\sigma = \sigma_{pe} + \sigma_{LB} + \sigma_{TDS} + \sigma_C \tag{5a}$$

where σ_{LB} is the cross section of the Laue–Bragg scattering and σ_{TDS} is the cross section of the thermal diffuse scattering. Experimentally, it should be possible to choose a sufficiently narrow X-ray beam and an appropriate crystal orientation with respect to the incident beam direction, so that no Laue–Bragg scattering occurs. In such a case equation (5a) reduces to

$$\sigma = \sigma_{pe} + \sigma_{TDS} + \sigma_C \tag{5b}$$

The photoeffect cross section is closely related to the anomalous dispersion correction in the forward scattering case. The scattering amplitude, f, of an isolated atom relative to that of a free electron is given by

$$f = f_0 + f' + if'' \tag{6}$$

The first term, f_0, is the atomic form factor or the atomic scattering factor. The second and third terms are the anomalous dispersion corrections. The photoeffect cross section is proportional to the imaginary part of the dispersion correction at the photon energy E:

$$\sigma_{pe} = \frac{2hcr_e f''}{E} \tag{7}$$

where h is Planck's constant, c is the velocity of light and r_e is the classical electron radius. It may be noted in passing that in practical units one has $hc = 12.398$ keV·Å.

If the absorber is a chemical compound or a mixture, it is generally assumed that the contribution of each element to the attenuation is additive. It follows that the *rule of mixture* can predict the resulting attenuation properties of the material. The mass attenuation coefficient, for example, is given by

$$\mu_m = \sum w_i (\mu_m)_i \tag{8}$$

where w_i is the proportion by weight of the ith constituent. The mixture rule applied to μ_m is also called Bragg's rule.

Finally, it should be mentioned that the equations in this section refer to the "narrow-beam" attenuation coefficient, i.e. it is assumed that the geometry of photon source, absorber and detector is such as to prevent any scattered photon, however small the scattering angle, from being detected. Departure from narrow-beam attenuation can arise in experimental situations.

2. EXPERIMENT

In quantitative analysis it would be desirable to know X-ray attenuation coefficients to within, say 3%. In order to discriminate between available theoretical data sets it is necessary to compare them with experimental data that are accurate to within 1% or even better (cf. Fig. 1 below). Very few measurements published in the past fulfill this requirement. There are many considerations that have to be taken into account when aiming for the 1% accuracy level. Experimental configurations and problems associated with the measurement of X-ray attenuation coefficients have been discussed by Creagh and Hubbell (1987, 1990) and Creagh (1992).

The existing experimental data situation for X-ray attenuation coefficients of the elements in the energy range from 0.1 to 100 keV has been amply reviewed by Hubbell *et al.* (1986), Saloman and Hubbell (1986), Saloman *et al.* (1988) and Manson (1989). At the higher energies the experimental data are reasonably good. Thus in the energy range 10–100 keV the experimental data are in good

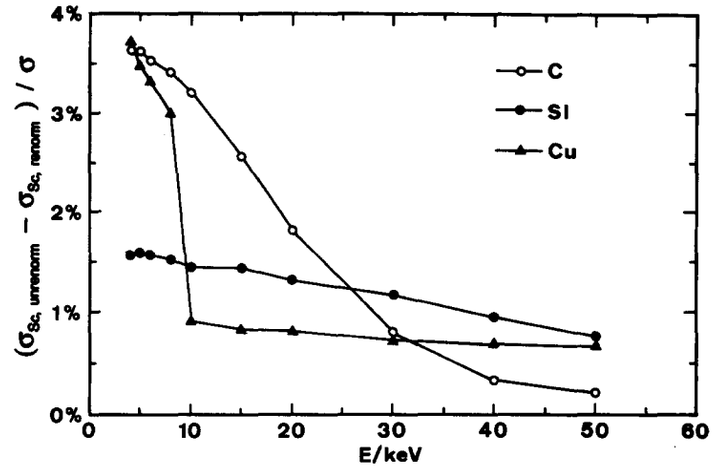

Fig. 1. Percentage reduction in the total attenuation cross section for C, Si and Cu caused by applying Hartree–Slater to Hartree–Fock renormalization to Scofield's photoionization calculation. E = photon energy. Data from Saloman and Hubbell (1986).

agreement with each other and with theory. Exceptions are energy regions just above absorption edges, where larger discrepancies are noted. Experimental results for atoms with atomic number $Z < 4$ are questionable because of the very small cross sections involved. Impurity corrections nullify accurate measurements for these elements and are important also in other low-Z absorbers.

