Compton profile of polycrystalline tungsten

Usha Mittal, B. K. Sharma, Farid M. Mohammad, and B. L. Ahuja
Department of Physics, University of Rajasthan, Jaipur 302 004, Rajasthan, India
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In this paper we report the experimental Compton profile of polycrystalline tungsten. The measurements have been made by scattering 59.54-keV γ rays and are compared with the band-structure calculation of Papanicolaou *et al.* These results have also been compared with our calculation based on the renormalized-free-atom model with different $5d$-$6s$ configurations. Best agreement with experiment is found for the $5d^{5.4}6s^{0.6}$ electron configuration.

I. INTRODUCTION

Tungsten, which belongs to the Cr group of metals, is one of the most important transition metals. Investigations on this metal seem to have begun in the early 1960s, when a model for its Fermi surface, proposed by Lomer,[1] was compared with band-structure calculations by Loucks[2] and Mattheiss.[3] Thereafter, a considerable amount of work was done to study the Fermi surface and other properties that depend on electronic structure. An excellent review of the work done on W up to 1970 can be found in the work of Cracknell[4] and we refer the reader to this reference for more details.

Within recent years there have been major advances in the development and implementation of accurate methods for predicting the structure and ground-state properties of solids. Accordingly, a number of *ab initio* calculations for both the electronic structure and structural properties of W have been published in the literature[5–13] and, whenever possible, compared with experiment.[14,15]

Compton scattering is one of the direct ways to probe the ground-state electronic structure of a material and therefore provides a useful test of *ab initio* electronic structure theories.[16] This technique has been used extensively in the last decade to study the electron momentum distribution in $3d$ transition metals and related systems.[16] Of late, our group has extended these studies to $4d$ transition metals[17–22] and interesting results have been obtained. As for the $5d$ metals, theoretical Compton profiles have already been computed for W and Ta by Papanicolaou *et al.*[23] using the wave functions from self-consistent augmented-plane-wave (APW) method. It was therefore thought to be of interest to measure the Compton profile of W in order to provide a possible check for this theoretical calculation. Besides this, we have also computed the Compton profile using the renormalized-free-atom (RFA) model[24] which has been successful in interpreting the experimental data on polycrystalline $3d$ and $4d$ metals. We have considered several $5d$-$6s$ electron configurations to obtain, as in other cases, the most favorable configuration for this metal. In Sec. II we describe briefly the experimental procedure and in Sec. III, the method of calculation. In Sec. IV we present our results and their discussion. The conclusions are given in Sec. V.

II. EXPERIMENT

The experimental setup used in this work is the same as reported earlier by Sharma *et al.*[19] and Dasgupta *et al.*[25] The experimental method is given here briefly. 59.54-keV γ rays from a 5-Ci annular ^{241}Am source were scattered at an angle of 159° (±2.5°) by a thin sheet of polycrystalline W metal (0.0125 cm) held vertically in the vacuum chamber kept at 10^{-1} mm Hg. The source-sample and sample-detector distances were 75 and 200 mm, respectively. The scattered radiation was detected using an intrinsic planar Ge detector. The momentum resolution of the spectrometer which depends upon the beam divergence and detector properties was about 0.6 a.u. full width at half maximum (FWHM). Over 68 000 counts per channel were accumulated at the Compton peak in a period of about 150 000 sec. The stability of the system was checked twice a day with a point source during the measurement.

