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Anomalous scattering factor using proton induced X-ray emission technique

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HIGHLIGHTS

- Anomalous scattering factors determined from the attenuation data.
- PIXE technique is used for getting the attenuation data.
- Our results are in close agreement with the available theoretical values.
- PIXE technique is a reliable tool for determining anomalous scattering factors.

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ABSTRACT

Atomic scattering factor is in general a complex number represented by the sum of normal scattering factor (f_0) and anomalous scattering factors [real (f') and imaginary (f'')]. Anomalous scattering factors in Ag, In, Cd and Sn were determined experimentally from attenuation data measured using PIXE and compared with theoretical values. The data cover the energy region from 10 to 30 keV and atomic number Z from 47 to 50 keV. Our results found to be in close agreement with theoretical values.

1. Introduction

In the X-ray energy range, the primary interactions of photons with atoms are photoabsorption, coherent (elastic) scattering and Compton (inelastic) scattering. Nuclear scattering and absorption including pair production and Delbrück scattering from the nuclear field; and nuclear resonant processes (such as nuclear Thomson scattering) are relevant at energies above around 1 MeV. The normal atomic scattering factor f_0 describes the strength of X-rays scattered by the electrons in an atom just like free oscillators. However, in actual situations the scattering electrons are bound in atomic orbitals and they act instead as a set of damped oscillators with resonant frequencies matched to the absorption frequencies of the electron shells. The total atomic scattering factor f is then a complex number, and is represented by the sum of the normal scattering factor (f_0) and anomalous scattering factor [real (f') and imaginary (f'') also called the dispersion correction]. Knowledge of complex X-ray scattering factors is very important in various applications such as crystallography, medical diagnosis, radiation safety, and X-ray absorption fine structure studies (XAFS). A detailed calculation of real and imaginary parts of anomalous scattering factor using the dispersion relation is carried out in this work. The absorption cross sections needed for this study are measured using Proton Induced X-ray Emission Technique (Appaji Gowda and Umesh, 2006). In the present work, we have used protons of 2 MeV energy to excite characteristic X-rays from a set of targets kept inside a scattering chamber (PIXE chamber). This technique has two distinct advantages as compared to photon induced x-ray emission. The X-ray flux available from the PIXE technique is much more than the flux available from radioactive sources. Also, the background effects from the PIXE technique are much less as compared to other methods.

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2. Theoretical description of anomalous scattering factor

Theory of anomalous scattering and dispersion of X-rays is treated in detail by James (1948). In this theory the atoms interacting with photons are treated like electric dipole oscillators having certain definite natural frequencies which correspond to the absorption frequencies of the atoms. The electric field of incident photon modifies the frequency and the amplitude of the oscillators by a dispersive term and an absorptive term. The dispersive term depends on the proximity of the impressed frequency to the natural resonant frequency of the system and the absorptive term depends on the damping factor.

At very low photon energy, the photon has no sufficient energy to excite any of the available electronic transitions. The elastic scattering cross-section (or the probability that the photon is scattered) may be adequately described by the normal atomic scattering coefficient f_0 only, with no phase delay (imaginary component f'' is zero).

When the incident photon has enough energy, some of them are scattered normally, while some of them are either absorbed and then re-emitted at lower energy (fluorescence) or absorbed and then re-emitted at the same energy (strong coupling to absorption edge energy). The scattered photon gains an imaginary component to its phase (f'' becomes non-zero); i.e. it is retarded compared to a normally scattered photon. Thus, in anomalous X-ray scattering from an atom the scattering factor becomes a complex quantity and is written as

$$f = f_0 + f' + if'' \quad (1)$$

where first term f_0 is the normal scattering form factor, f' is the real part of anomalous scattering factor representing the dispersion effect in scattering near the resonant level and f'' is the imaginary part of anomalous scattering factor representing the absorptive part of the elastic scattering near a resonant state of the bound scattering electron. f' and f'' are together known as dispersion corrections. From the optical theorem

$$f'' = \frac{mc\epsilon_0 E}{e^2 \hbar}\sigma_{tot} \quad (2)$$

In terms of classical electron radius r_0, we obtain the expression as

$$f'' = \frac{E}{2hcr_0}\sigma_{tot} \quad (3)$$

Here, $r_0 = e^2/4\pi\epsilon_0 mc^2$ is the classical electron radius. The total cross section $\sigma_{\rm tot}$ is given by $\sigma_{tot} = \tau + \sigma_{BBT} - \sigma_{BPP}$, where τ, σ_{BBT}, and σ_{BPP} are the photo effect, photo excitation, and bound pair production cross-sections, respectively. For energies sufficiently away from absorption edges of a particular element, σ_{BBT}, σ_{BPP} are expected to be insignificant for $Z > 10$, below the pair production threshold (Wang, 1986; Wang and Pratt, 1983). In the energy region of current interest, if we neglect the spin flip process, the f' and f'' are connected by the modified Kramers–Kronig transform (Zhou et al., 1992; Henke et al., 1982)

