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Abstract. Using wavefunctions from energy band calculations the Compton profiles of the electron momentum distribution in scandium metal have been calculated along the crystallographic directions (100), (110) and (111). The results show a considerable amount of anisotropy in the Compton profiles.

1. Introduction

Measurements of the Compton profiles of the electron momentum distribution in scandium metal are available from techniques using both x-rays (Manninen 1971, Weiss 1972) and γ-rays (Paakkari *et al* 1976). These profiles are, however, isotropic in nature and, as such, fail to show the dependence of the shape of the profiles on crystallographic directions. On the theoretical side, attempts have been made to interpret these data on the basis of a free-atom model as well as the renormalized-free-atom (RFA) model (Paakkari *et al* 1976). While the latter model may be a better approximation than the free-atom model, it cannot describe satisfactorily the elecron states, and particularly the band states in a solid. To our knowledge, calculations of the Compton profiles for scandium metal using band wavefunctions and for different crystallographic directions are not available. To bridge this gap we have made an attempt to determine the shape dependence of the Compton profiles on crystallographic directions. For this purpose, energy eigenfunctions of scandium metal have been calculated using a non-local model potential. The paper is organized as follows. In section 2, we briefly describe the procedure for the calculation of the Compton profiles. Section 3 summarizes the results of the present calculation. Conclusions are given in section 4.

2. Procedure

In the impulse approximation (Platzman and Tzoar 1965) the cross section for the scattering of a photon by an electron in a fixed direction k is given (Rath *et al* 1973) by

$$J_{\hat{k}}(q) = \frac{\Omega}{(2\pi)^3} \int d^3 p\, \rho(p)\delta(q - p \cdot \hat{k}) \tag{1}$$

where Ω is the volume of the unit cell, p is the initial momentum of an electron and ρ is the momentum distribution function.

In the present work, each of the 1s–3p core electrons in scandium metal is represented by a single tight-binding function

$$\phi_i(g, r) = \frac{1}{\sqrt{2N}} \sum_\mu \exp(ig \cdot R_\mu)\, U_i(r - R_\mu) \tag{2}$$
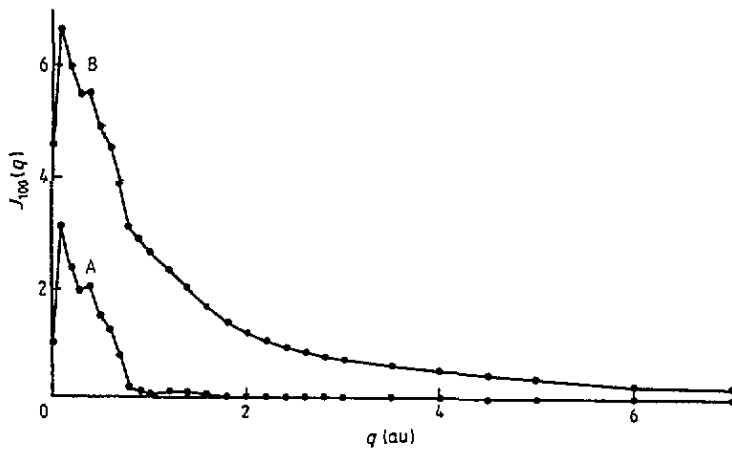
Figure 1. $J_{\hat{k}}(q)$ for scandium with $\hat{k}$ along the (100) direction: curve A, band contribution; curve B, total contribution (core + band).

where N is the number of unit cells, g is a wavevector in the Brillouin zone (BZ), R_μ is the lattice vector in the direct lattice and U_i is the ith atomic core function. The conduction electron states, on the other hand, are constructed by orthogonalizing the model wavefunction, determined in the model potential calculation, to the core states. The model wavefunctions expanded in the plane-wave basis set are determined in the standard band calculation procedure (Mahapatra *et al* 1977) employing a model potential or pseudo-potentials. Thus a band state in this procedure is expressed as

$$\Psi_t(g, r) = \sum_K C_t(g + K)\left(PW(g + K, r) - \sum_i \langle \phi_i(g)|PW(g + K)\rangle \phi_i(g, r)\right) \qquad (3)$$

where t denotes the band index, the C_t are the coefficients determined in the variational procedure and PW is the plane wave given by

$$PW(k, r) = (1/\sqrt{N\Omega})\exp(ik \cdot r). \qquad (4)$$

The momentum distribution function is given by

$$\rho(p) = \sum_{t,g}|\Psi_t(g, p)|^2 + \sum_{i,g}|\phi_i(g, p)|^2 \qquad (5)$$

where

$$\Psi_t(g, p) = \frac{1}{\sqrt{N\Omega}}\int \exp(-ip \cdot r)\,\Psi_t(g, r)\,d^3r. \qquad (6)$$