The background was measured by running the system without sample for 45 000 sec and it was subtracted from the data point by point after scaling it to the time of measurement for the sample. Thereafter, the profile was corrected for the effects of instrumental resolution,[26] sample absorption, and the energy dependence of the Compton scattering cross section following the usual method (see, for example, Benedek *et al.* in Ref. 16). The profile was then converted to the momentum scale to obtain $J(p_z)$. Since our sample was not very thin, the Monte Carlo procedure of Halonen *et al.*[27] which removes the contribution of elastic- and inelastic-double-scattering events was also applied. Finally, the experimental profile (high-energy side) was normalized to have the area of corresponding free-atom profile (core$+5d^4 6s^2$) in the momentum range 0–7 a.u. In our arrangement, $1s$ electrons do not contribute to the Compton scattering events because of their large binding energy[28] and therefore their contribution was excluded in determining the area. Likewise, the contribution of $L_{\rm I}$, $L_{\rm II}$, and $L_{\rm III}$ electrons was included only up to those values where the recoil energy exceeded their binding energies (Ref. 28). In particular in the high-energy side of the Compton spectrum, the recoil energy decreases from about 11 to 7 keV (0 to +7 a.u. of momentum). Therefore, in this region only the $I_{\rm III}$ electrons contribute from 0 to 1.0 a.u. However, in the low-energy side of the peak

(i.e., −7–0 a.u.) $L_{\rm I}$ and $L_{\rm II}$ electrons contribute between −7.0 and −2.0 a.u., and −7.0 and −1.0 a.u., respectively. On the other hand, the contribution of $L_{\rm III}$ electrons would be present over the entire range. This would be expected to produce asymmetry in the Compton peak. Besides this asymmetric contribution from L-shell electrons, the use of ^{241}Am radioisotope for W produces some interesting features. First of these is the intense peak around 60 keV which can be expected due to the elastically scattered photons. Then, there is a small peak on the left side of the elastic peak whose energy is 57.98 keV and in fact is the $K\alpha_2$ x rays of W produced by the high-energy radiation emitted by the ^{241}Am source (Ref. 25). The $K\alpha_1$ line, more intense than $K\alpha_2$ by a factor of 2, has an energy of 59.32 keV. It is therefore merged in the elastic peak and hence is not seen separately.

III. CALCULATIONS

As is well known,[24] the Compton profile, $J(p_z)$, measured for a polycrystal along the p_z direction is related to the electron momentum density $\rho(\mathbf{p})$ through the equation

$$J(p_z)=2\pi\int_{p_z}\langle\rho(\mathbf{p})\rangle p\,dp\ , \tag{1}$$

where the integration is made over a constant-p_z plane.

Thus, in order to calculate $J(p_z)$ one must know $\langle\rho(\mathbf{p})\rangle$. For inner-core electrons it is sufficient to use free-atom wave functions to obtain $\rho(\mathbf{p})$ and their values for W are available in the literature.[29] However, for band electrons the use of free-atom values is not proper and for them the wave functions based on APW or other methods are required.[16] As mentioned earlier, Compton profiles for band electrons of W have been calculated by Papanicolaou *et al.*[23] along the three principal directions from their self-consistent APW wave functions. We used their values and determined their spherical average using the standard formula.[30] This was checked for proper normalization and taken as the valence-electron contribution. To obtain the total Compton profile, the contribution of inner electrons was then suitably added to it. For them, the free-atom values from Ref. 29 were used as discussed below.

An alternative method for computing spherically averaged Compton profiles from transition metals is due to Berggren.[24] It is based on the simple RFA model. In this approach the Compton profile, $J_{6s}(p_z)$, due to the 6s electrons of W was computed using the relation

$$J_{6s}(p_z)=4\pi\sum_{n=0}^{\infty}|\psi_0^c(\mathbf{K}_n)|^2G_n(p_z)\ , \tag{2}$$

where $\psi_0^c(\mathbf{K}_n)$ is the Fourier transform of the RFA wave function and the auxiliary function $G_n(p_z)$ involves the reciprocal-lattice vector $\mathbf{K}_n$, Fermi momentum p_F, and the number of points in the nth shell in reciprocal space as given in Ref. 24.

