

Compton Scattering from Heavier Metals*

B. K. Sharma

Department of Physics, University of Rajasthan, Jaipur, India

Z. Naturforsch. **48a**, 334–342 (1993); received December 31, 1991

The use of Compton scattering in the determination of electronic structure has grown considerably in the last two decades. With the advent of synchrotron radiation it has become possible, even with good resolution, to measure several single-crystal orientations to determine three-dimensional electron momentum distributions. Although most of the earlier work has been directed to low- Z materials, in the last few years medium and high- Z metals have also been investigated with this technique. In this paper we present a review of these studies on heavier metals with particular attention to the difficulties encountered. Compton profile measurements from techniques based on energetic ion beams are also considered briefly.

Key words: Compton profiles; Electron momentum distributions; Electronic structure; Bremsstrahlung; Ion Compton profile.

I. Introduction

The use of Compton scattering in the determination of the electronic structure of a material has grown considerably within the last two decades. The use of synchrotron radiation has made it possible to study systematically, even with good resolution, several single-crystal orientations and to determine three-dimensional electron momentum distributions. This has been due to the fact that, within the framework of the impulse approximation, the non-relativistic double-differential Compton cross-section is proportional to the Compton profile, $J(p_z)$, which is the projection of the electron momentum density along the direction of the scattering vector. Compton profiles can thus provide a useful test of ab-initio electronic structure theories [1]. Extensive experimental and theoretical work has been carried out on low- Z materials comprising simple metals, ionic crystals, semi-conductors and 3d transition metals. Excellent review papers covering these results are available [1–4]. In the last few years such investigations have been extended to heavier metals.

In this paper a review of these studies is presented. Particular attention has been paid to the difficulties encountered in the interpretation. Newer techniques to determine Compton profiles from high-energy ion collision are also briefly considered.

II. Studies of 4d and 5d Metals

Transition metals have always received considerable attention because of their interesting properties and importance from a technological point of view. In the monumental review paper of Cooper [4] the table of Compton studies of transition metals shows only Nb [5], Pd [6], Ce [7], and Lu [8] amongst the high- Z metals. Since then the situation has changed considerably. Among the 4d metals, in 1985 Tomak et al. [9] reported the Compton profile for polycrystalline Nb measured by using 59.54 keV gamma rays and interpreted their data in terms of the Renormalised Free Atom (RFA) model. Thereafter, Sharma et al. [10] published data on polycrystalline Ag and observed that the RFA model for $4d^{10}5s^1$ showed better agreement with their measurement than the orthonormalized LCAO approach.

A year later, the experimental Compton profile for valence electrons in Pd was reported by the author's group [11]. The measurements were made by scattering 59.54 keV γ -rays, and theoretical calculations were carried out using the RFA model and the APW method. A comparison of computed and measured profiles is shown in Figure 1. As seen, none of these calculations is in close agreement with the experiment. The APW values show large differences in the low-momentum region (~ 0.2 e/a.u. at $p_z=0$). Within the RFA model, best agreement was obtained when 0.3 ± 0.1 electrons were assigned to the 5s band. This value of 5s band occupancy came out to be in remarkable agreement with the conclusions of dHvA studies, but even in this case the theoretical values differed

* Presented at the Sagamore X Conference on Charge, Spin and Momentum Densities, Konstanz, Fed. Rep. of Germany, September 1–7, 1991.

Reprint requests to Prof. Dr. B. K. Sharma, Department of Physics, University of Rajasthan, Jaipur-302004, India.

