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Experimental studies on atomic form factors at 2.216 Å^{-1} photon momentum transfer

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Abstract: Differential cross sections for coherent scattering of 59.5 keV γ-rays 55° (scattering) by Ti, Fe, Ni, Cu, Zn, Zr, Nb, Mo, Ag, Sn, Ta, Au and Pb were measured using a Ge(Li) detector. From these accurately measured cross sections atomic form factors are extracted corresponding to 2.216 Å^{-1} photon momentum transfer. The results are compared with predictions of form-factor theories, and the appropriateness of these theories is discussed.

Key-words: Scattering cross sections and atomic form factors.

Abbreviations: EDXRD, energy dispersive X-ray diffraction; EPMA, electron probe microanalysis; EXAFS, X-ray absorption fine structure; FWHM, Full width at half the maximum; NRFF, non-relativistic form-factor; PIXE, proton induced X-ray emission; RMFF, relativistic modified form-factor; XRF, X-ray fluorescence.

INTRODUCTION

The terms "atomic scattering factor," "atomic form factor" and "atomic structure factor" have been used in describing the elastic scattering of photons by atoms. The "atomic scattering factor" F was defined by Hartree (cited by Crasemann [2] as the "ratio of the amplitude of the wave scattered by this atom to the amplitude scattered by an electron". Here we define F as $A = F A^T$, the ratio of the isolated-atom total-atom elastic

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scattering amplitude A to the Thomson scattering amplitude A^T. Since the Thomson amplitude is the low-energy limit of the Klein-Nishina formula, the Thomson amplitude is the correct low-energy quantum-mechanical prediction for elastic scattering by a free electron. Hence, our F function may be considered as another definition of Hartree's F funtion. In general F depends on the atom (or ion) that scatters the photon, the photon energy $\hbar\omega$ and the scattering angle θ [2]. Atomic form factors are important because of their relevance in basic atomic physics investigations [24]. The systematic use of the form-factor in calculations of Rayleigh scattering from isolated atoms has led to significant progress in understanding this process and to wide range of agreement with experiment. A description of the interaction of X-rays with condensed matter may be obtained from the atomic scattering factors. For example the atomic form-factor is used extensively for the quantitative analysis of data from X-ray scattering experiments and from X-ray fluorescence analysis. The atomic form-factor also serves as an input to theoretical predictions of various physical applications. For these applications such data are useful in power reactor shielding, industrial radiation processing, analysis of nuclear physics experiments, energy deposition and medical physics [13]. Atomic form factors provide information about the inner structure of the atoms and macromolecules [15], and are of interest in medical diagnostics and imaging [1]. They are used in studies of the local environments of atoms in molecules and in condensed matter by considering the X-ray absorption fine structure (EXAFS), X-ray fluorescence spectroscopy (XRF), electron probe microanalysis (EPMA) and proton-induced X-ray emission (PIXE). Atomic form factors are also used in investigation of composition of materials. Finally atomic form factors are used in energy dispersive X-ray diffraction (EDXRD) in order to be informed about crystal structures and changes in the composition of materials [3].

In the present study we report values of form factors for 13 elements in the region $22 \leq Z \leq 82$. These results constitute a report at 2.216 $Å^{-1}$ photon-momentum transfer. The experimental results are used to decide about the relative appropriateness of the different formalisms of the form-factor theory. Theoretical predictions of form factors are based on nonrelativistic [11], relativistic [12] and relativistic modified [21] form-factor formalisms.

EXPERIMENTAL

The geometry employed in our present work is similar to that described by previous authors [6]. 59.5 keV γ-rays emitted from a filtered low energy photon point source of ^{241}Am (100 mCi) were made to hit the target at an angle of 55° to the sample surface and the angle of the scattered γ-rays with the target was also 55°. The source was housed at the centre of a cylindrical lead shield of 1.2 cm diameter and 1.9 cm length. The radiation scattered from the target was detected through a Ge(Li) detector 8 mm in diameter and 5 mm in depth. The detector connected to a ND66 multichannel analyser was also shielded by a lead collimator. The energy resolution of the Ge(Li) detector (FWHM) was found to be 190 eV at 5.9 keV Mn Kα. This detector was coupled to a computerized 1024-multichannel analyser through a spectroscopy automatic fine-tuning research amplifier. High-purity, thin elemental foils of Al, Ti, Fe, Ni, Cu, Zn, Zr, Nb, Mo, Ag, Sn, Ta, Au and Pb (all of purity higher than 99.9%) were used as scatterers. Foils of all samples were chosen in the thickness range from 0.0074 to 0.0072 g/cm^2. Each

circular target had an area of 16 π mm^2. The pulse height spectrum of the γ-rays scattered by all foil samples was collected for 21.6 × 10^3 s live time. To obtain the net pulse height spectra of the scattered γ-rays, a background spectrum without the scatterer was stripped from the spectrum acquired for an equal period of time under experimental conditions. A representative spectrum of 59.5 keV γ-rays scattered at 55° by Sn is shown in Fig. 1.