The free-atom Hartree-Fock wave functions needed for this calculation were taken from the tables of Herman and Skillman.[31] The lattice parameter for bcc tungsten was taken as 5.9715 a.u.,[15] which gave a value of 2.94 a.u. for the Wigner-Seitz radius. It turned out that only 38% of the 6s wave function was contained in the Wigner-Seitz sphere whereas this number for 5d electrons was about 90%. Therefore, only 6s electrons were considered in the RFA scheme. The effect of renormalization of the 6s wave function is shown in Fig. 1. $J_{6s}(p_z)$ was calculated using the 15 shortest K_n values in Eq. (2) for several 5d-6s configurations. The values of p_F and normalization of the 6s contribution were based on the number of 6s electrons. For 5d electrons the values were taken directly from the tables of Biggs *et al.*[29] The core contribution was added to them. In determining the core contribution, we did not include K-, $L_{\rm I}$-, and $L_{\rm II}$-shell electrons because, as discussed earlier, they do not contribute to the profile in the range of 0–7 a.u. Also, the contribution of $L_{\rm III}$ electrons was taken only up to 1.0 a.u., because above this value the recoil energy became less than the binding energy. The total theoretical profiles obtained after adding the contribution of core and valence electrons were normalized to an area of 25.89 electrons being equal to that of the corresponding free-atom profile area in this momentum range with a $5d^46s^2$ configuration.

IV. RESULTS AND DISCUSSION

Figure 2 shows the raw data for W metal accumulated in about 1.5×10^5 sec. The broad peak (around channel 792) is due to Compton-scattered γ rays. The sharp peak on the right is due to the elastically scattered radiations and also contains $K\alpha_1$ x rays of W. The peak just on the

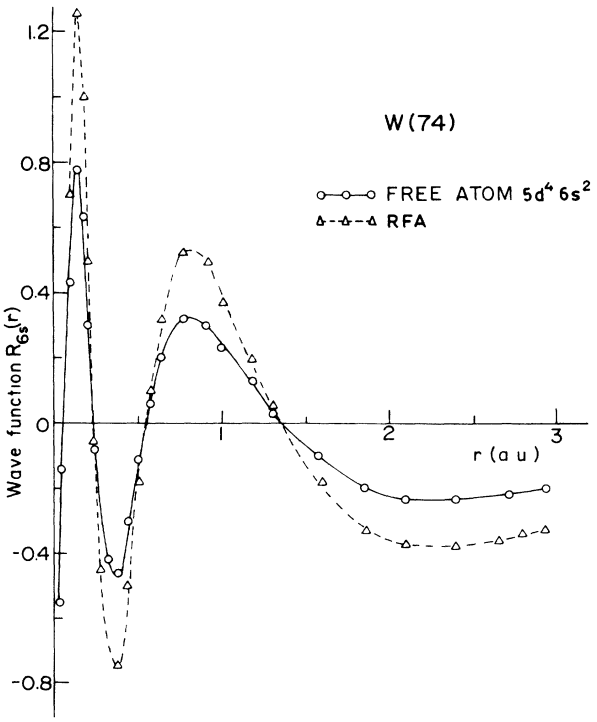

FIG. 1. Free-atom and RFA wave functions for 6s electrons in W.

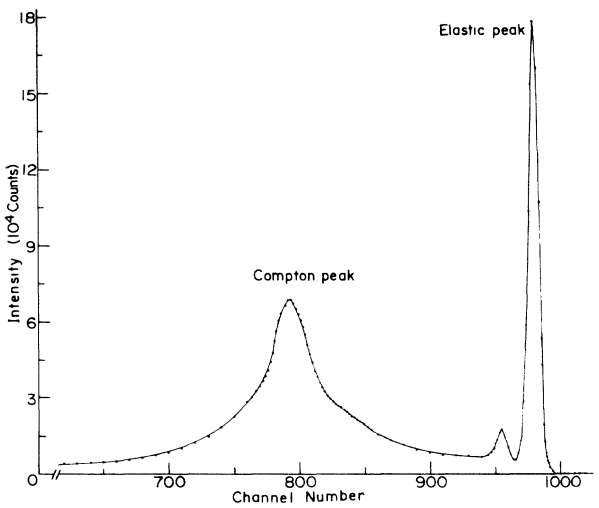

FIG. 2. Energy distribution of 59.54-keV photons scattered at 159° (±2.5°) from polycrystalline W. Each channel corresponds to about 63 eV.

