Multiple scattering and the Compton profile of titanium

J. Felsteiner*
Department of Physics, Technion–Israel Institute of Technology, Haifa, Israel

P. Pattison†
Department of Physics, University of Warwick, Coventry CV4 7AL, England, United Kingdom
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Monte Carlo methods recently introduced to correct for the effect of multiple scattering in Compton-profile measurements have been extended to take better account of the behavior of bound electrons. This procedure was applied to experimental Compton profiles of polycrystalline titanium measured with 60-keV γ rays for two thicknesses. The resultant profiles show good agreement with a recent calculation based on a renormalized-free-atom model for a $3d^2 4s^2$ electronic configuration.

It has recently become evident that multiple photon scattering can have a significant effect on Compton-profile measurements.[1–5] It has been shown that Monte Carlo procedures can successfully correct experimental Compton profiles for multiple-scattering effects. In this paper we report an extension of the Monte Carlo procedure described earlier in Refs. 2–4 which now enables us to make a reliable correction to Compton profiles of higher-atomic-number materials. In order to test the method we measured the Compton profile of polycrystalline titanium in two samples of different thickness.

The measurements were made using 59.54-keV γ rays from a 300-mCi ^{241}Am source scattered at an angle of $150° \pm 2°$ and detected with a Ge(Li) counter. The experimental arrangement and the data processing were similar to those described in Refs. 3 and 6. The two sample thicknesses were 0.120 and 0.013 cm, and about 20 000 counts were accumulated in each channel at the Compton peak for both samples. The separation between channels corresponded to an interval of approximately 0.03 a.u. per channel. The final profiles before a multiple-scattering correction has been made are shown in Table I.

The general form of the Monte Carlo procedure is essentially the same as that described previously.[2] However, we now take into account the way in which the binding of the electrons modifies the scattering cross sections.

First, the nature of the interaction, whether photoelectric absorption, Compton scattering, or elastic scattering, is determined according to the cross sections given in the compilation of Ref. 7.

For a Compton-scattering event the Klein-Nishina differential cross section is given by

$$\left(\frac{d\sigma}{d\Omega}\right)_{\mathrm{KN}} = \tfrac{1}{4} r_0^2 \left(\frac{\omega'}{\omega}\right)^2 \left(\frac{\omega}{\omega'} + \frac{\omega'}{\omega} - 2 + 4(1 - \sin^2\theta \cos^2\eta)\cos^2\beta\right), \quad (1)$$

where r_0 is the classical electron radius, ω and ω' are the energies of the incident and scattered photons, θ and η are the polar and azimuthal angles, and β is the polarization angle as described in Ref. 2. To take account of the motion of the bound electrons the differential cross section can be modified by including the Compton profile $J(q)$ to give the following:

$$\frac{d^2\sigma}{d\Omega\, dq} = \left(\frac{d\sigma}{d\Omega}\right)_{\mathrm{KN}} \frac{\omega}{\omega'} \frac{m}{\Delta k} \frac{d\omega'}{dq} J(q), \quad (2)$$

where m is the rest energy of the electron and $\Delta k = (\omega^2 + \omega'^2 - 2\omega\omega' \cos\theta)^{1/2}$. It can easily be shown that Eq. (2) reduces in the nonrelativistic case to the expression given by Eisenberger.[8] The energy ω' of the scattered photon can be derived from the electron-momentum component q and the scattering angle θ by solving the equation

$$q = \frac{137}{m}\left(\frac{\Delta k}{2} + \frac{m\Delta\omega}{\Delta k} - \frac{(\Delta\omega)^2}{2\Delta k}\right), \quad (3)$$

where q is in a.u., and $\Delta\omega = \omega' - \omega$. When a photon is Compton scattered, values of $\cos\theta$, η, β, and q are chosen at random, and a Monte Carlo rejection procedure[9] is used to force the distribution to follow the behavior given by Eq. (2). If the energy transfer to the electron is insufficient to overcome the electron binding, then a Compton-scattering event cannot occur. In the Monte Carlo procedure the atomic shell of the scattering electron is selected at random, taking into account the number of electrons in each shell. If the binding energy of this shell is sufficient to prevent a scattering then such an event is rejected.

For an elastic-scattering event the Thomson differential cross section is

$$\left(\frac{d\sigma}{d\Omega}\right)_{\mathrm{Th}} = r_0^2(1 - \sin^2\theta \cos^2\eta) \ . \quad (4)$$

TABLE I. Compton profile of polycrystalline titanium.

