

On the bremsstrahlung background correction to the high-energy Compton spectroscopy

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Abstract. A methodology for bremsstrahlung (BS) background correction to extract a true Compton profile in high-energy Compton scattering experiments is presented. The BS background profiles for Hg, computed within the Born approximation, are estimated for different values of incident energy. It is seen for the first time that the BS background contribution in high-energy Compton profile experiments like those employing third generation synchrotron radiation sources comes out to be significant and non-linear. Further, it is found that the incorporation of BS correction in data reduction of such an experiment performed on Hg at 662 keV energy helps in reconciliation of theory and experiment.

Keywords. Bremsstrahlung radiation; Compton spectroscopy; γ -ray scattering.

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1. Introduction

Compton scattering is a very powerful technique for testing the electronic properties of various materials [1]. Experimentally, within the impulse approximation, the measured double differential scattering cross-section $D(\omega_2)$ can be written in terms of the scattered photon energy ω_2 as

$$D(\omega_2) = C(\omega_2)J(p_z), \quad (1)$$

where $J(p_z)$ is the Compton profile (CP) and $C(\omega_2)$ is the Ribberfors cross-section [1]. The aim of Compton data analysis is to extract $D(\omega_2)$ from the measured energy spectrum $M(\omega_2)$. This is achieved by the removal of background and the energy dependent effects like instrumental resolution, sample absorption, detector efficiency, etc. In fact, to remove these effects from $M(\omega_2)$ one requires application of various correction procedures that are additive, factorial or convolutive [2].

After such corrections, the profile is corrected for the multiple scattering using a Monte-Carlo simulation [3,4]. After careful data reduction, in several high-energy CP measurements, a poor agreement between the duly processed experiment and

the theory in the high-momentum side is seen. In fact, the high-momentum side of the CP corresponds to core electrons, which remain almost unaffected by solid-state effects and hence a good agreement between theory and experiment for $p_z \geq 4$ a.u. is quite expected. This discrepancy in the high-momentum region has been explained by several workers [5–12] in terms of an additional bremsstrahlung (BS) background. In the case of experimental CPs of Ag and Cd measured with 662 keV γ -ray energy, Andrejczuk *et al* [11] and Reniewicz *et al* [12] have considered the BS and other background as a constant which is a single adjustable parameter. They have fitted the background iteratively, preserving the profile normalization, to get the best agreement between theory and experiment in the high-momentum side.

Here we present a methodology for a quantitative determination of the BS background in high-energy Compton scattering experiments using synchrotron radiations (SR) or γ -rays and see the effect of BS correction on the Compton profile of a representative high Z sample, namely Hg.

2. Methodology

In a Compton scattering experiment, mainly two types of electrons (a) the photoelectrons (PE) and (b) the recoil Compton electrons (CE) are liberated from the target atoms. These electrons may produce a continuous spectrum of bremsstrahlung radiation (BS) on interaction with the electric field due to neighbouring atomic nuclei. To obtain the BS spectrum due to PE and CE, the required BS cross-section can be obtained by using the Born approximation (BA)–BS cross-section formula. The relativistic BA–BS cross-section formula of Bethe and Heitler (formula 3BN of [13]), in the field of atomic nucleus is given by

$$\frac{\partial\Phi_\omega}{\partial\omega} = \frac{\alpha r_e^2 Z^2}{\omega} M_{\text{Born}}^{\text{unscr}}, \quad (2)$$

where $\alpha = 1/137.036$ is the fine structure constant, $r_e = 2.81793 \times 10^{-13}$ cm is the classical electron radius and $M_{\text{Born}}^{\text{unscr}}$ is a dimensionless quantity involving E_0, E (the initial and the final total energy of the electron in a collision in m_0c^2 units), ω (photon energy in m_0c^2 units), p_0, p (the initial and the final momentum of the electron in a collision in m_0c units), etc [13]. The total energy and momentum of the electron are obtained from its kinetic energy using the relativistic relations. The initial kinetic energy of the PE from different shells of the target atom is worked out from the difference of the incident energy and the binding energy of the respective shell and the average initial kinetic energy of CE is taken as the difference of the incident energy and the energy of the Compton peak.

In the case of heavy materials, the screening effect of the nuclear charge by atomic electrons is taken into account by a form factor correction [14] on eq. (2). Further, in the high-frequency limit of the emitted photons, eq. (2) is multiplied by Elwert factor [14] given by

$$f_E = \frac{\beta_0 [1 - \exp(2\pi\alpha Z/\beta_0)]}{\beta [1 - \exp(2\pi\alpha Z/\beta)]}, \quad (3)$$

where $\beta_0 = p_0/E_0$ and $\beta = p/E$.