A similar integral holds for $\phi_i(g, p)$. The summation in equation (5) is taken over all the occupied band states (first term) and the core states (second term). Using $\rho(p)$ for the core state in equation (1) it can be easily shown (Berggren 1972) that the contribution per atom from core electron is given by

$$J_{\hat{k}}(q) = \frac{2}{\pi}\sum_{nl}(2l + 1)\int_q^\infty I_{nl}^2(p)p\,dp \qquad (7)$$

where n, l are the quantum numbers of the core states and I_{nl} is the integral given by

$$I_{nl}(p) = \int_0^\infty j_l(pr)P_{nl}(r)r\,dr \qquad (8)$$

involving the radial part of the atomic core function P_{nl} and the spherical Bessel function j_l of order l.
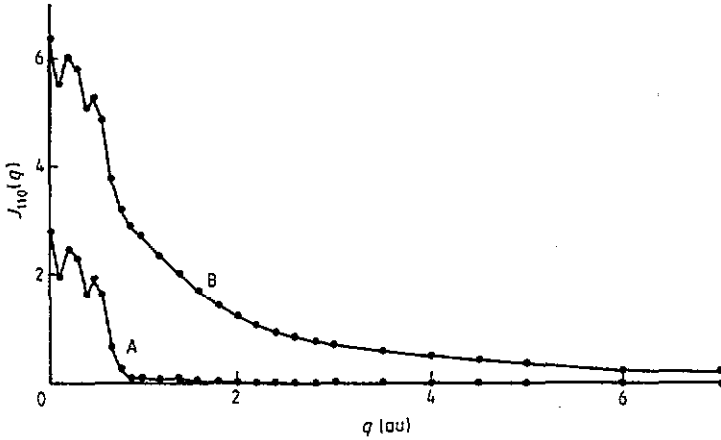
Figure 2. $J_{\hat{k}}(q)$ for scandium with $\hat{k}$ along the (110) direction: curve A, band contribution; curve B, total contribution (core + band).

Table 1. Present results of the Compton profiles $J_{\hat{k}}(q)$ of scandium along the (100) direction.

q (au)	Core contribution (au)	Band electrons (au)	Total (au)
0.0	3.590	0.999	4.589
0.1	3.584	3.094	6.678
0.2	3.562	2.410	5.972
0.3	3.518	1.974	5.492
0.4	3.450	2.055	5.505
0.5	3.359	1.515	4.874
0.6	3.245	1.263	4.508
0.7	3.111	0.776	3.887
0.8	2.959	0.152	3.111
0.9	2.795	0.092	2.887
1.0	2.623	0.056	2.679
1.2	2.270	0.100	2.370
1.4	1.936	0.091	2.027
1.6	1.643	0.049	1.692
1.8	1.397	0.009	1.406
2.0	1.200	0.008	1.208
2.2	1.046	0.011	1.057
2.4	0.924	0.010	0.934
2.6	0.834	0.008	0.842
2.8	0.756	0.001	0.757
3.0	0.698	0.000	0.698
3.5	0.583	0.001	0.584
4.0	0.497	0.000	0.497
4.5	0.421	0.000	0.421
5.0	0.355	0.000	0.355
6.0	0.229	0.000	0.229
7.0	0.206	0.000	0.206

In order to obtain the band contribution to $J_{\hat{k}}(q)$, the band part of $\rho(p)$ from the equation (5) is used in equation (1) and the summation with respect to g-vectors over the BZ is replaced by a combination of the weighted sum over a number of sample g-vectors chosen in the irreducible part and a symmetry sum over the point group of the crystalline lattice. In this respect the procedure is similar to that of Rath *et al* (1973). Replacing the Dirac δ-function in equation (1) by the derivative of the step function θ, the contribution to

