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X-ray Attenuation Coefficients of Beryllium in the Energy Range 5 to 20 keV

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Abstract

Mass attenuation coefficients for beryllium have been determined by an X-ray energy-dispersive method with a relative experimental error of 1-2%. Results are given for Cr, Fe, Co, Cu and Mo $K\alpha_1$ lines and compared with recent experimental and theoretical results.

1. Introduction

Accurate X-ray attenuation coefficients are required in a variety of applications, such as dosimetry, spectrometry, radiography and crystallography. Beryllium is widely used as a window material for X-ray tubes, synchrotron-radiation beam lines and semiconductor detectors [Si(Li) and Ge]. Attenuation cross sections of beryllium are therefore important in order to correct for the attenuation in the window, in particular at photon energies below 10 keV. However, there are large differences among experimental data reported for beryllium. Values of the attenuation cross section may differ by as much as 50%, as can be seen, for example, by comparing the 1968 and 1974 volumes of *International Tables for X-ray Crystallography.*

The present work describes the determination of mass attenuation coefficients of beryllium using an energy-dispersive method developed for the Attenuation Project of the International Union of Crystallography. The method was considered the most reliable one in the energy range from 4 to 50 keV in a report on the IUCr project results for silicon (Creagh & Hubbell 1987).

The experimental results are compared with theoretical data based on relativistic photoeffect calculations. Particular attention is paid to a comparison with the theoretical data set of Scofield (1973) and the question of whether a renormalization procedure from the Hartree–Slater to the Hartree–Fock atomic model improves the agreement between theory and experiment or not.

2. Experimental procedure

The narrow-beam mass attenuation coefficient, μ/ρ, is determined by the exponential law

$$I = I_0 \exp[-(\mu/\rho)x]$$

where I and I_0 are the observed intensities with and without the absorber and x is the mass per unit area of the absorber.

The experimental arrangement corresponds to configuration no. 3 as described by Creagh & Hubbell (1987). Slit-collimated X-rays were monochromatized by a perfect silicon crystal using the 220 or 440 reflection. The reflected X-rays were recorded by a Si(Li) detector connected to a multichannel pulse-height analyser. The absorber was placed between the X-ray source and the monochromator. The absorber thickness was chosen to give a value of $\ln(I_0/I)$ near 3, giving optimum attenuation conditions (Nordfors, 1960). Details on the elimination of harmonic contamination and dead-time effects have been described in previous work on silicon and carbon (Gerward & Thuesen, 1977; Gerward 1981, 1983). Errors in counting statistics were always kept less than 0·25%.

The beryllium specimens are squares with lateral dimensions 15 × 15 mm and thickness 2 mm, delivered by Goodfellow Metals Ltd, Cambridge, England. The purity is 99·3%. The mass per unit area was determined with a relative standard deviation of 0·10–0·14% by weighing and measuring the lateral dimensions. The mass density was determined as 1·839 (4) g cm^{-3}. This is close to literature data, showing that the specimens do not contain any voids that could contribute to the narrow-beam attenuation coefficient through small-angle scattering. Several specimen squares could be stacked together to give the optimum thickness as discussed above.

The measured mass attenuation coefficients were corrected for contributions from the impurities using attenuation coefficients tabulated in *International Tables for X-ray Crystallography* (1974). The most severe correction is due to the 530 p.p.m. content of iron. Moreover, a slight correction was necessary to take into account the air displaced by the specimen. Attenuation coefficients of air were taken from the tabulation by Hubbell (1982).

3. Results and discussion

The mass attenuation coefficient is proportional to the total photon interaction cross section per atom,

$$\sigma = (\mu/\rho)M/N_A,$$

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Table 1. *Calculated scattering contributions to the mass attenuation coefficient of beryllium*

E = photon energy, R = Rayleigh scattering, C = Compton scattering. The values are given in units of cm^2 g^{-1}.

Line	E (keV)	$(\mu/\rho)_R$	$(\mu/\rho)_C$
Cr $K\alpha_1$	5·415	0·180	0·099
Fe $K\alpha_1$	6·404	0·156	0·106
Co $K\alpha_1$	6·930	0·144	0·110
Cu $K\alpha_1$	8·048	0·125	0·116
Cu $K\beta_1$	8·905	0·112	0·121
Mo $K\alpha_1$	17·479	0·044	0·145

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

$$\sigma = \sigma_{\rm pe} + \sigma_R + \sigma_C$$

where $\sigma_{\rm pe}$ 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 wave for a single atom. Rayleigh scattering assumes an assembly of independent scattering atoms. Smooth continuous Debye rings recorded on transmission pinhole photographs showed that the samples are made of a fine-grained polycrystalline material. It has been shown that the coherent scattering in such a material is best described by the Rayleigh scattering cross section (Gerward, 1982).

Calculated scattering cross sections useful for comparisons with other experimental or theoretical work are summarized in Table 1. Rayleigh scattering cross sections and bound-electron Compton scattering cross sections have been interpolated from the tabulation by Hubbell & Øverbø (1979) and Hubbell, Veigele, Briggs, Brown, Cromer & Howerton (1975), respectively.