left is due to $K\alpha_2$ x rays. A close look on the Compton peak clearly reveals its asymmetry. This point was mentioned briefly above and will be considered below. We first consider, as usual, the high-energy side of the Compton profile. The experimental data after applying the various corrections (as given in Sec. II) are presented in Table I along with errors for some points. Also included in this table are theoretical results from band-structure (BS) calculations of Ref. 23 and our RFA calculation for five different configurations, namely $5d^{4.8}6s^{1.2}$, $5d^{6}6s^{1}$, $5d^{5.2}6s^{0.8}$, $5d^{5.4}6s^{0.6}$, and $5d^{5.6}6s^{0.4}$. The free-atom values for the $5d^{5}6s^{1}$ configuration are also given for comparison (column 11).

First we compare the experimental data given in columns 9 and 10. It is seen that the correction due to double scattering is not negligible and increases the $J(0)$ value by 1.2% despite the fact that the sample was only 0.0125 cm thick. Next we consider the comparison of the theoretical results (columns 2–7) with experiment (column 10). The values given in columns 2–7 were first convoluted with the residual instrumental function (RIF) (column 8) in order to facilitate a proper comparison with our deconvoluted data. This is essential because no deconvolution scheme can remove the instrumental broadening effects completely due to statistical noise ever-present in the experiment.[16,26] It turned out that this convolution with the RIF modified the values only in the low-momentum region and particularly around and up to the Fermi momentum (P_F). The high-momentum values remained almost unchanged. We can, therefore, consider the values of Table I for comparison in this region. It is to be noted that for $p_z > 3$ a.u. the theoretical values from the BS, RFA, and free-atom calculations are nearly equal. This is understandable because the core contribution is the same in all cases. What is most interesting is the fact that they are very close to the experiment. It is known that the contribution of valence electrons is very small in this region and, hence, it is to be expected that most of the contribution would be due to the inner-core electrons. These inner electrons are reasonably described by the free-atom values of Biggs *et al.*[29] This good agreement also provides confidence to our

TABLE I. Theoretical (unconvoluted) and experimental Compton profiles of polycrystalline W. All quantities are in atomic units. The values have been normalized to 25.89 electrons being the area between 0 and +7 a.u. DS means double scattering. The residual instrumental function (RIF) is also given at some points.