The differential cross-section for the coherent scattering of γ-rays by a target atom is obtained using the relation [14]

$$\frac{n_c}{n} = \frac{T}{T_{Al}} \frac{N}{N_{Al}} \frac{\varepsilon}{\varepsilon_c} \left[\frac{d\sigma_{Al}}{d\Omega} \right]^{-1} \frac{d\sigma_c}{d\Omega} \qquad (1)$$

where T^{Al} and T are, respectively, the transmission factors for Al at Compton energy and for 59.5 keV energy with the target, N^{Al} and N are the numbers of scattering atoms in Al and the scatterer, ε_c and ε are, respectively, the detector photopeak efficiencies for Compton and coherent scattered γ-rays [$(\varepsilon / \varepsilon_c) \approx 1$ at 59.5 keV energy] and $d\sigma^{Al}/d\Omega$ is the Compton scattering cross section of the aluminium atom

$$\frac{d\sigma^{Al}}{d\Omega} = \frac{d\sigma^{KN}}{d\Omega} S(x, Z = 13) \qquad (2)$$

In the latter equation $d\sigma^{KN}/d\Omega$ is the Klein-Nishina cross section per electron, $S(x, Z = 13)$ is the incoherent scattering function for Al, x is the photon-momentum transfer

$$x = \frac{\sin(\theta / 2)}{\lambda} \qquad (3)$$

θ is the angle of scattering and λ is the wavelength of the incident radiation in Ångström.

The theoretical coherent scattering differential cross sections are calculated by using

$$\frac{d\sigma_{coh}}{d\Omega} = \frac{1}{2} r_e^2 (1 + \cos^2 \theta) [F(x, Z)]^2 \qquad (4)$$

where r_e is the classical electron radius, Z is the atomic number of the scattering atom and $F(x, Z)$ is the atomic form-factor. The atomic form-factor $F(x, Z)$ was then extracted from the measured cross sections using relation (4). The self-absorption in the present investigation is similar for all samples to that described in our previous work [10].

RESULTS AND DISCUSSION

The form factor values which we have determined in our present work are given in Table 1. The error in the experimental form factors is of order of 4.4%. This error originates from the various parameters in equation 1 used to evaluate the cross section. To the best of our knowledge no experimental data on atomic form factors have been reported previously in the literature for 59.5 keV at this angle. Our experimental results

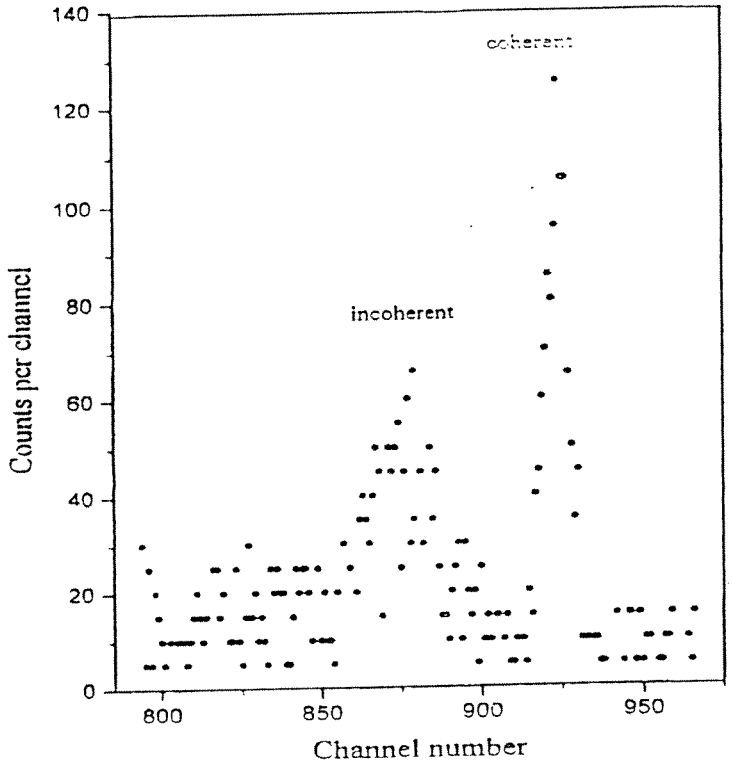


FIG. 1. Representative spectrum of 59.5 keV photons scattered at 55° by Sn.