On the whole, the experimental data are reasonably satisfactory also in the range 1–10 keV. This is true in particular for the medium Z elements. It is surprising, however, to find that good experimental data are lacking for several elements (Saloman *et al.* 1988). In the energy region below 1 keV, the situation is poorer, both experimentally and theoretically. There are many elements for which good experimental data are lacking (Saloman *et al.* 1988). Thus, it is obvious that the quality of the experimental attenuation cross sections degrades with decreasing photon energy. There is a need for more experimental work at the 1% accuracy level or better, particularly in the vicinity of absorption edges and at lower energies.

The discussion so far has dealt with neutral atoms. For excited states and ions the experimental data situation is rather poor (Manson, 1989). Turning to components, the mixture rule (8) is valid only when the effects of molecular bonding and chemical or crystalline environment are negligible. The validity of the mixture rule is uncertain in the soft X-ray region generally, and close to absorption edges (Jackson, 1982). The modulation of the cross section known as the extended X-ray absorption fine structure (EXAFS) is sensitive to the atomic environment. It has been estimated (Deslattes, 1969; Hubbell, 1990) that errors are generally less than 1 or 2% for photon energies 1 keV away from an absorption edge. However, recent experimental work (Kerur *et al.*, 1992, 1993) has shown that the range of non-validity of the mixture rule extends beyond 1 keV to, say about 1.5 keV above an absorption edge.

In X-ray absorption spectroscopy it is also important to know the absolute energy of absorption edges. Until now experimenters have relied on tables produced by Bearden (1967) and Bearden and Burr (1967), but the tabulated values can only be trusted to about 1 part in 10^4 (Arndt, 1992). There is an urgent need for a revision of these tables and for developing precise methods for energy calibration of X-rays. The availability of synchrotron radiation should facilitate such measurements as shown in recent experiments by Stümpel *et al.* (1991). It should be mentioned that the position of an edge depends on the valence state of the element involved.

3. THEORY

Computational developments have significantly improved the theoretical description of photon interactions with atoms. Calculations of photoeffect cross sections using relativistic wavefunctions have been reported, among others, by Cromer and Liberman (1970, 1981), Storm and Israel (1970) and Scofield (1973), the latter reference being of particular interest in the present work.

Scofield (1973) has calculated photoeffect cross sections using a model where the electrons are treated relativistically as moving in a Hartree–Slater central potential. For elements with atomic number from $Z = 1$ to 54, Scofield has provided correction factors for individual atomic subshells. Using these factors, the photoeffect cross sections can be renormalized so that they correspond to a relativistic Hartree–Fock model rather than the Hartree–Slater model used in the original calculation. The renormalization, which always is a decrease of the photoeffect cross section, has its greatest effect for outer shells.

Figure 1 shows the effect of renormalization for carbon, silicon and copper in the photon energy range 5–50 keV. It is seen that the percentage reduction of the total cross section is about 4% for carbon at 5 keV and that it has dropped to below 0.5% at 50 keV. For copper there is a marked decrease from 3 to 1% at the K absorption edge. Silicon shows a slow decrease from 1.5 to 1% over the whole energy range considered.

Kissel *et al.* (1980) have developed a method for accurate evaluation of total-atom Rayleigh amplitudes using the relativistic second-order S matrix of quantum electrodynamics. The S matrix formalism is considered the most rigorous method now available, even though it is difficult to program and costly in computer time. In practice, the contributions of the inner-shell electrons are calculated using the S matrix formalism, and the contributions of outer-shell electrons are estimated using form-factor approximations (Roy *et al.*, 1983). Recent progress has produced new S matrix results for scattering, beyond the impulse approximation and beyond the usual anomalous scattering factors (Pratt, 1993).