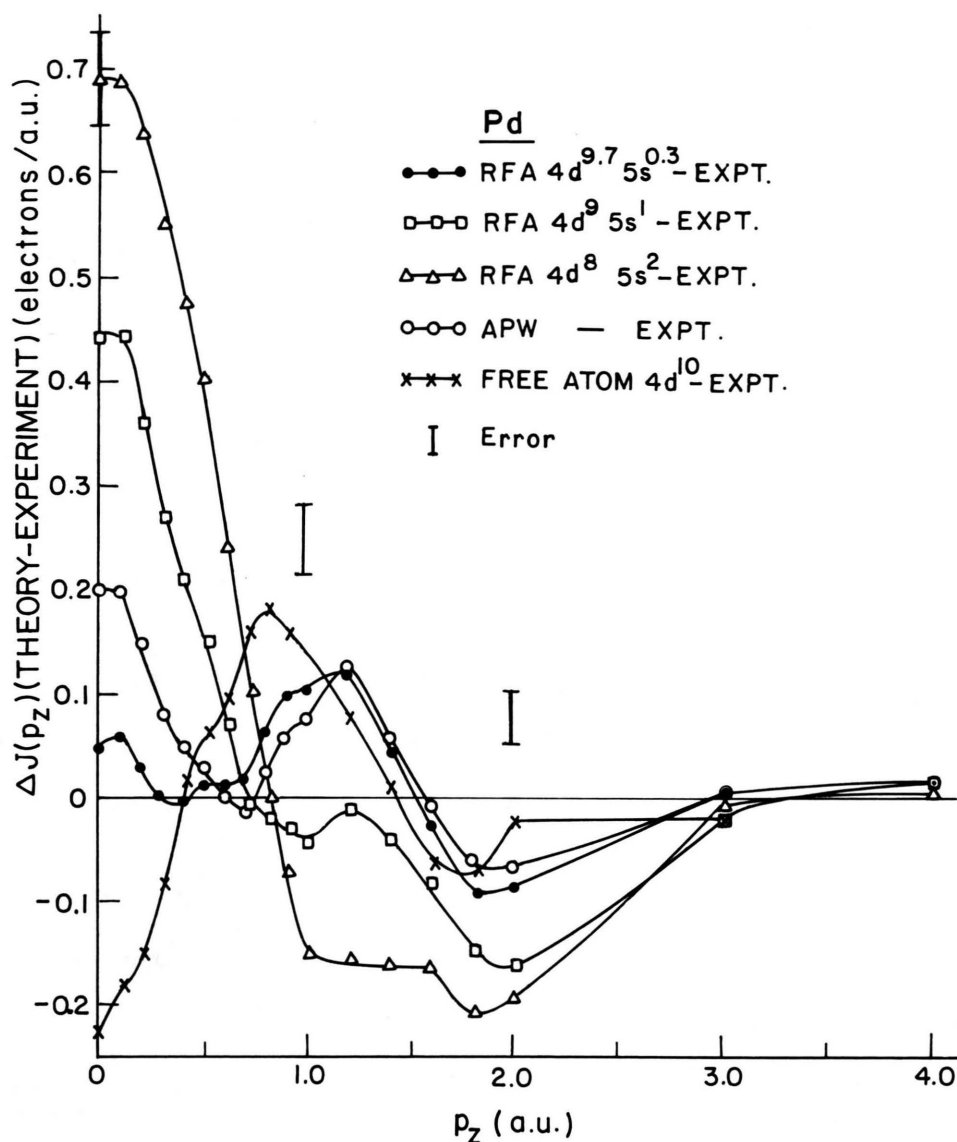


Fig. 1. Difference (ΔJ) profiles for valence electrons in polycrystalline Pd. The theory has been convoluted with the RIF (from [11]).

from the measurement particularly in the region around 1 a.u. This, perhaps, was the single case where the data were explained better by the crude RFA model than by the APW model. Gamma-ray Compton profile measurements and an RFA calculation were carried out for Rh, too [12]. When compared with two theoretical calculations based on Hubbard's exchange scheme [13] and linear combinations of Gaussian orbitals (hereafter called LCGO) [14], the data showed relatively better agreement with the

LCGO calculation. In the case of the RFA model the agreement was not good at all.

Although in all the above-mentioned cases the samples were polycrystalline sheets, perhaps it did encourage theorists to think of these metals also with respect to their Compton profiles, and soon theoretical Compton profiles for the valence electrons along the three principal directions in the cubic metals Nb [15], Mo [16], Rh [14], Pd [17], and Ag [18] were published by the group of Callaway. They employed the self-