		Core	Core	Core	Core	Core		Experiment		Free atom
	Band	+RFA	+RFA	+RFA	+RFA	+RFA	RIF of	Before	After	core+
p_z	struct.	$5d^{4.8}6s^{1.2}$	$5d^{5.0}6s^{1.0}$	$5d^{5.2}6s^{0.8}$	$5d^{5.4}6s^{0.6}$	$5d^{5.6}6s^{0.4}$	expt.	DS	DS	$5d^{5}6s^{1}$
0.0	9.475	9.214	9.166	9.114	9.051	8.975	0.2009	8.898	9.004±0.068	9.861
0.1	9.406	9.180	9.133	9.080	9.017	8.941	0.1861	8.876	8.982	9.703
0.2	9.292	9.111	9.063	9.010	8.942	8.871	0.1468	8.808	8.913	9.319
0.3	9.136	8.950	8.903	8.850	8.787	8.710	0.0931	8.695	8.796	8.883
0.4	8.904	8.778	8.730	8.676	8.613	8.536	0.0398	8.538	8.635	8.513
0.5	8.649	8.457	8.408	8.353	8.288	8.279	−0.0035	8.338	8.431	8.207
0.6	8.417	8.138	8.087	8.029	8.064	8.111	−0.0278	8.098	8.185	7.961
0.7	8.091	7.713	7.756	7.801	7.845	7.889	−0.0327	7.822	7.903	7.716
0.8	7.775	7.472	7.511	7.552	7.592	7.632	−0.0260	7.516	7.587	7.462
1.0	7.045	6.891	6.922	6.954	6.986	7.016	0.0038	6.844	6.895±0.059	6.875
1.2	6.098	6.186	6.209	6.234	6.258	6.280	0.0119	6.153	6.189	6.167
1.4	5.483	5.588	5.604	5.622	5.639	5.655	0.0029	5.521	5.540	5.567
1.6	4.858	5.058	5.069	5.081	5.093	5.104	−0.0045	5.002	5.010	5.039
1.8	4.438	4.608	4.615	4.624	4.632	4.641	−0.0029	4.607	4.609	4.595
2.0	4.146	4.254	4.259	4.265	4.272	4.279	0.0011	4.304	4.301±0.047	4.246
3.0	3.258	3.296	3.295	3.295	3.295	3.295		3.270	3.249	3.288
4.0	2.640	2.660	2.660	2.659	2.659	2.659		2.671	2.649	2.656
5.0	2.034	2.049	2.050	2.050	2.050	2.051		2.100	2.076±0.030	2.049
6.0	1.533	1.544	1.545	1.545	1.546	1.540		1.618	1.595	1.544
7.0	1.172	1.179	1.179	1.180	1.180	1.180		1.260	1.235	1.179

measurement and data analysis. It also suggests that impulse approximation (IA) can be considered valid for all the electrons that are contributing in the scattering. We examine this in terms of the binding-energy criterion. As pointed out earlier, in these data the electrons from K, $L_{\rm I}$, and $L_{\rm II}$ shells do not contribute to single Compton scattering. They can contribute via double elastic scattering for which a suitable correction has been included through a multiple-scattering-correction program. As for the $L_{\rm III}$ electrons, they contribute only up to 1.0 a.u. Thus, beyond 1.0 a.u. the condition of the IA is satisfied by all electrons because their binding energies are much smaller than the recoil energy.

In order to study the behavior of valence electrons, we consider the values between 0 and 3 a.u. It is seen that near $p_z=0$, BS values are higher than the experiment but between 1.2 and 3 a.u., the trend is reversed. As for the RFA values, for low-momentum values $J(p_z)$ decreases as the number of $6s$ electrons decreases but beyond 0.7 a.u., the trend gets reversed. This is so because the contribution of $6s$ electrons is parabolalike and the contribution of $5d$ electrons is very flat. For $p_z=2.0$ a.u. the various values are nearly equal. In order to examine this comparison more clearly, we plot in Fig. 3 the difference profiles (ΔJ), i.e., the difference between theory and experiment for different calculations. Here, the theoretical values have been convoluted with the RIF of our spectrometer. It can be seen that the BS values show significant deviation. For the RFA model, the configuration $5d^{5.4}6s^{0.6}$ shows the best overall agreement. The values of ΔJ for the $5d^{5.6}6s^{0.4}$ configuration are all negative up to 0.8 a.u. and then become positive and remain higher than for all other cases. Similarly, in the region 0–0.4 a.u. the $5d^{5}6s^{1}$ configuration has a large positive value of ΔJ while the $5d^{5.2}6s^{0.8}$ configuration has approximately equal positive and negative values of ΔJ up to 2 a.u. Between 2 and 3 a.u. the overall trend of difference profiles is identical in all cases. The difference decreases as the number of $5d$ electrons decreases. But the BS values show a rather different behavior.