Photoeffect cross sections can be obtained from the imaginary part of the S matrix forward-scattering amplitudes using the optical theorem [cf. equation (7)]. However, only a few sets of cross sections are at hand because of the considerable computing time needed for the calculations. Recently, Creagh and McAuley (1992) have developed a model based on the use of relativistic Dirac–Slater wavefunctions. The Creagh and McAuley approach has been shown to give similar results to those of many S-matrix calculations (Creagh, 1990). For this reason it was chosen for producing the new set of photoeffect cross sections used in the *International Tables for Crystallography, Vol. C* (Creagh and Hubbell, 1992).

Theory also appears to degrade with decreasing energy as well as near absorption edges (Manson, 1989). Physically, this occurs because the photoelectrons emerge more slowly and many-body interactions become important. This is true in particular just above an absorption edge, where the photoelectron has almost zero energy. The many-body interactions lead to the X-ray absorption fine structure and, at low energies, to an energy dependence that is different from the traditional "sawtooth" shape.

4. COMPILATIONS

Tables of X-ray attenuation coefficients are purely theoretical, purely experimental or a mixture of theoretical and experimental information. Compilations that are widely used are for example those produced by Storm and Israel (1970), McMaster *et al.* (1969), Hubbell *et al.* (1974), Henke *et al.* (1982) and Hubbell (1982b). A more exhaustive listing has been given by Creagh (1990). It may be noted that the tabulation of Hubbell (1982b) is based on the calculated photoeffect cross sections of Scofield (1973) modified for $Z = 1$–54 using the relativistic Hartree–Fock renormalization factors supplied by Scofield (1973).

Coherent (Rayleigh) scattering cross sections have been calculated and tabulated by Hubbell and Øverbø (1979) using relativistic atomic form factors. The tables cover all elements and energies from 100 eV to 100 MeV. Similar tables of incoherent (Compton) scattering cross sections have been produced by Hubbell *et al.* (1975, 1977).

In practice it is not possible to meet all needs adequately by means of printed tables. Several authors (Loi *et al.*, 1977; Hawkes and Jackson, 1980;

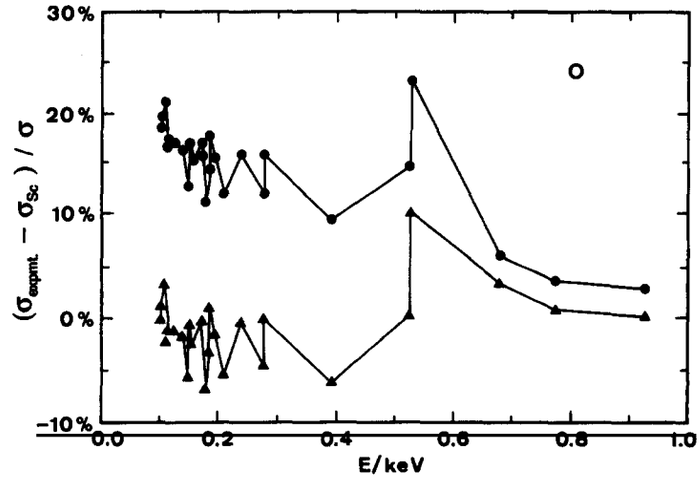

Fig. 2. Oxygen cross section data. Deviation from the experimental data (in %) of cross sections calculated using Scofield cross section with renormalization (●) and without renormalization (▲). A positive deviation corresponds to the experimental data being larger than the theoretical result. Data from Saloman and Hubbell (1987).