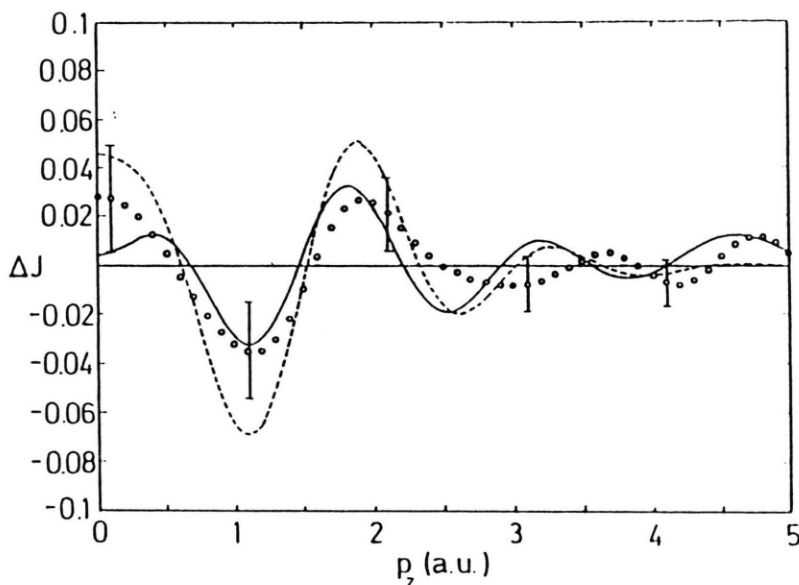


Fig. 2. Difference between the directional Compton profiles $J_{111} - J_{110}$. The experimental result is given by circles and the statistical error bars are shown at some points. The solid line corresponds to the LCGO model and the dashed lines to the APW calculation (from [24]).

consistent form of the LCAO method in which the wave function was expanded into a set of independent Gaussian orbitals; relativistic effects were, however, neglected. In another work, Papanicolaou and co-workers computed Compton profiles using the electron wavefunctions from their scalar relativistic self-consistent APW method [19–21]. In the case of Nb, there are no recent experimental results on single-crystals for comparison with the directional anisotropies. As mentioned by Jani et al. [15], their results for the anisotropy along the [100] and [110]-directions were apparently in good agreement with those of Wakoh et al. [5], but detailed comparison with individual values could not be done because no appropriate table of data was presented by those authors. With respect to the anisotropy data of Alexandropoulos and Reed [5], not corrected for instrumental resolution and only along the [100] and [110]-directions, the LCGO values were larger, but the positions of maxima and minima were found to match quite well. Noteworthy in this context is the comparison with the recent APW calculations of Papanicolaou et al. [19], where it was observed that in the two calculations the overall general features like the position of the wiggles in the anisotropy curves were almost identical, but that for small value of p_z the LCGO values were smaller than these APW results, whereas for large p_z the trend was reversed. These authors could not find any reason for this discrepancy and suggested that the difference could possibly be due to different approaches

for the generation of wavefunctions and different numbers of reciprocal lattice vectors used in the two calculations. This thus represents an example where Compton profile measurements, particularly on single crystals, would be valuable to test the two approaches. Recently, it has been suggested by Wakoh and co-workers [22] that the Lam-Platzman correction would, in general, contain both isotropic and anisotropic terms, the latter arising due to band-structure effects. It would therefore be interesting to calculate the Lam-Platzman correction in order to see how important this contribution is in this metal. None of the above papers reported on this correction. Sharma et al. [23] have made a comparison of the LCGO values with their polycrystalline data on Nb, Mo, and Rh. It was observed that the LCGO values showed consistently better overall agreement than the simple RFA model, but there remained differences, larger than the experimental errors, in the region up to 2 a.u. To our knowledge there are no measurements on single-crystals of Mo and Rh to compare with. Manninen and Paakkari [24] have measured the Compton profiles for Ag along the three principal directions using 59.54 keV gamma-rays and compared these results with the two calculations mentioned above. In Fig. 2 we reproduce some of their results. It is seen that their observed anisotropy is explained better by the LCGO calculation [18] than by the APW model [20]. The spherically averaged electron momentum distribution measured using a poly-crystalline sheet

also showed very good agreement with the LCGO model. This study has thus already provided a test for the two different schemes of calculation. On the basis of the close agreement between their isotropic results and the LCGO model these authors have suggested that for this case the Lam-Platzman correction term could be represented by an isotropic contribution and that the effect of the correction term arising from the band structure did not exceed the experimental error.

The metals with hexagonal structure have not received much attention. There are no rigorous theoretical calculations, perhaps because of the complexities introduced by the combination of uniaxial symmetry and two atoms in the unit cell. The only reported calculation is on Zr (along with ZrH_2) and assumes an f.c.c. structure [21]. Experimental data, however, have been published on polycrystalline Zr metal by Sharma and Ahuja [25]. They had also carried out a theoretical calculation using the RFA model and found that the RFA model was unable to interpret the data; however, on the basis of lowest overall deviations this model supported a $4d^3 5s^1$ configuration for the metal. This result was surprisingly in good agreement with the 4d band occupancy as estimated by Jepsen et al. [26] in their LMTO calculation. A Compton profile study of Cd has recently been published [27]. The

gamma-ray measurement on a polycrystalline sample has been compared with the calculations based on an RFA model ($4d^{10} 5s^2$) and the orthonormalised LCAO approach. The agreement was, as in the case of Zn, found to be slightly better for the RFA model.