To determine the most favorable configuration we have calculated a quantity Δ^2 given as $\sum_{p_z=0}^{7}|\Delta J(p_z)|^2$, which is a measure of overall deviation. It was found that this quantity was lowest for the $5d^{5.4}6s^{0.6}$ configuration and nearly the same for the $5d^{5.2}6s^{0.8}$ configuration. For the other three RFA configurations, $5d^{5.6}6s^{0.4}$, $5d^{5}6s^{1}$, and $5d^{4.8}6s^{1.2}$, the values of Δ^2 were somewhat higher. For the BS calculation the value of Δ^2 was obviously much larger. With this analysis and also the nature of the ΔJ curve shown in Fig. 3, we conclude that the present data show clear disagreement with the BS calculation up to ~ 2 a.u. As for the RFA model, the agreement, though not very satisfactory, is clearly better. This analysis suggests that the most favorable configuration for bcc tungsten can be taken as $5d^{5.4}6s^{0.6}$. This may seem surprising because the simple RFA calculations yielded results which are in much better agreement with the experiment than the BS calculations. Interestingly, in a similar study on Mo (another member of this group), the favored configuration was found as $d^{5.4}s^{0.6}$, in agreement with the present conclusion.[22]

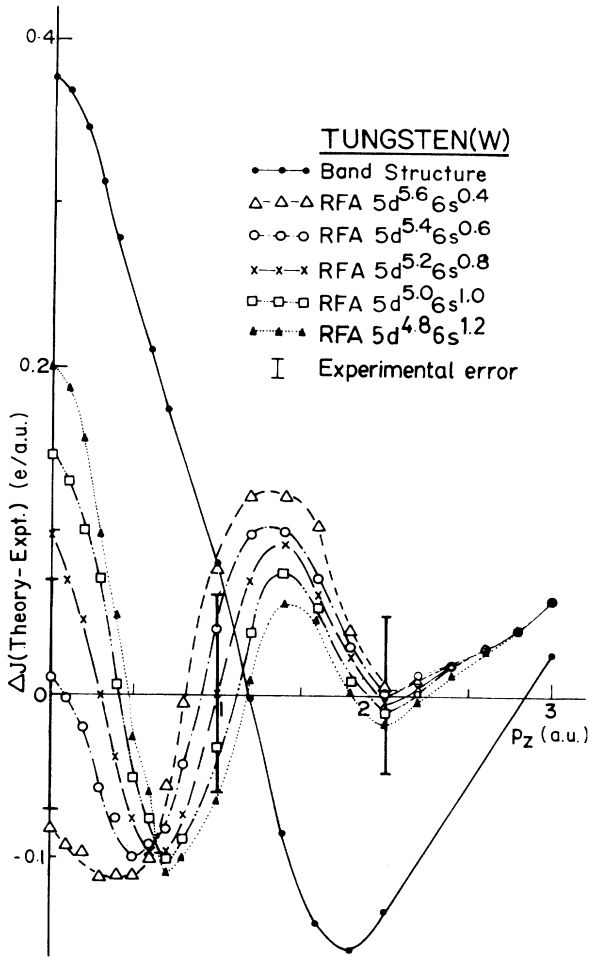

FIG. 3. Difference of the theoretical and experimental Compton profiles (ΔJ) for polycrystalline W. Theory has been convoluted with the RIF as discussed.

It may be worth pointing out that Papanicolaou *et al.*[23] did not include the spin-orbit effects in their calculations. It is therefore likely that this large discrepancy could be due to this. For the RFA model it is encouraging, but the agreement is not as good as has been seen for $3d$ and $4d$ metals. It may be mentioned that we had also computed the Compton profile for the d^4s^2 configuration in the RFA model but the disagreement was very large and hence the values have not been presented. This is quite interesting because in a study of cohesive and structural properties, Chan *et al.*[32] have suggested d^5s^1 to be the ground-state atomic configuration for both Mo and W. However, our conclusion that the $5d^{5.4}6s^{0.6}$ configuration is most favorable is in disagreement with the work of Bylander and Kleinman[9] who reported 4.8, 0.25, and 0.84 electrons in the $5d$, $6s$, and $6p$ bands, respectively. We cannot explain the cause for this discrepancy but perhaps it could be due to $6p$ occupancy neglected in our work.