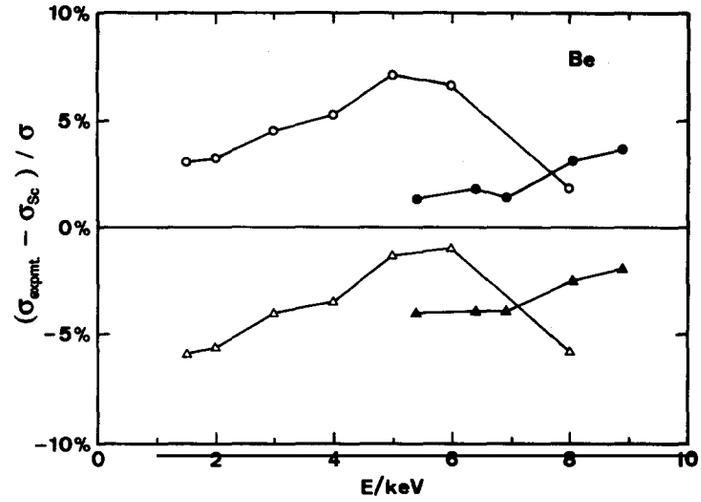

Fig. 3. Beryllium cross section data. Deviation from the experimental data (in %) of cross sections calculated using Scofield photoeffect cross sections with renormalization (○, ●) and without renormalization (△, ▲). A positive deviation corresponds to the experimental data being larger than the theoretical result. Experimental data from Gowda and Powers (1985) (open symbols) and Gerward (1989a) (solid symbols).

Jackson and Hawkes, 1981; Gerward, 1981, 1986) have derived formulae which give a parametrization of the X-ray attenuation coefficient in appropriate ranges of energy and/or atomic number. Cromer (1983) has made a Fortran program and a photoelectric cross section data file available for calculating anomalous scattering factors f' and f'' at arbitrary X-ray wavelengths. The output also includes the photoelectric mass absorption coefficient.

Berger and Hubbell (1987) have developed a computer program which can be used to calculate, with a personal computer, photon cross sections for scattering, photoelectric absorption and pair production, as well as total attenuation coefficients in any element, compound or mixture, at energies from 1 keV to 100 GeV. The program, based on conclusions developed from comparisons with measurements in the Saloman *et al.* (1988) work, uses the unrenormalized Scofield photoeffect values. The official version of the program is available as XGAM from the NIST office of Standard Reference Data (National Institute Standards and Technology Special Publication 782, 1992).

The new tables of X-ray attenuation coefficients in the *International Tables for Crystallography, Vol. C* (denoted by ITVC in the following) are based on a fully theoretical data set, because reliable experimental data do not exist for the range of elements $Z = 1$–98 and the range of photon energies 5–25 keV. The rationale underlying the production of the ITVC data set has been discussed by Creagh (1990). The data entries listed in ITVC agree with experimental and other theoretical values to better than 3% for most elements. Discrepancies of greater than 3% are most likely to occur for atomic numbers in the ranges $1 \leqslant Z \leqslant 4$ and $60 \leqslant Z \leqslant 90$.

The theoretical photoeffect cross sections used for the production of the ITVC data set are those of Creagh and McAuley (1992). The ITVC data are generally consistent with the unrenormalized Scofield calculation as shown by Gerward (1992). There is perfect agreement between the ITVC values and the unrenormalized Scofield values for the low- and medium-Z elements. For the lanthanides the agreement is better than 1.5%. Somewhat larger differences are found for the high-Z elements: general agreement to $\pm 4\%$ exists; however, differences up to 7% are observed for some entries.

5. COMPARISON BETWEEN EXPERIMENTAL AND THEORETICAL CROSS SECTIONS

An important issue is to establish which of the existing tabulations of photon interaction cross sections are to be preferred. This was one of the aims set for the IUCr Attenuation Project, but so far no definite conclusions have been drawn (Creagh and Hubbell, 1987, 1990). Creagh (1990) has compared data on X-ray attenuation coefficients tabulated in *International Tables for Crystallography, Vol. C* with other empirical, semi-empirical and theoretical data.

In a critical analysis of soft X-ray cross section data, Saloman and Hubbell (1987) have compared experimental results with the Scofield photoeffect cross sections with and without renormalization. The authors conclude that the Scofield theoretical values, taken as a whole, are not improved by the Hartree–Slater to Hartree–Fock renormalization. Thus the unrenormalized results seem to agree better

with the experimental results. Figure 2 illustrates the point for oxygen cross section data. There are exceptions, however, to the rule. Thus the results of the IUCr Attenuation Project have shown that carbon is an example in which the renormalization would improve the agreement between theory and experiment (Creagh and Hubbell, 1990). In the 10–100 keV range the effect of renormalization is only about 1% (cf. Fig. 1) and no conclusion can yet be drawn about the value of renormalization in this decade (Saloman and Hubbell, 1986).