$J_{\hat{k}}(q)$ (per atom) from the band states can be expressed as

$$J_{\hat{k}}(q) = \mathrm{d}F_{\hat{k}}(q)/\mathrm{d}q \tag{9}$$

where

$$\begin{aligned}
F_{\hat{k}}(q) = \sum_{g_{\text{irred}}} w_g \sum_{K} \Bigg(&\left(\sum_{\alpha} \theta[q - (g + K) \cdot \alpha\hat{k}] \right) \left(\sum_t |C_t(g + K)|^2 \right) \\
&- \frac{16\pi}{\Omega} S(K) \sum_t C_t^*(g + K) \sum_{K'} C_t(g + K') \sum_{nl} (2l + 1) \\
&\times I_{nl}(|g + K|) I_{nl}(|g + K'|) P_l(\cos\beta_{KK'}) \Bigg) \\
&+ \left(\frac{8\pi}{\Omega} \right)^2 \sum_{g_{\text{irred}}} \sum_{K_s} S^2(K_s) \sum_{\alpha} \theta[q - (g + K_s) \cdot \alpha\hat{k}] \\
&\times \sum_t \Bigg(\sum_{K} C_t^*(g + K_s) S(K) \\
&\times \sum_{nl} (2l + 1) I_{nl}(|g + K|) I_{nl}(|g + K_s|) P_l(\cos\beta_{KK_s}) \Bigg)^2
\end{aligned} \tag{10}$$

where w_g is the weighting factor associated with the g-vector in the irreducible part of the BZ, P_l is the Legendre polynomial of order l, $\beta_{KK'}$ is the angle between the vectors $g + K$ and $g + K'$, α is the point-symmetry operator and $S(K)$ is the structure factor of the lattice. In equation (10) the first three lines arise from the plane wave and the hybrid part (i.e. the plane-wave–tight-binding combination) and the last three lines give the contribution from the tight-binding part of the band state Ψ_t. It may be noted that, when the core states are completely filled, the contribution to $J_{\hat{k}}(q)$ from these states is found to be isotropic.
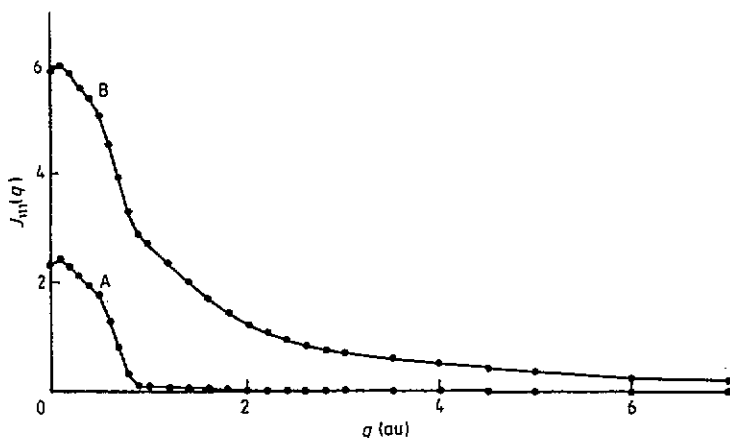
Figure 3. $J_{\hat{k}}(q)$ for scandium with $\hat{k}$ along the (111) direction: curve A, band contribution; curve B total contribution (core + band).

The results for $J_{\hat{k}}(q)$ obtained for any arbitrary direction $\hat{k}$ satisfy (Rath *et al* 1973)

$$\int_0^\infty J_{\hat{k}}(q)\,\mathrm{d}q = n \tag{11}$$

where n is equal to half the number of electrons per atom. Equation (11) may be used as a test for the accuracy of the band as well as the core contribution to $J_{\hat{k}}(q)$.

Table 2. Present results of the Compton profiles $J_{\vec{k}}(q)$ of scandium along the (110) direction.

q (au)	Band electrons (au)	Total (au)	q (au)	Band electrons (au)	Total (au)
0.0	2.783	6.373	1.8	0.022	1.419
0.1	1.938	5.523	2.0	0.012	1.212
0.2	2.471	6.033	2.2	0.011	1.057
0.3	2.297	5.815	2.4	0.007	0.931
0.4	1.618	5.069	2.6	0.006	0.840
0.5	1.924	5.283	2.8	0.003	0.760
0.6	1.618	4.863	3.0	0.001	0.699
0.7	0.645	3.757	3.5	0.001	0.583
0.8	0.237	3.196	4.0	0.000	0.497
0.9	0.080	2.875	4.5	0.000	0.421
1.0	0.090	2.713	5.0	0.000	0.355
1.2	0.065	2.335	6.0	0.000	0.229
1.4	0.085	2.021	7.0	0.000	0.206
1.6	0.048	1.690			