Before we conclude the review on 4d metals, it is important to mention here two recent investigations. Manninen et al. [28] have measured the Compton profile for 1s electrons in Zr using a 59.54 keV γ -ray source and the coincidence technique. These results established that at least at moderate resolution the effects of non-validity of the impulse approximation for 1s electrons in medium-Z metals were not very significant. In another experiment using 141 keV synchrotron radiation from HASYLAB, Manninen et al. [29] studied Compton scattering from the 1s electrons of Ag and observed that, in the energy region close to the K-absorption edge, the theoretical values based on the impulse approximation were in good agreement with their data. Both these results have provided considerable consolation to the experimentalists and confidence in the use of low-energy gamma-ray sources (e.g. ^{241}Am) in such studies.

In Table 1 we present a summary of this work. The application of Compton scattering to investigate the electronic structure in heavy metals of the 5d group is relatively new. Papanicolaou et al. [30] reported the first theoretical Compton profiles for the transition metals Ta and W using electron wave functions from self-consistent APW band structure calculations. They included relativistic effects, but neglected the spin-orbit interaction. The Compton profiles of Ta showed a more pronounced structure than W, and also the anisotropies were smaller for W than for Ta, which were explained by the authors on the basis of the topology of the Fermi surfaces in these cases.

As regards experiments, Mittal et al. [31] have measured the Compton profile of polycrystalline W using 59.54 keV γ -rays and compared their data with the above calculations. They also reported Compton profiles calculated on the basis of the RFA model. The agreement was not good with either band-structure or RFA calculations. A careful analysis of the various corrections has revealed that in this work the multiple scattering correction was somewhat underestimated owing to a programming error [32]. When incorporated correctly, these data showed closer agreement with the band structure calculation than reported before, but some differences, between 1 and 2 a.u., remained. Similar measurements of Compton profiles

Table 1. Summary of recent CP studies on 4d/5d metals.

Metal	Measurement	Theory	Ref.
Zr	—	APW for f.c.c. Zr	[21]
	^{241}Am	RFA	[25]
Nb	—	LCGO	[15]
	^{241}Am	APW	[19]
		RFA	[9]
Mo	—	LCGO	[16]
	^{241}Am	—	[23]
Rh	—	Hubbard	[13]
	^{241}Am	LCGO	[14]
		RFA	[12]
Pd	—	LCGO	[17]
	^{241}Am	RFA + APW	[11]
Ag	—	LCGO	[18]
	^{241}Am	APW	[20]
	^{241}Am	RFA	[10]
	^{241}Am	—	[24] *
Cd	^{241}Am	RFA + LCAO	[27]
Ta	—	RAPW	[30]
	^{241}Am	RFA	[33]
W	—	RAPW	[30]
	^{241}Am	RFA	[31]
Pt	^{241}Am	RFA	[34]
Au	^{241}Am	RFA	[34]

* Measurement on single crystal.