TABLE 1

Experimental and atomic form-factors ($d\sigma/d\Omega$) (b/sr) at 2.216 $Å^{-1}$ photon momentum transfer

Element	Experimental	Theoretic		
		[11]	[12]	[21]
^{22}Ti	1.815 ± 0.172	1.911	1.941	1.914
^{26}Fe	2.547 ± 0.242	2.642	2.693	2.645
^{28}Ni	2.994 ± 0.202	3.051	3.109	3.049
^{29}Cu	3.047 ± 0.211	3.248	3.310	3.244
^{30}Zn	3.289 ± 0.224	3.452	3.516	3.444
^{40}Zr	4.756 ± 0.334	5.018	5.115	4.978
^{41}Nb	4.812 ± 0.343	5.124	5.228	5.084
^{42}Mo	5.028 ± 0.333	5.228	5.341	5.189
^{47}Ag	5.586 ± 0.377	5.793	5.969	5.907
^{50}Sn	6.194 ± 0,387	6.257	6.482	6.428
^{73}Ta	10.161 ± 0.630	11.868	12.408	11.806
^{79}Au	11.647 ± 0.752	12.928	13.584	12.853
^{82}Pb	12.168 ± 0.767	13.364	14.096	13.293

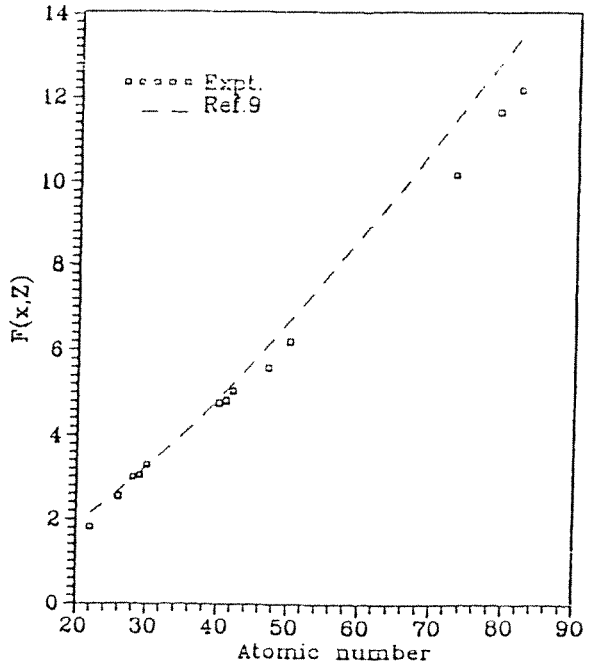


FIG. 2. Graphical comparison of the experimental results with predictions of the form-factor theory.

are also compared graphically with predictions of relativistic modified form factor [21] theories in Fig. 2.

It is clear from Table 1 that our experimental results are in good agreement with predictions of all three formalisms. It is, however, also clear from Fig. 2 that the best agreement is achieved by using RMFF [21] theory. Moreover, the agreement is better with the RMFF theory, although our experimental results also agree with the NRFF [11] theory. The sensitiveness of the RMFF theory is determined by the least squares methods. As visible in Fig. 2, the agreement of our experimental results agree with the RMFF theories is all the better as the atom number increases. The present experimental work upholds the superiority of the RMFF theory as reported by earlier authors [4, 5, 7 to 9, 14, 16, 19 to 22, 24]. As it can be seen from Table 1 and Fig. 2, theoretical form-factors are greater than experimental form-factors. These deviations are probably caused by small differences in the values of some of the parameters employed in the calculations. Similar deviations have also been observed by previous authors [8, 10, 18, 23].

When the experimental results are compared with predictions by form factors theories the deviations are larger with atoms with large atomic numbers than they are with small atomic number. These deviations may be related to the fact that the K-edges of some elements (especially 67.4 keV for Ta, 80.7 keV for Au and 83 keV for Pb) are close to the energy of coherently scattered γ-rays. Such deviations are attributed to the dispersion effects near K-edges. Earlier authors have observed such dispersion effects [8, 16, 19, 22, 24].

CONCLUSION

We have found that the modified form factor gives better results when calculated with relativistic wave functions. This is the reason why this approximation was employed in the present work and denoted as RMFF. This is another subtle correction to the nonrelativistic nature of the form-factor approximation [17]. As a result, the RMFF theory may be more appropriate in predicting the form factor in the intermediate photon momentum transfer region ($1 < x < 10$ Å^{-1}). For three elements experimental results confirm the occurrence of dispersion effects near the K-edges.

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