Table 3. Present results of the Compton profiles $J_{\vec{k}}(q)$ of scandium along the (111) direction.

q (au)	Band electrons (au)	Total (au)	q (au)	Band electrons (au)	Total (au)
0.0	2.326	5.916	1.8	0.027	1.424
0.1	2.433	6.017	2.0	0.015	1.216
0.2	2.296	5.858	2.2	0.009	1.055
0.3	2.074	5.592	2.4	0.006	0.930
0.4	1.941	5.392	2.6	0.004	0.838
0.5	1.732	5.091	2.8	0.002	0.758
0.6	1.306	4.551	3.0	0.001	0.699
0.7	0.793	3.905	3.5	0.000	0.583
0.8	0.303	3.263	4.0	0.000	0.497
0.9	0.092	2.887	4.5	0.000	0.421
1.0	0.091	2.713	5.0	0.000	0.355
1.2	0.072	2.342	6.0	0.000	0.229
1.4	0.058	1.994	7.0	0.000	0.206
1.6	0.043	1.686			

3. Results and discussions

Scandium metal has a hexagonal close-packed lattice structure. The lattice parameters $a = 6.2391$ au and $c = 9.9316$ au used in the present work are those given by Das (1976). In carrying out the energy band calculations, the non-local model potential parameters given by Animalu (1973) have been used. The model potential is first screened by a suitable dielectric function (Animalu 1973) before being used in the evaluation of the Hamiltonian matrix elements. The energy and band wavefunctions are calculated at 3456 representative g-points chosen throughout the BZ. For this purpose, in the one-twentyfourth irreducible part of the BZ, 144 g-points distributed suitably over nine equidistant planes sliced perpendicular to c axis are chosen. To each of the g-points a weighting factor w_g in proportion to the volume that it represents is assigned. At each g-point the model wavefunction is expanded in 23 plane waves corresponding to the shortest 23 wavevectors $|g + K|$ for that g-point. With this choice the convergence of energy and eigenfunctions is found to be good. The bands have converged to within 0.001 Ryd.

In an evaluation of the core contribution to $J(q)$, the atomic wavefunctions of Clementi (1967) have been used. As the core states are localized, the corresponding momentum distribution is delocalized and this requires $J(q)$ to be integrated over a very large distance on the q scale in order to satisfy equation (11). This is particularly true for 1s states whose contribution to $J(q)$ varies very slowly with q. Since the impulse approximation is not good for 1s electrons, one may ignore them. By ignoring 1s electrons, we find that the integrated result from equation (11) is 7.56 which is close to 8, the number of core electrons in half an atom. There still remains some contributions from 2s and 2p electrons which accounts for the above discrepancy.

Unlike the core states, the band states are delocalized, and hence their momentum distribution is fairly localized. To evaluate the band contribution to $J_{\vec{k}}(q)$, equations (9) and (10) are used. It may be noted that the plane-wave and hybrid (the first three lines in equation (10)) contributions were found to be well converged with 23 reciprocal-lattice vectors. However, to obtain convergence of the tight-binding contribution we have summed over the lowest 297 K_s-vectors. This number of K_s-vectors was also used for the three crystallographic directions (100), (110) and (111). In each case, equation (11) gives the number of conduction electrons per half-atom as approximately equal to 1.48. The latter value is very close to the exact result of 1.5 in scandium.

In tables 1–3, the results for $J_{\vec{k}}(q)$ are listed for the three crystallographic directions. In addition, these results are also plotted in figures 1–3. In table 1, the core contribution, the band contribution and the total $J_{\vec{k}}(q)$ are given. As the core contribution in the present work is the same for all the directions, it is not listed in tables 2 and 3 with a view to avoiding repetition. It may be noted from the tables as well as the figures that the anisotropy of the Compton profiles is quite appreciable. Considerable structures in the band contributions are seen from the figure. Similar but less prominent structures were also noted in the work of Rath *et al* (1973). Experimental data for the crystallographic directions are not available to compare with the present results.

4. Conclusions

Using the wavefunctions from energy band calculations, the Compton profiles of the electron momentum distribution are calculated along the (100), (110) and (111) directions. The results show a considerable amount of anisotropy in the profiles. It would be interesting to have measurements to compare with the theoretical predictions.

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