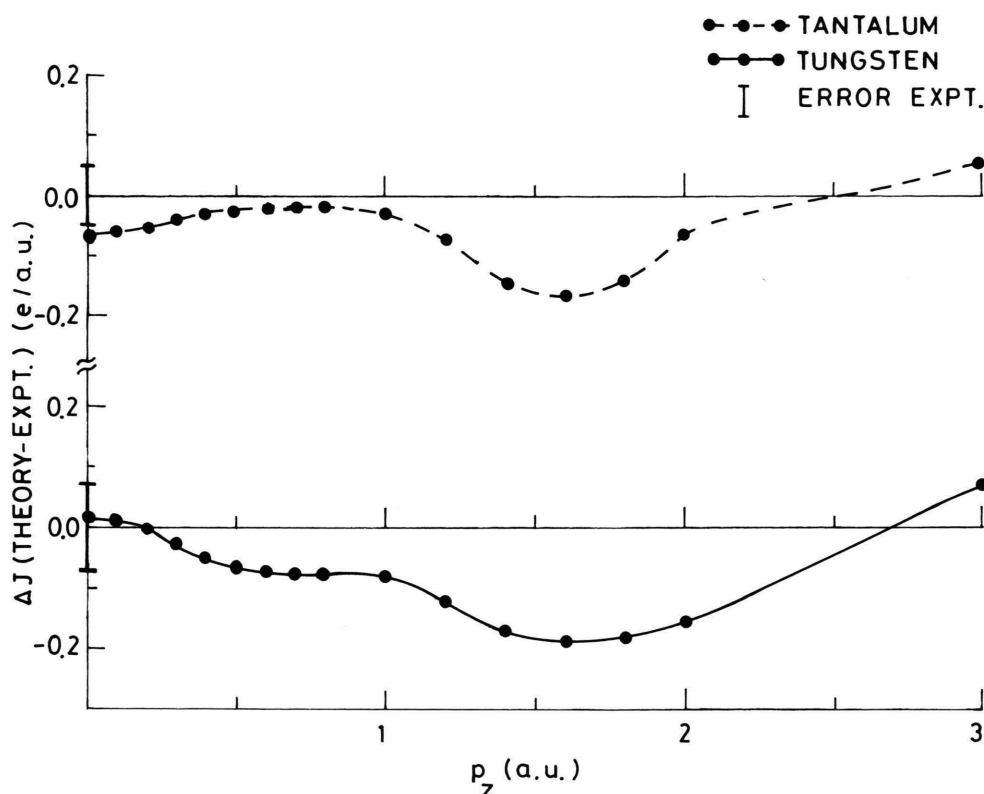


Fig. 3. The difference of the theoretical profiles [30] convoluted with the RIF of the experiment and the experimental profiles for Ta [33] and W [31].

were carried out for Ta [33], Pt, and Au [34]. For Ta, the experimental data were in good overall agreement with the above theory (spherically averaged Compton profiles); however, also here some differences, particularly between 1 to 2 a.u., were seen. In Fig. 3 we show these results for both Ta and W where, as usual, the differences ΔJ have been plotted. The theoretical values for valence electron Compton profiles have been taken from [30], and the core contribution was added properly. These values were then convoluted with the residual instrumental function (RIF). The measurement on Ta was made with the Helsinki set-up, and the numerical values can be found in [33]. The experimental data for W were obtained at Jaipur. The two difference curves look quite similar. There is an obvious bump of 1 to 2 a.u. that is beyond the experimental errors in this region. It may be worthwhile to point out that in a recent work on W, Rozing et al. [35] have observed that the spin-orbit coupling may affect the Fermi surface (and hence the electron momentum distribution). At present it is not clear whether the

discrepancy observed here is due to the neglect of spin-orbit effects or of the Lam-Platzman correction in the calculation, or whether it has arisen from some other effects. In the case of Pt and Au, comparison of the data could only be made with the RFA calculation, since no rigorous calculations of Compton profiles are reported. The agreement, though not quite satisfactory, favours a $5d^{8.4}6s^{1.6}$ and a $5d^{10}6s^1$ configuration for the two metals, respectively. As can be seen in Table 2, except for Au these results do not agree with the “5d” occupancies for Ta and Pt reported in the literature. This once again points out the fact that the simple RFA model cannot be used to interpret the Compton profiles of these medium and large- Z metals. Timms and Cooper [36] have recently reported their data on Compton profiles along the three principal directions in Pb using 412 keV and 59.54 keV γ -rays. It was observed that both measurements were in mutual agreement and showed very little anisotropy. Their spherically averaged data clearly favoured relativistic Hartree-Fock (RHF) wave functions in comparison to

Table 2. Estimates of 5d band occupancies.

Metal		Q_{6s}	Q_{6p}	Q_{5d}
Ta	Lytle [48]	—	—	4.2
	Davenport et al. [49]	0.82–0.89	0.67–0.92	3.51–3.19
	Papaconstantopoulos [50]	0.85	0.36	3.78
	Sharma et al. [33] *	2	—	3
Pt	Lytle [48]	—	—	9.2
	Davenport et al. [49]	0.82–0.89	0.67–0.92	8.51–8.41
	Papaconstantopoulos [50]	0.75	0.50	8.74
	Mittal et al. [34] *	1.6	—	8.4
Au	Lytle [48]	—	—	10
	Davenport et al. [49]	—	—	9.36
	Papaconstantopoulos [50]	0.86	0.25	9.89
	Mittal et al. [34] *	1	—	10.0

Lytle [48]: X-ray measurement. — Davenport et al. [49]: Linear augmented Slater-type-orbital method. — Papaconstantopoulos [50]: APW method. — * Compton scattering (further details are given in [33] and [34]).