The BS intensity for photons of energy ω due to PE (χ^P) and CE (χ^C) is then given by

$$\chi^P = \frac{\omega}{E_0} \sum_i \sigma_{PE,i} \left(\frac{d\Phi_\omega}{d\omega} \right)_i \quad \text{and} \quad \chi^C = \frac{\omega}{E_0} \sigma_C \left(\frac{d\Phi_\omega}{d\omega} \right) \quad (4)$$

where $\sigma_{PE,i}$ is the photoelectric cross-section for the i th shell and σ_C is the Compton cross-section of the target atom respectively. The total BS intensity (I_{BS}^{Total}) for all the photon energies is then written as

$$I_{BS}^{\text{Total}} = \int_0^{T_0} (\chi^P + \chi^C) d\omega, \quad (5)$$

where T_0 is the initial kinetic energy of the electrons in keV.

BS spectrum is obtained by plotting $I_{BS}(= \chi^P + \chi^C)$ vs. ω for the entire range of the emitted photon energies. The area under this BS curve in the Compton region (-7 to $+7$ a.u. in momentum space) gives I_{BS}^{CP} whereas the area under the curve for the entire energy range gives I_{BS}^{Total} . In order to get the BS profile, we compute the ratio $I_{BS}^{\text{Total}}/I_C^{\text{Total}}$ using the relations given in [15], where I_C^{Total} is the total intensity of Compton electrons. Then $I_{BS}^{\text{CP}}/I_C^{\text{Total}}$ is obtained from the product of $I_{BS}^{\text{CP}}/I_{BS}^{\text{Total}}$ and $I_{BS}^{\text{Total}}/I_C^{\text{Total}}$ which is then multiplied by the free atom Compton profile area in the momentum range -7.0 to $+7.0$ a.u. to get the total electronic contribution (n) of the BS background profile. The area under the BS curve (in the Compton region) is then normalized to n to get the BS background profile in $e/\text{a.u.}$ at different momentum values.

3. Results and discussion

BS spectra due to photo- and Compton electrons produced by 662 keV γ -rays incident on Hg and scattered at an angle of 160° within Born approximation (incorporating the screening effect and the Elwert factor corrections) are shown in figure 1. The two vertical arrows mark the Compton region (-7 to $+7$ a.u.). It is seen that the computed total BS curve (figure 1) is almost flat in the Compton region resulting in almost linear BG profile shown in column 4 of table 1. This figure shows that the major contribution to the total BS spectrum comes from the Compton and the K-shell electrons, which is expected because of higher values of their cross-sections as compared to those of the L, M and N shell electrons. The kinetic energy of the Compton and the K-shell electrons in this case is 473 and 580 keV respectively which is reflected in the two sharp discontinuities in the BS curves at these energies. In the inset of figure 1, we have also plotted the BS curve and its contributions from the Compton and different shell photoelectrons for a representative energy 200 keV (like that from advanced synchrotron radiation sources) with the same scattering angle. The BS curves in the inset have been plotted in the same arbitrary units as those for the 662 keV energy. A comparison of BS spectra (total) shown in the main part and inset of figure 1 shows that the amplitude of the BS intensity for 200 keV is much higher than that at 662 keV which may lead to a significant BS background contribution to the Compton profile. Further, a

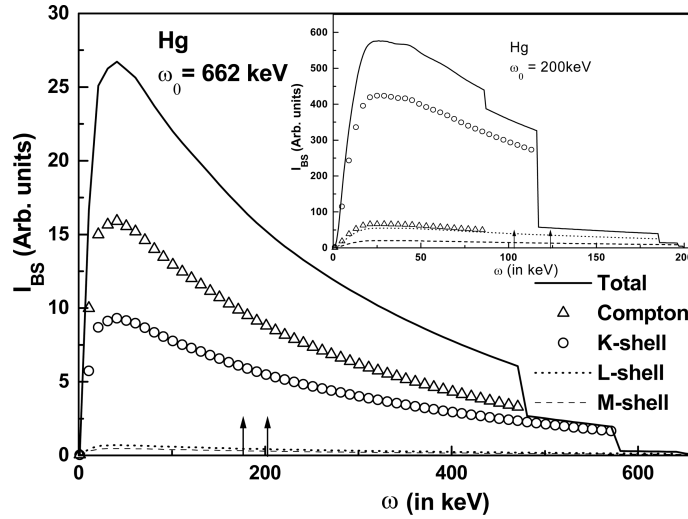


Figure 1. Spectrum of the BS intensity in the Born approximation (corrected for Elwert factor and screening effect) for Compton electrons and photoelectrons knocked out from K, L and M shells of Hg by 662 keV incident energy (ω_0). In the inset, we have shown a similar spectrum computed for Hg employing 200 keV photon energy representing the third and higher generation synchrotron radiation sources. Vertical arrows show the Compton region (-7 to 7 a.u.) for 160° scattering angle. The solid line corresponds to total (photo K, L, M + Compton) BS contribution.