The experimental results are summarized in Table 2 and compared with published data. Recent measurements are scarce, as can be seen in the table. Also included are the results of two compilations. The values given in *International Tables for X-ray Crystallography* (1974) are interpolated from an evaluated cross-section compilation by McMaster, Del Grande, Mallett & Hubbell (1970). This compilation is based on experimental as well as theoretical data. In contrast, the compilation by Veigele (1973) is based solely on experimental data. It is seen that the values of the Veigele compilation are larger than those of McMaster *et al.* The latter values appear to be too low in the energy range considered here.

Relativistic quantum mechanics is used by many authors in their calculation of the photoeffect cross section. In Table 3 the experimental results are compared with total mass attenuation coefficients calculated by Cromer & Liberman (1970, 1981), Storm & Israel (1970) and Scofield (1973). The first two calculations give nearly the same results, which is natural, because they are both based on the code of Brysk & Zerby (1968).

The theoretical photoeffect cross section data of Scofield (1973) are based on Hartree–Slater wavefunctions. The tabulation by Hubbell (1982) uses Scofield's data modified for Z = 1 to 54 using relativis-

Table 2. *Comparison with recent measurements and two compilations of mass attenuation coefficients of beryllium*

Ka = Karev (1964), Be = Bearden (1966), De = Del Grande, Stinner & Oliver (1969), PC = Phillips & Chin (1973), Na = Nathuram, Rao & Mehta (1984), GP = Gowda & Powers (1985), IT = *International Tables for X-ray Crystallography* (1974) and Ve = Veigele (1973); E = photon energy. The values are given in units of cm^2 g^{-1}.

Line	E(keV)	This work	Ka	Be	De*	PC	Na*	GP*	IT	Ve*
Cr $K\alpha_1$	5·415	3·30 (5)		3·50	3·08			3·40	3·18	3·40
Fe $K\alpha_1$	6·404	2·01 (3)		2·19	2·00			2·06	1·91	2·07
Co $K\alpha_1$	6·930	1·61 (2)		1·70*	1·57			1·63	1·52	1·65
Cu $K\alpha_1$	8·048	1·08 (2)	1·15	1·01	1·05			1·04	1·00	1·10
Cu $K\beta_1$	8·905	0·841 (15)			0·830				0·774	0·849
Mo $K\alpha_1$	17·479	0·255 (5)	0·266		0·231	0·303	0·254		0·245	0·257

* Interpolated

Table 3. *Comparison with theoretical total mass attenuation coefficients of beryllium*

CL = Cromer & Liberman (1970, 1981), SI = Storm & Israel (1970), Sc = Scofield (1973): renormalized values from Hubbell (1982) and unrenormalized from Saloman & Hubbell (1986). The values are given in units of cm^2 g^{-1}.

Line	E(keV)	This work	CL	SI	Sc renormalized	Sc unrenormalized
Cr $K\alpha_1$	5·415	3·30 (5)	3·16	3·16	3·26	3·43
Fe $K\alpha_1$	6·404	2·01 (3)	1·93	1·94	1·99	2·09
Co $K\alpha_1$	6·930	1·61 (2)	1·55	1·55	1·59	1·67
Cu $K\alpha_1$	8·048	1·08 (2)	1·035	1·040	1·059	1·11
Cu $K\beta_1$	8·905	0·841 (15)	0·803	0·805	0·818	0·853
Mo $K\alpha_1$	17·479	0·255 (5)	0·250	0·252	0·252	0·255

tic Hartree–Fock renormalization factors supplied by Scofield (1973). However, in recent studies Saloman & Hubbell (1986, 1987) have suggested that the Scofield values without renormalization are in better agreement with the experiments than the renormalized values in the photon energy range from 0·1 to 1 keV.

Table 3 shows that the renormalized Scofield values are smaller than the corresponding unrenormalized values. The table also shows that the experimental results of the present work are larger than the renormalized Scofield values but not so large as the unrenormalized values. The few other experimental data available in the literature (Table 2) give no clear evidence to establish which of the theoretical tables is to be preferred in the energy range considered here.

The experimental error in the present work ranges from 1 to 2%. It is mainly determined by uncertainties in the impurity corrections. Thus, in order to improve the results one should use beryllium of a purity that is at least a factor of ten better than in the present work, *i.e.* 99·93% purity or better.

4. Concluding remarks

Mass attenuation coefficients of beryllium have been measured with a relative experimental error of 1-2% using an energy-dispersive technique. Theoretical attenuation coefficients derived from relativistic photoeffect cross sections are in good agreement with the experimental results, although some systematic deviations can be noticed. In particular, it is found that the present results fall between the renormalized and the unrenormalized theoretical Scofield data.

Furthermore, it has been shown that a meaningful comparison between high-precision attenuation coefficients for a low-Z material, such as beryllium, is possible only when the contributions from the impurities are carefully analysed.

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