A few years ago, Heller and Moreira[33] measured the Compton profile of W with 662-keV γ rays. They observed that the measured FWHM agreed within errors with that calculated using the free-atom wave functions

of Biggs *et al.*[29] In order to check this we computed the Compton profile from these free-atom values choosing the $5d^5 6s^1$ configuration.[32] This is given in the last column in Table I. The differences in the low-momentum region are quite obvious. It is worth mentioning here that the errors in the work of Heller and Moreira[33] were rather large. Also, the FWHM parameter that they have considered is not a parameter physically related to the valence-electron distribution directly. In fact, the contribution of valence electrons might hardly be significant in FWHM of this magnitude. This possibly was the reason for their observed agreement on the basis of free-atom wave function. It was not their intention to study precisely the line shape and thus those measurements cannot be compared with ours.

Now we consider the asymmetry of the Compton peak shown in Fig. 2. These data after all corrections were applied as per Sec. II exhibited clear asymmetry. To examine this, in Fig. 4 we plot the difference between the Compton profiles corresponding to the left-hand (-7–0 a.u.) and right-hand (0–7 a.u.) sides of the Compton profile.

It is seen that the asymmetry observed experimentally is negligible up to 0.8 a.u. but rises to a maximum (~ 0.3 e/a.u.) and then decreases for higher values of p_z. Some asymmetry is to be expected because the contribution from L-shell electrons is not symmetric for the reasons explained earlier. The L_{III} electrons contribute from -7 to $+1$ a.u. while the L_I and L_{II} shells contribute from -7 to -1.86 and -1.0 a.u., respectively. As is known, for these electrons the free-atom model provides a reasonable description. In order to understand the cause of asymmetry we calculated the contribution due to L-shell electrons using the values from Ref. 29. They are also plotted in Fig. 4. It is seen that the agreement between the two curves is quite good up to 0.8 a.u. This is essentially due to the fact that in this region only the L_{III} contribution exists which is present on both the sides and thus cancels in the difference. It is interesting to note that between 0.8 and 2.4 a.u., the free-atom curve is somewhat higher than the experimental curve. The theoretical curve shows discontinuities at places (shown by arrows pointing downwards) where L_{II} and L_I shells start contributing in the Compton scattering. These sharp edges will be smoothed out in the measurement because of the instrumental smearing. There, however, remains an obvious difference between theory and experiment between 1 and 3 a.u. One of the possible causes could be the Compton scattering of K-fluorescent x rays of W in backward directions. Their energies for 180° were calculated and are shown by the dotted arrows (pointing upwards) for $K\alpha_1$ and $K\alpha_2$ lines. There is, however, no indication in the data and hence this can be ruled out. The most probable causes could be (i) the nonvalidity of the impulse approximation for L-shell electrons, (ii) the effect of multiple scattering, and (iii) the residual effects of the tail in the detector response. However, the behavior of the asymmetry curve in the low-momentum regime suggests that at least for L_{III}-shell electrons these effects are not very significant. In our analysis based on the right-hand side of the Compton profile, only L_{III} contribution is present and thus this part of the data can be considered reliable. It would be most interesting to include the occupation of the 6p band as suggested by Bylander and Kleinman's work (Ref. 9). It has, however, been neglected in our simple calculation; qualitatively it would flatten the low-momentum region of the Compton profile. This can be expected to lead to some improvement in the agreement in this region. However, to our knowledge, no such calculation has so far been performed.

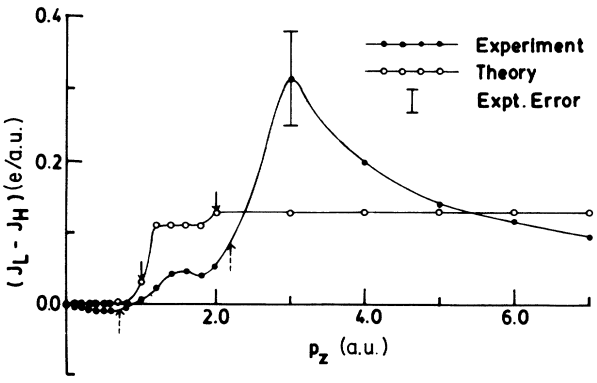

FIG. 4. Plot of the asymmetry in experimental Compton profile of W. Open circles represent the contribution due to L-shell electrons. (See text for details.)