Figure 2 illustrates another striking fact, namely that the renormalized and the unrenormalized Scofield values tend to satisfy the inequality

$$\sigma_{\mathrm{Sc,renorm}} < \sigma_{\mathrm{expmt.}} < \sigma_{\mathrm{Sc,unrenorm}} \quad (9)$$

where $\sigma_{\mathrm{expmt.}}$ is the experimental cross section and σ_{Sc} is the Scofield value under consideration. In other words, it appears that the Scofield theoretical values with and without the Hartree–Slater to Hartree–Fock renormalization could be used as lower and upper limits to the experimental photoeffect cross sections. Figure 3 shows the same point for beryllium cross sections in the energy range from 1.5 to 9 keV. More examples on the inequality (9) have been given by Gerward (1989b, 1992).

The validity (or non-validity) of the mixture rule (8) has attracted a recent experimental interest (Kerur *et al.*, 1992, 1993). In addition to the chemically-dependent fine structure (EXAFS) just above absorption edges, smooth monotonic curves drawn through this fine structure depart systematically from theory by as much as 10%. These systematic effects have been observed and discussed by Del Grande (1986) and Del Grande *et al.* (1987).

In conclusion, accurate experimental work is needed to provide X-ray attenuation data for various applications, but also for use as benchmarks for comparison with theory. The ultimate aim would be to develop theory to the point where photon interaction cross sections could be accurately predicted over the periodic table and the whole energy range considered.

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REFERENCES

Arndt U. W. (1992) Generation of X-rays. In *International Tables for Crystallography, Vol. C* (Edited by Wilson A. J. C.), p. 167. Kluwer Academic, Dordrecht.

Bearden J. A. (1967) X-ray wavelengths. *Rev. Mod. Phys.* **39,** 78.

Bearden J. A. and Burr A. F. (1967) Reevaluation of X-ray atomic energy levels. *Rev. Mod. Phys.* **39,** 125.

Berger M. J. and Hubbell J. H. (1987) XCOM: Photon cross sections on a personal computer. National Bureau of Standards Internal Report, NBSIR 87-3597.

Campbell J. L., Cookson J. A. and Paul H. (1983) Uncertainties in thick-target pixe analysis. *Nucl. Instrum. Meth.* **212,** 427.

Creagh D. C. (1990) Tables of X-ray absorption coefficients and dispersion corrections: the new versus the old. *Nucl. Instrum. Meth.* **A295,** 417.

Creagh D. D. (1992) X-ray absorption spectra. In *International Tables for Crystallography. Vol. C* (Edited by Wilson A. J. C.), p. 182. Kluwer Academic, Dordrecht.

Creagh D. C. and Hubbell J. H. (1987) Problems associated with the measurement of X-ray attenuation coefficients. I. Silicon. Report on the International Union of Crystallography X-ray attenuation project. *Acta Cryst.* **A43,** 102.

Creagh D. C. and Hubbell J. H. (1990) Problems associated with the measurement of X-ray attenuation coefficients. II. Carbon. Report on the International Union of Crystallography X-ray attenuation project. *Acta Cryst.* **A46,** 402.

Creagh D. C. and Hubbell J. H. (1992) X-ray absorption (or attenuation) coefficients. In *International Tables for Crystallography. Vol. C* (Edited by Wilson A. J. C.), p. 189. Kluwer Academic, Dordrecht.

Creagh D. C. and McAuley W. J. (1992) X-ray dispersion corrections. In *International Tables for Crystallography, Vol. C* (Edited by Wilson A. J. C.), p. 206. Kluwer Academic, Dordrecht.

Cromer D. T. (1983) Calculation of anomalous scattering factors at arbitrary wavelengths. *J. Appl. Cryst.* **16,** 437.

Cromer D. T. and Liberman D (1970 Relativistic calculation of anomalous scattering factors for X-rays. *J. Chem. Phys.* **53,** 1891.

Cromer D. T. and Liberman D (1981) Anomalous dispersion calculations near to and on the long-wavelength side of an absorption edge. *Acta Cryst.* **A37,** 267.

Cullity B. D. (1978) *Elements of X-ray Diffraction*, 2nd edn. Addison-Wesley, Reading.

D'Amico K. L., Dunsmuir J. H., Ferguson S. R. and Flannery B. P. (1992) The Exxon microtomography beam line at the National Synchrotron Light Source. *Rev. Sci. Instrum.* **63,** 574.