HF wave functions. The above discussion, particularly on 5d transition metals, clearly suggests that there is a lack of experimental data, mainly on single-crystals, and also that there is a need for proper theoretical calculations, primarily on h.c.p. metals. For the heavy metals it will be interesting to calculate Compton profiles with and without the spin-orbit effects along the lines of Rozing et al. [35] in order to examine the effects of this correction in the electron momentum distribution.

III. Experimental Difficulties

Having presented an overview of the present status of the Compton scattering studies on heavy metals, we now turn to the difficulties encountered in these materials. The first and most serious one is the low counting rate resulting from the relatively small Compton cross-section compared to the photo-electric absorption cross-section. With increasing Z , the relative Compton intensity decreases rapidly. Moreover, since the measured Compton cross-section consists of contributions from all electrons, the solid-state effects related to the valence electrons only are relatively small. In addition to these, there are a number of other

features, discussed below, that become important, and considerable care has therefore to be taken in the data processing to obtain reliable results.

(i) *Elastic scattering*. As discussed several years ago [9], the elastic scattering cross-section increases with Z and the result is an intense elastic line. With a ^{241}Am source this becomes a problem as the low-energy tail of the detector response and the Ge K-escape peaks overlap with the Compton profile and these have to be carefully eliminated. This can be done by the procedure described in [9] and has worked reasonably, but depends on the nature of the weak source used for the purpose.

(ii) *Fluorescent X-rays*. In the case of 4d metals, the 59.54 keV radiation induces K X-rays with a considerably larger intensity than that of the Compton radiation. These would cause pile-up effects, which have to be minimised through the use of a pile-up rejector (see [24]) or even standard filters. The situation can be similar for other metals and more severe when large energy windows are used in the measurements. The problem assumes an entirely different dimension if the energy of the fluorescent radiation happens to overlap with the Compton spectrum.

(iii) *Bremsstrahlung (BS)*. As the photons interact with the material, photoelectrons and Compton electrons are produced. Both emit bremsstrahlung when they slow down in the material. The attenuation coefficient increases with Z , and so does the cross-section for bremsstrahlung. As a result, this radiation would also be measured and thus produce a sample-dependent background. If it overlaps with the region of interest, a proper correction has to be applied. This problem was realised long ago [37] and has been re-examined by Alexandropoulos et al. [38] with particular attention to the low-energy spectrum from inelastic scattering. Mittal et al. [39] have recently examined this problem in detail using different schemes of calculating the spectral distribution of BS. They have also determined theoretically the intensity of BS in the region of the Compton profile relative to the Compton intensity for a number of 4d and 5d metals for 59.54 keV γ -rays. The results are interesting. For Mo, Ta and W the BS to Compton ratios are 0.05%, 0.6% and 0.7%, respectively. Here the contributions are only due to photoelectrons. Clearly for the accurate determination of Compton profiles in 5d metals a correction for BS would be necessary. When higher energy γ -rays are used, even Compton electron contributions would have to be considered. The biggest

problem in this correction is the lack of availability of accurate photoionization and Compton cross-sections for different shells at the desired energies.

(iv) *Impulse approximation (IA)*. As pointed out earlier, the validity of the impulse approximation is the basis on which a Compton profile is deduced from the energy spectrum. In heavier metals, the IA may not remain valid for some of the inner electrons because the electron binding energies may not be much smaller than the recoil energy. For 60 keV γ -rays, the 1s electrons do not contribute to Compton scattering in most of the 4d and other heavier metals. For the 1s-electrons in Zr these effects were insignificant [28]. A method to estimate quantitatively the effect of such a correction for 1s, 2s and 2p-electrons has been suggested recently by Holm and Ribberfors [40]. According to it, the first-order correction produces a maximal error, in percent of $J(0)$, of $20\varepsilon/q$, where ε is a measure of the binding energy E_{nl} for the (nl) shell given as $\varepsilon = n(2m|E_{nl}|)^{1/2}$ and q is the momentum transfer. This correction produces an asymmetry in the profile. However, the correction term has opposite signs for 2s and 2p-shells and leads to some cancellation effects. For the case of Ag, Manninen and Paakkari [24] have estimated this error to be about 0.016 e/a.u. at $J(0)$. The above formula may perhaps be invalid for L-electrons in 5d metals, as the criterion for the above formula demands $\varepsilon/q \sim 1$, which is certainly not true for these cases. We must, however, mention that an asymmetry has been observed in the case of W and other metals that cannot be explained on the basis of an asymmetric L-shell contribution. We are studying this in order to see how much of the observed asymmetry can be accounted for by this effect.

