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Compton profile of tantalum

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Abstract. The Compton profile of tantalum (Ta) has been measured using IGP type coaxial photon detector. The target atoms were excited by means of 59.54 keV γ-rays from Am-241. The measurements were carried out on a high purity thin elemental foil. The data were recoreded in a 4 K multichannel analyzer. These data duly corrected for various effects are presented and compared with theoretical and measured values. Best agreement with experiment is found for the $5d^3 6s^2$ electron configuration.

Keywords. Compton scattering; Compton profile.

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1. Introduction

When radiation is inelastically scattered from a body of electrons the emerging beam is Doppler-broadened because of the motion of the target electrons. The momentum density of electrons in a solid has been investigated by measuring the energy spectrum of Compton scattered γ-rays at a fixed scattering angle. The energy spectrum in momentum scale-Compton profile is directly related to the momentum distribution of the electrons. The spectral analysis of the Compton scattered radiation reveals the line shape which according to impulse approximation can be reduced to the 'Compton profile'. The impulse approximation assumes that the reaction time involved in the Compton scattering is so small that the initial and final electrons see the same constant potential. In the impulse approximation, the Compton profile $J(q)$ is the projection of the target's electron momentum distribution, $n(p)$, along the scattering vector axis, i.e.,

$$J(q) = \int\int n(p) \mathrm{d}p_x \mathrm{d}p_y. \quad (1)$$

Hence, it is used as a powerful tool for the investigation of electronic structure of materials, provided the impulse approximation remains valid [1–4]. This technique is particularly sensitive to the behaviour of the slowly moving outer electrons involved in bonding in condensed matter and serves as a reliable test of the accuracy of the calculated wave functions. Such basic infomation is useful in the study of all the physical properties of a system.

In this paper we report a systematic study of the Compton profile of Ta. In §2, we briefly describe the experimental arrangement and results and discussion are given in §3.

2. Experimental details

In the present work Compton profiles of a thin elemental foil of Ta (purity more than 99.9%) were measured using an IGC 15190 HPGe photon detector supplied by M/s Princeton Gamma-Tech. Inc., NJ. It has dimensions of 5.05 cm of active diameter and 4.9 cm of active depth providing an active volume of 90 cc. Thin elemental foil of Ta having thickness of 0.2560 gm/cm^2 and dimensions 2.5$\times$2.5 cm was used as target in the present work. The target atoms were excited using 59.54 keV γ-rays from 300 mCi Am-241 source. The optimum distance between the source and the scatterer was chosen to be 25 cm and that between the scatterer and detector, 25 cm. The γ-rays scattered at a mean angle 165° were detected by the HPGe detector having a resolution of 2 keV at 1332 keV and 780 eV at 122 keV.

The geometry and shielding arrangement of the experimental set up employed for the present study is shown in figure 1. A well-collimated beam of photons from the source S was made to fall on the target scatterer T mounted on a target holder. These scattered photons were made to fall on the detector D which was shielded properly with lead and graded shielding to minimize the background radiation. The source S was kept in a lead source holder H having a cylindrical hole 1 cm in length and 0.5 cm in diameter. A collimator C made from lead in the form of a disc having cylindrical hole of diameter 1 cm was placed suitably in front of the source. The source was properly shielded with lead so that the detector sees only the scattered γ-rays from the scatterer.

The linearity of the spectrometer was studied by using standard γ-ray sources and was found that it possesses very good linearity. The stability was also tested and it was observed that the shift in the peak channel was less than a channel over a period of 3 days. The data were collected and analyzed using a PC based 4 K MCA. A separate measurement was made without the sample to obtain background contribution that was scaled to the measurement time of the foil and then subtracted point by point from the measured data.

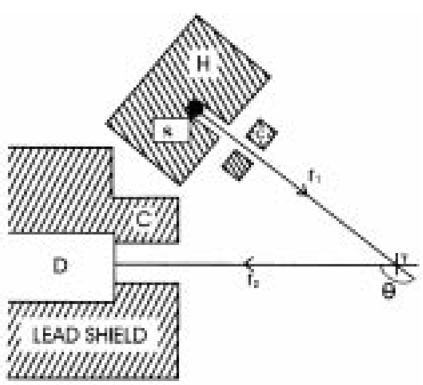

Figure 1. Schematic layout of the geometry and shielding arrangement. T - target; S - source; C - collimator; D - HPGe detector; H - Source collimator; r_1-source to target distance; r_2-target to detector distance.

The-signal-to-noise ratio was found to be 50:1. About 50,000 counts were collected at the Compton peak. The raw data were corrected for background, absorption in the sample, instrumental resolution and differential scattering cross-section [5].