Del Grande N. K. (1986) Measured 1 to 40 keV photoabsorption cross sections for: Fe, Ni, Sn, Ta, Pt, Au, Pb, U. *SPIE Proc.* **691,** 2.

Del Grande N. K., Tirsell K. G., Schneider M. B., Garrett R. F., Kneedler E. M. and Manson S. T. (1987) Resonances in near-threshold X-ray photoabsorption of inner shells. *J. Phys. Colloq.* **48,** C9–951.

Deslattes R. D. (1969) Estimates of X-ray attenuation coefficients for the elements and their compounds. *Acta Cryst.* **A25,** 89.

Gerward L. (1981) Analytical approximations for X-ray attenuation coefficients. *Nucl. Instrum. Meth.* **181,** 11.

Gerward L. (1986) Empirical absorption equations for use in X-ray spectrometric analysis. *X-ray Spectrom.* **15,** 29.

Gerward L. (1989a) X-ray attenuation coefficients of beryllium in the energy range 5 to 20 keV. *Acta Cryst.* **A45,** 1.

Gerward L. (1989b) Atomic photoeffect cross sections for beryllium, carbon, silicon and copper from 5 to 20 keV. *J. Phys. B: At. Molec. Opt. Phys.* **22,** 1963.

Gerward L. (1992) Theoretical upper and lower limits to experimental X-ray attenuation coefficients. *Nucl. Instrum. Meth.* **B69,** 407.

Gowda R. and Powers D. (1985) Photon-attenuation cross sections for beryllium from 1.5 to 8.0 keV. *Phys. Rev.* **A32,** 2637.

Hawkes D. J. and Jackson D. F. (1980) An accurate parametrisation of the X-ray attenuation coefficient. *Phys. Med. Biol.* **25,** 1167.

Henke B. L., Lee P., Tanaka T. J., Shimabukuro R. L. and Fujikawa B. K. (1982) Low-energy X-ray interaction coefficients: photoabsorption, scattering, and reflection, $E = 100$–2000 eV, $Z = 1$–94. *Atom. Data Nucl. Data Tables* **27,** 1.

Higgins P. D., Attix F. H., Hubbell J. H., Seltzer S. M., Berger M. J. and Sibata C. H. (1992) Mass energy-transfer and mass energy-absorption coefficients, including in-flight positron annihilation for photon energies 1 keV to 100 MeV. National Institute of Standards and Technology Internal Report, NISTIR 4812.

Hubbell J. H. (1982a) Photon attenuation coefficients and cross section data 100 eV to 100 GeV. Current status and prospects. In *Proc. 2nd Int. Symp. Radiation Physics (ISRP-2)*, Penang, Malaysia.

Hubbell J. H. (1982b) Photon mass attenuation and energy-absorption coefficients from 1 keV to 20 MeV. *Int. J. Appl. Radiat. Isot.* **33**, 1269.

Hubbell J. H. (1990) Annotated and indexed bibliography of experimental photon-attenuation coefficients for compounds. National Institute of Standards and Technology Internal Report, NISTIR 90-4282.

Hubbell J. H. and Øverbø I. (1979) Relativistic atomic form factors and photon coherent scattering cross sections. *J. Phys. Chem. Ref. Data* **8**, 69.

Hubbell J. H., Gerstenberg H. M. and Saloman E. B. (1986) Bibliography of photon total cross section (attenuation coefficient). Measurements 10 eV to 13.6 GeV. National Bureau of Standards Internal Report, NBSIR 86-3461.

Hubbell J. H., McMaster W. H., Del Grande N. K. and Mallett J. H. (1974) X-ray cross sections and attenuation coefficients. In *International Tables for X-ray Crystallography, Vol. 4* (Edited by Ibers J. A. and Hamilton W. C.), p. 47. Kynoch Press, Birmingham.

Hubbell J. H., Veigele Wm. J., Briggs E. A., Brown R. T., Cromer D. T. and Howerton R. J. (1975) Atomic form factors, incoherent scattering functions, and photon scattering cross sections. *J. Phys. Chem. Ref. Data* **4**, 471.