(v) *Impurity of primary radiation*. The problem of spectral contamination in the γ -ray source is well established [41]. Inelastic scattering within the source material (self-scattering) produces an additional low-energy tail in the spectral distribution of the primary radiation. The effect of such radiation is to produce Compton spectra shifted in energy and weighted by the intensity of the low-energy tail [41]. In heavy metals this can produce additional contributions through large elastic scattering. Several authors have considered this problem, and for the case of the Au source, a confident correction is now possible [42]. A novel scheme based on an iterative method has been proposed and tested by Schütz et al. [43]. It is also designed for overcoming the problem of source scattering for Am sources. Having presented the ex-

perimental difficulties, it is somewhat fortunate that when one considers directional differences in Compton profiles, several of these problems arising due to the impulse approximation, BS etc. cancel automatically. Moreover, if the scattering geometry remains the same then even the multiple-scattering contribution cancels to a large extent. This way one hopes to obtain more reliable data. Coupled with the fact that the electron momentum density is intrinsically a directional property, it is always very important to measure it on single-crystals. It is hoped that this paper will stimulate more measurements in this direction.

IV. New Techniques

For the sake of completeness we now consider results from other techniques. In the last decade, a new method based on proton-electron scattering has been developed to determine the so-called ion-Compton profiles, which resemble in many details conventional γ -ray Compton profiles. The idea is to observe and energy-analyse the recoiling electron after an inelastic ion-electron encounter. Spies and Bell [44] have used this technique to extract valence Compton profiles of Ag and Au. Their results for Ag were found to be in agreement with our data [10]. They have considered in detail the merits and demerits of this technique vis-a-vis conventional Compton scattering and concluded that because of the absence of any competitive scattering process this technique is specially suitable for heavy elements. They have estimated that owing to the combined influence of cross-section and beam intensity one can gain a factor of 10^5 to 10^6 in the intensity, and thus this method holds enormous promises for thin samples and clusters where other methods would obviously not be applicable. Another approach has been proposed by Mowat [45] and is called the method of "kinetic tuning". It involves tuning of Radiative Electron Capture X-rays, produced in ion-atom collisions, across a sharp absorption edge. It has been shown that through an elaborate mathematical procedure, the Compton profile can be extracted from these data with a momentum resolution of 0.001 a.u. (an improvement of over two orders of magnitude over the γ -ray method). The principle of the method is well founded [46, 47], and it will be interesting to see some results based on this method. Thin and gaseous targets are the obvious areas where this technique would be most effective.

Summary

In this paper a review of Compton profiles have been reported for the metals of the 4d group and for two of the 5d group. However, except for Ag there are no measurements on single crystals. For the case of Ag, the LCGO model works better than the APW method. For other 4d metals the polycrystalline data have shown better agreement with the LCGO values than with the simple RFA model. For the h.c.p metals even theoretical calculations have not been attempted. For the two 5d metals, the RAPW calculation shows good agreement with the polycrystalline data, but there are obvious discrepancies in the region beyond 1–2 a.u. Here also the RFA model has not been able to explain the data. The effects of Lam-Platzman correlations have not been considered, and once accurate single-crystal data are available, it will be interesting

to see how significant this correction is in the heavier metals. Problems encountered particularly with the use of γ -rays from a ^{241}Am source are considered at depth. Two techniques based on ion-atom collisions are also briefly mentioned. It is hoped that this review will stimulate work in the area where there is an obvious need, namely accurate data on single crystals and theoretical calculations on h.c.p metals.

Acknowledgement

This work has been partially supported by the B.R.N.S. India. It is a matter of great pleasure to thank my collaborators at Jaipur and Helsinki for their valuable contributions. Discussions with Prof. W. Weyrich, Prof. M. Cooper, Prof. T. Paakkari, Dr. S. Manninen, and Dr. B. L. Ahuja are gratefully acknowledged.

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