q (a.u.)	Core $1s^2 \ldots 3p^6$	RFA $3d^3 4s^1$	RFA $3d^2 4s^2$	0.013 cm (not corrected)	0.120 cm (not corrected)	0.013 cm (corrected)	0.120 cm (corrected)
0.0	3.449	5.225	5.551	5.461 ±1.2%	5.262 ±1.2%	5.510 ±1.3%	5.508 ±1.6%
0.1	3.441	5.194	5.521	5.412	5.253	5.461	5.494
0.2	3.416	5.101	5.428	5.300	5.148	5.347	5.375
0.3	3.376	4.948	5.275	5.113	4.972	5.157	5.177
0.4	3.317	4.728	5.057	4.889	4.832	4.930	5.022
0.5	3.240	4.442	4.772	4.691	4.560	4.729	4.725
0.6	3.145	4.085	4.420	4.469	4.347	4.504	4.491
0.7	3.033	3.874	4.001	4.205	4.017	4.236	4.131
0.8	2.907	3.720	3.544	3.910	3.761	3.936	3.854
0.9	2.770	3.549	3.380	3.541	3.433	3.561	3.501
1.0	2.625	3.362	3.202	3.297 ±1.6%	3.163 ±1.6%	3.314 ±1.7%	3.211 ±2.3%
1.1	2.475	3.166	3.016	3.077	2.938	3.090	2.971
1.2	2.322	2.964	2.824	2.815	2.829	2.824	2.858
1.3	2.176	2.767	2.638	2.577	2.612	2.583	2.628
1.4	2.025	2.566	2.446	2.386	2.382	2.389	2.383
1.5	1.882	2.373	2.263	2.216	2.174	2.218	2.162
1.6	1.750	2.193	2.092	2.035	2.003	2.033	1.982
1.7	1.625	2.023	1.931	1.882	1.927	1.878	1.905
1.8	1.511	1.868	1.782	1.761	1.780	1.756	1.751
1.9	1.405	1.724	1.645	1.662	1.697	1.656	1.666
2.0	1.311	1.597	1.523	1.542	1.562	1.534	1.523
2.2	1.150	1.381	1.317	1.311	1.394	1.299	1.349
2.4	1.022	1.208	1.156	1.188	1.205	1.177	1.153
2.6	0.920	1.070	1.028	1.048	1.114	1.034	1.062
2.8	0.838	0.959	0.925	0.930	1.008	0.916	0.957
3.0	0.774	0.872	0.844	0.862 ±4%	0.910 ±4%	0.848 ±4.5%	0.862 ±5.5%
3.5	0.657	0.716	0.701	0.693	0.769	0.681	0.736
4.0	0.572	0.609	0.600	0.587	0.631	0.579	0.592
5.0	0.438	0.452	0.449	0.448	0.449	0.444	0.423
6.0	0.331	0.337	0.336	0.336	0.343	0.330	0.321
7.0	0.249	0.251	0.251	0.251 ±6%	0.258 ±6%	0.248 ±6.5%	0.252±7.5%

To take account of coherent scattering from an atom this distribution was modified to be

$$\frac{d\sigma}{d\Omega} = \left(\frac{d\sigma}{d\Omega}\right)_{\mathrm{Th}} F^2 \ , \tag{5}$$

where F is the atomic form factor. The value of F, for particular values of θ and ω, is taken from the tables of Ref. 10. In the Monte Carlo calculation, when there is an elastic-scattering event values of $\cos\theta$ and η are chosen at random, and the distribution is then forced by the rejection procedure to follow Eq. (5).

An additional improvement to the previous Monte Carlo code was the introduction of photon splitting. Since the multiple-scattering intensity is much smaller than the single-scattering intensity, each photon which scattered more than once was "split" after the first collision into, say, ten photons, while still preserving the initial probability. This procedure increases the statistical accuracy of the multiple-scattering calculation.

The Monte Carlo procedure described above was employed to correct our experimental data for the effects of double and triple scattering. The corrected profiles for the two thicknesses are shown in Table I and are seen to agree within the experimental error. Triple scattering, al-

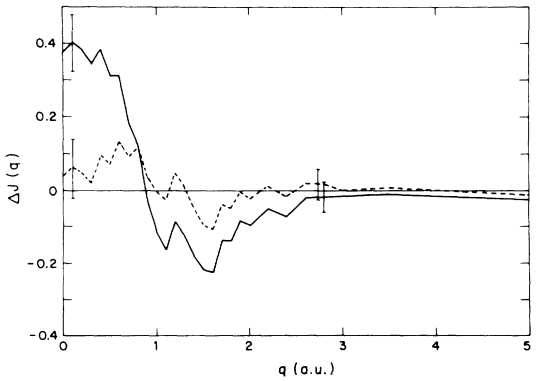

FIG. 1. Difference curves between corrected thick-sample data and convoluted-deconvoluted RFA theory. ——: $3d^3 4s^1$; – – –: $3d^2 4s^2$. The range of statistical uncertainty is indicated by the error bars.

though negligible for the thin sample, was noticeable for the thick-sample profile, where $J(0)$ was increased by a further $\frac{1}{2}\%$.

Table I also shows results of a calculation by Berggren *et al.*[11] using a renormalized-free-atom model (RFA) for the two different electronic configurations $3d^3 4s^1$ and $3d^2 4s^2$. Since the deconvolution procedure does not remove all of the effects of instrumental broadening, a more reliable comparison between theory and experiment can be achieved by convoluting the theory with the instrumental resolution function (full width at half maximum 0.65 a.u.) and then deconvoluting it.[12] Figure 1 shows the difference between the corrected experimental results for the thick sample and the RFA theory after the theory has been convoluted and deconvoluted. It is clear that the present experimental results support the assumption that the electronic configuration in titanium is closer to $3d^2 4s^2$ than to $3d^3 4s^1$. This is in contrast to the conclusions of an earlier γ-ray measurement[11] where multiple-scattering effects were not taken into account. On the other hand, the results of lower-energy x-ray measurements,[13] where multiple scattering should be negligible,[4] show better agreement with the present data.

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