Hubbell J. H., Veigele Wm. J., Briggs E. A., Brown R. T., Cromer D. T. and Howerton R. J. (1977) Erratum: Atomic form factors, incoherent scattering functions, and photon scattering cross sections. *J. Phys. Chem. Ref. Data* **6**, 615.

Jackson D. F. (1982) Chemical effects in X-ray transmission measurements. *Nucl. Instrum. Meth.* **193**, 387.

Jackson D. F. and Hawkes D. J. (1981) X-ray attenuation coefficients of elements and mixtures. *Phys. Rep.* **70**, 169.

Jenkins R. (1974) *An Introduction to X-ray Spectrometry*. Heyden, London.

Kerur B. R., Thontadarya S. R. and Hanumaiah B. (1992) A study on the range of non-validity of the Bragg's additive law for compounds at photon energies below 10 keV. *Appl. Radiat. Isot.* **43**, 893.

Kerur B. R., Thontadarya S. R. and Hanumaiah B. (1993) X-ray attenuation coefficients at 6.46 keV and the validity of the mixture rule for compounds. *X-Ray Spectrom.* **21**, In press.

Kissel L., Pratt R. H. and Roy S. C. (1980) Rayleigh scattering by neutral atoms, 100 eV to 10 MeV. *Phys. Rev.* **A22**, 1970.

Lindegaard-Andersen A., Notea A., Bushlin Y. and Rheinländer J. (1990) Image-centered frame of reference in rotational film-based X-ray tomography. *NDT Int.* **23**, 332.

Loi T. H., Remy M. and Zeller C. (1977) A semi-empirical law for the determination of mass absorption coefficients for X-rays. *J. Phys. D: Appl. Phys.* **10**, 717.

Manson S. T. (1989) Photoionization cross sections: Present status and future needs. *Nucl. Instrum. Meth.* **A280**, 173.

McMaster W. H., Del Grande N. K., Mallett J. H. and Hubbell J. H. (1969) Compilation of X-ray cross sections. Lawrence Livermore Nat. Lab. Rep. UCRL-50174, Sec. II, Rev. 1.

National Institute for Standards and Technology Special Publication 782, 1992 Ed. (1992) *Reliable Evaluated Data for Global Problems* (Edited by Chase M. W. and Sauerwein J. C.), p. 18.

Pratt R. H. (1993) New relativistic S matrix results for scattering—beyond the usual anomalous factors/beyond impulse approximation. In *X-Ray Resonance (Anomalous) Scattering* (Edited by Fischer K., Materlik G. and Sparks C. J.). Elsevier Science, Amsterdam, to appear in 1993.

Roy S. C., Kissel L. and Pratt R. H. (1983) Elastic photon scattering at small momentum transfer and validity of form-factor theories. *Phys. Rev.* **A27**, 285.

Saloman E. B. and Hubbell J. H. (1986) X-ray attenuation coefficients (total cross sections): Comparison of the experimental data base with the recommended values of Henke and the theoretical values of Scofield for energies between 0.1–100 keV. National Bureau of Standards Internal Report, NBSIR 86-3431.

Saloman E. B. and Hubbell J. H. (1987) Critical analysis of soft X-ray cross section data. *Nucl. Instrum. Meth.* **A255**, 38.

Saloman E. B., Hubbell J. H. and Scofield J. H. (1988) X-ray attenuation cross sections for energies 100 eV to 100 keV and elements $Z = 1$ to $Z = 92$. *Atom. Data Nucl. Data Tables* **38**, 1.

Scofield J. H. (1973) Theoretical photoionization cross sections from 1 to 1500 keV. Lawrence Livermore Nat. Lab. Rep. UCRL-51326.

Storm E. and Israel H. I. (1970) Photon cross sections from 1 keV to 100 MeV for elements $Z = 1$ to $Z = 100$. *Nucl. Data Tables* **A7**, 565.

Stümpel J., Becker P., Joksch St., Frahm R. and Materlik G. (1991) Measurement of the energy of X-ray absorption edges. *Phys. Stat. Sol. (A)* **124**, 565.

Williams D. B. (1984) *Practical Analytical Electron Microscopy in Materials Science*, p. 75. Verlag Chemie International, Basel.