In order to reduce the absorption in the scatterer very thin foil was employed as target scatterer and the criterion $\mu t < 1$ (μ is the linear attenuation coefficient and t is the target thickness) [6] was satisfied. Hence error due to bremsstrahlung and multiple scattering are expected to be negligibly small. The uncertainty in setting the target foil angle was about 2%, which contributes a negligible error in the measured Compton profile. The statistical error due to count rate were reduced and kept within 2% by counting the data for a long time. The counts under the peak were determined accurately after subtracting the background counts and applying Gaussian fitting. The error due to the uncertainty in evaluating the solid angles was less than 1%. The estimated error in the determination of photopeak efficiency of the detector using the standard weak sources was about 2%. The errors associated in evaluating the source strength was estimated to be about 3%. All the errors were compounded according to the well-known rules of propagation of errors and the resultant error was quoted on the measured Compton profiles. Finally, the experimental profile was normalized to have the area of corresponding free atom profile in the momentum range 0–7 a.u. [7].

3. Results and discussion

The Compton profile of Ta was measured with the aid of experimental set up described in §2. The present experimental results for Ta are compared in table 1 and figure 2 with the calculation based on the renormalized free atom (RFA) model of Sharma *et al* [8] and the

Table 1. The Compton profiles of Ta.

q a.u	$J_{(q)\text{Expt.}}$ Present	$J_{(q)\text{Expt.}}$ [8]	$J_{(q)\text{Theo.}}$ Band structure [9]	$J_{(q)\text{Theo.}}$ RFA $5d^4 6s^1$ [8]	$J_{(q)\text{Theo.}}$ RFA $5d^3 6s^2$ [8]
0.0	9.390±0.281	9.460±0.050	9.319	9.204	9.392
0.1	9.349±0.280	9.414	9.362	9.166	9.348
0.2	9.305±0.279	9.310	9.324	9.088	9.275
0.3	9.123±0.273	9.145	9.164	8.905	9.093
0.4	8.789±0.262	8.923	8.922	8.696	8.889
0.5	8.450±0.253	8.650	8.620	8.336	8.538
0.6	8.131±0.244	8.334	8.316	7.962	8.182
0.7	7.884±0.236	7.981	8.031	7.671	7.648
0.8	7.576±0.227	7.600	7.705	7.399	7.190
0.9	7.147±0.214	–	–	–	–
1.0	6.601±0.198	6.812	6.702	6.777	6.618
1.2	6.035±0.181	6.114	6.048	6.136	6.025
1.4	5.413±0.162	5.535	5.399	5.546	5.472
1.6	4.962±0.148	5.041	4.862	5.036	4.989
1.8	4.553±0.136	4.605	4.428	4.621	4.592
2.0	4.178±0.125	4.225	4.141	4.218	4.197
3.0	3.287±0.098	3.240	3.287	3.311	3.313
4.0	2.625±0.078	2.597	2.632	2.643	2.644
5.0	1.989±0.059	1.945	1.999	2.008	2.007
6.0	1.537±0.046	1.482	1.495	1.503	1.502
7.0	1.142±0.034	1.120	1.139	1.143	1.141

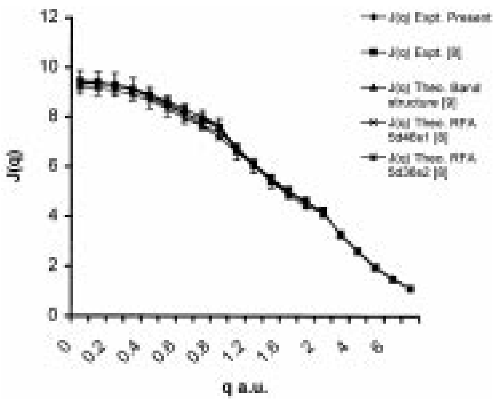

Figure 2. Comparison of the present results of Ta with experimental results [8] and with theoretical values based on RFA model [8] and band structure [9] calculations.

band structure calculation of Papanicolaou *et al* [9]. For $q = 0$ a.u., the value for $5d^4 6s^1$ configuration is lower by about 2% than the experiment. Between 0 and 1 a.u. the values of this configuration are slightly lower than the experiment, but beyond 1 a.u. the trend gets changed. It can be seen that for $q > 4$ a.u., all theoretical and experimental results are close together. It is known that the contribution of valence electrons is very small in this region and hence most of the contributions may be due to the innercore electrons. Between 0.1 and 1.2 a.u., band structure values are slightly broader than the measured profiles, but for $1.4 \leq q \leq 2$ a.u., the trend gets reversed. To obtain the most favoured configuration, the quantity Δ^2 was calculated for all cases [10].

$$\Delta^2 = \sum_{q=0}^{7.0} |\Delta J_{(q)} / \sigma_{(q)}|^2,$$

where $\sigma_{(q)}$ represents the corresponding experimental error. It was observed that the value of Δ^2 was the lowest for $5d^3 6s^2$ configuration of RFA model and thus gives the best fit to the present data for Ta. For the band structure calculation this quantity was larger. It is interesting to note that the results of the simple RFA model are in better agreement with the experiment than the result of band structure calculations. It may be worthwhile to point out that the band structure calculation of Papanicolaou *et al* did not include the spin-orbit effects in their calculations and the discrepancy could be due to this. But Sharma *et al* [8] suggested that their experimental results for Ta agree well with the band structure calculations than with the RFA model calculations.

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