$$f_R'(E) = f'(\infty) - \frac{2}{\pi}P\int_0^{\infty}\frac{E'f''(E')}{E^2 - E'^2}dE' \quad (4)$$

where P is the Cauchy principal value of the dispersion integral. The second term on the R.H.S. of the above equation represents the non-relativistic values $f_{NR}'(E)$. The factor $f'(\infty)$ is called the high energy limit or relativistic correction. The $f'(\infty)$ values of Cromer and Liberman (1970) [CL], Creagh and McAuley (1992) [CM] and Kissel and Pratt (1990) [KP] for elements Ag, Cd, In and Sn which have been used in the present work are given in Table 1. Cromer and Liberman (1970) and Henke et al. (1982) considered electric dipole approximation in their estimate of the relativistic correction to the high energy limit $f'(\infty)$ of forward scattering. Kissel and Pratt (1990) used numerical S-matrix approach to determine $f'(\infty)$ to a high degree of accuracy and the values have been tabulated for all neutral atoms. The attenuation coefficient data were determined experimentally for the elements Ag, Cd, In and Sn using the PIXE method, for evaluating the dispersion correction in these elements. Details of the calculation and the results obtained therefrom are given in the following section.

Table 1
Relativistic corrections (high energy limit, $f'(\infty) = \Delta$).

Element	Δ_{KP} S-matrix correction	Δ_{CM} Multiple correction	Δ_{CL} Dipole corrections
Silver	−0.264	−0.285	−0.471
Cadmium	−0.277	−0.300	−0.496
Indium	−0.291	−0.315	−0.522
Tin	−0.305	−0.331	−0.548

3. Analysis

For evaluating the dispersion corrections, it is essential to determine the total mass attenuation coefficients of the elements of interest over a wide range of energies around the corresponding K-edges. Using these values, the total attenuation cross section σ was determined. From the measured values of total attenuation cross section, the total photoelectric cross sections were estimated by subtracting the sum of the coherent and incoherent scattering contributions. The scattering contributions required for this were extracted from the XCOM (Berger et al., 1990) data base.

3.1. Calculation of imaginary part of the anomalous scattering factor f''

The photo effect cross sections obtained as mentioned above were used to calculate f'' using Eq. (3). These values are tabulated in Tables 2–5.

Table 2
Photo effect cross-sections (σ_{ph}), imaginary part (f'') and real part (f') of the anomalous scattering factor for **Ag**.

Energy (keV)	σ_{ph} (barns/atom)	f''	Real part, f' (KP)	(CM)	(CL)
10.50	17,068.02 ± 1016.23	2.56 ± 0.15	−0.03	−0.05	−0.23
11.51	12,113.44 ± 721.53	1.99 ± 0.12	−0.35	−0.37	−0.56
12.62	11,482.46 ± 683.59	2.07 ± 0.12	−0.55	−0.57	−0.76
12.94	11,013.89 ± 658.85	2.04 ± 0.12	−0.46	−0.48	−0.66
13.38	8945.25 ± 536.84	1.71 ± 0.10	−0.50	−0.52	−0.71
14.76	7971.52 ± 476.49	1.68 ± 0.10	−0.65	−0.67	−0.86
15.73	6010.05 ± 357.70	1.35 ± 0.08	−0.74	−0.76	−0.94
16.57	5635.10 ± 335.40	1.34 ± 0.08	−0.84	−0.86	−1.05
17.43	4762.85 ± 283.50	1.19 ± 0.07	−0.95	−0.97	−1.16
17.67	4879.42 ± 290.81	1.23 ± 0.07	−0.98	−1.00	−1.19
18.62	4295.08 ± 256.10	1.14 ± 0.07	−1.01	−1.04	−1.22
19.61	3575.74 ± 213.24	1.00 ± 0.06	−1.12	−1.14	−1.32
21.10	2903.72 ± 172.91	0.88 ± 0.05	−1.33	−1.36	−1.54
22.08	2429.22 ± 144.68	0.77 ± 0.05	−1.53	−1.55	−1.74
23.08	2109.89 ± 125.76	0.70 ± 0.04	−1.83	−1.85	−2.04
23.82	2100.52 ± 125.72	0.72 ± 0.04	−2.08	−2.10	−2.29
24.11	1800.37 ± 107.38	0.62 ± 0.04	−2.22	−2.25	−2.43
24.94	1687.62 ± 101.13	0.60 ± 0.04	−2.98	−3.00	−3.19
25.16	1498.78 ± 89.46	0.54 ± 0.03	−3.40	−3.42	−3.60
25.51	1244.00 ± 74.76	3.36 ± 0.20	−4.89	−4.91	−5.10
26.10	8933.09 ± 542.19	3.33 ± 0.20	−2.91	−2.93	−3.12
27.28	8428.03 ± 515.94	3.29 ± 0.20	−1.74	−1.76	−1.94
28.49	7161.69 ± 441.15	2.92 ± 0.18	−1.22	−1.24	−1.42