Finally, we discuss the estimation of cohesive energy which has been calculated by other workers also (Refs. 8 and 9). It has already been discussed that the calculation of cohesive energy from the experimental Compton profile is a very difficult task because the p^2 weighting of the high-momentum tails magnifies the systematic errors alarmingly.[34] We, however, calculated cohesive energy for W using theoretical Compton profiles for the $5d^5 6s^1$ configuration using the formula of Ref. 34 given as

$$E_{\text{coh}} = \int_0^{p_{\max}} p^2 [J_s(p) - J_{\text{fa}}(p)] dp \ .$$

where the subscripts s and fa refer to solid and free-atom profiles, respectively. The values for $J_s(p)$ were taken from the present RFA calculation and those for J_{fa} were computed using the data of Biggs *et al.* (last column of Table I). The purpose of this calculation was to see the contribution of the 6s electrons because the contributions of the 5d as well as other electrons were the same in the two calculations and, hence, got canceled in the difference seen above. The value so obtained was 7.382 eV, which compares reasonably with the calculation of Zunger and Cohen[8] but is lower than other values including the experiment.

Subsequently, we used this method to compute the cohesive energy for other configurations investigated here. The results are summarized in Table II. Here $p_{\max}$ was taken as 7 a.u. because the contribution of the 5d electrons became nearly zero after this. Our results for the $5d^{5.4}6s^{0.6}$ configuration which showed the best agreement for the Compton profile came out to be 9.22 eV which is very close to the other values. It, however, shows an increasing trend as the 6s contribution de-

TABLE II. Comparison of cohesive energy (E_{coh}) in eV for W.

This work (configuration)	ZC[a]	BK[b]	Expt.[c]
	7.90	8.93	8.90
7.382 ($5d^{5.0}6s^{1.0}$)			
7.166 ($5d^{5.2}6s^{0.8}$)			
9.220 ($5d^{5.4}6s^{0.6}$)			
11.366 ($5d^{5.6}6s^{0.4}$)			

[a]Reference 8.
[b]Reference 9.
[c]Reference 56 in Zunger and Cohen (Ref. 8).

creases because of the flatter contribution of the 5*d* electrons, which is weighted heavily due to p^2 factor. This, however, is not reasonable because for these configurations the theoretical Compton profiles show a significant difference from the experimental Compton profile and, hence, they cannot be given more weight. This discrepancy could be possibly resolved by considering a realistic computation of cohesive energy for 5*d* electrons along the line suggested by Gelatt *et al.*[35] This simple calculation suggests that as was seen for 3*d* and 4*d* metals (Ref. 35), the RFA model might predict reasonably well the cohesive energies for 5*d* metals also. Such a calculation has not been reported to our knowledge. However, as suggested by Zunger and Cohen,[8] the calculation of cohesive energy involves the uncertainties associated with the atomic energy, and therefore the disagreement between the computed and experimental cohesive energies should not be taken strictly as characteristic of the accuracy of the other bulk properties.

V. CONCLUSION

In this work we have reported accurate experimental data for the Compton profile of polycrystalline W. Despite some difficulties the use of 60-keV γ rays has shown some encouraging results. The data show disagreement with the band-structure calculation but the simple RFA model gives fairly good description. It is concluded that the favorable structure for W must be close to $5d^{5.4}6s^{0.6}$. The calculated cohesive energy compares well with the other investigations. Improvement in the calculations and more measurements particularly with high-energy γ rays would be of tremendous value in this context.

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