remarkable feature of this curve is the loss of linearity of the BS contribution in the Compton range. It is due to the abrupt fall of the BS intensity around 116 keV arising due to the fact that the K-electron contribution vanishes beyond this region and only the L and M shell electrons contribute to BS, the contribution of the Compton electrons being already zero beyond 86 keV.

In table 1, we have also listed the background profiles for Hg computed for two lower values of energy (200 and 400 keV) for the same scattering angle. To check the effect of BS correction on Compton measurements, we have corrected the experimental Compton profile of Hg (column 5 of table 1) measured at 662 keV incident energy using our 20 Ci ^{137}Cs γ -ray spectrometer [10]. After subtracting the BS background (column 4) from the experimental profile of Hg (column 5) and preserving the normalization of the experimental profile, it is seen that at $J(0)$ the Hg profile comes out to be $9.768 e/\text{a.u.}$. Therefore, the BS background correction enhances $J(0)$ by $0.045 e/\text{a.u.}$ which is more than twice that of the statistical error $\pm\sigma$. It is seen from column 2 of this table that the BS background contribution at lower momenta ($p_z < 3$ a.u.) for 200 keV incident energy is significant and non-linear. Looking at the trend of the BS correction effect in Hg using 662 keV γ -rays, the overall effect of BS on the SR-based experimental profile after preserving the normalization seems to be about $0.06 e/\text{a.u.}$ at $J(0)$. Therefore, the BS correction in SR-based experiments where the statistical error is almost negligible is quite important in deducing the high-precision experimental CP. In table 1, a

Table 1. Bremsstrahlung (BS) background profiles for Hg sample within Born approximation corrected for Elwert factor and screening effect for three different representative incident energies (ω_0) and a scattering angle of 160° . Also listed is the experimental Compton profile of Hg measured with a 662 keV γ -ray spectrometer (Gaussian FWHM of 0.4 a.u.) [10] and the convoluted renormalized free atom (RFA) profile of Hg [10]. The effect of the BS correction on the experimental profile (CP with BS correction – CP without BS correction) of Hg at 662 keV after preserving normalization is also shown in column 6.

p_z (a.u.)	Quantitative BS background for Hg (e/a.u.)			Experimental $J(p_z)$ for Hg (e/a.u.) [10]	Effect of BS correction (e/a.u.) (662 keV)	Convoluted RFA $J(p_z)$ for Hg (e/a.u.)
	$\omega_0 = 200$ keV	$\omega_0 = 400$ keV	$\omega_0 = 662$ keV			
0.0	0.044	0.031	0.035	9.723±0.021	+0.045	10.054
0.1	0.044	0.031	0.035	9.662	+0.044	10.012
0.2	0.044	0.031	0.035	9.542	+0.044	9.885
0.3	0.044	0.031	0.035	9.371	+0.042	9.669
0.4	0.044	0.031	0.035	9.149	+0.041	9.368
0.5	0.044	0.031	0.034	8.888	+0.038	8.998
0.6	0.044	0.031	0.034	8.607	+0.037	8.597
0.7	0.044	0.031	0.034	8.335	+0.034	8.216
0.8	0.044	0.031	0.034	8.064	+0.032	7.894
1.0	0.044	0.031	0.034	7.511±0.018	+0.027	7.391
1.2	0.043	0.031	0.034	7.018	+0.024	6.910
1.4	0.043	0.031	0.034	6.435	+0.019	6.394
1.6	0.043	0.031	0.034	5.892	+0.014	5.865
1.8	0.043	0.031	0.034	5.369	+0.010	5.356
2.0	0.033	0.031	0.034	4.907	+0.006	4.892
3.0	0.008	0.030	0.034	3.358±0.010	-0.007	3.451
4.0	0.008	0.030	0.034	2.906	-0.010	2.849
5.0	0.008	0.030	0.033	2.443±0.008	-0.013	2.379
6.0	0.007	0.030	0.033	1.981	-0.017	1.931
7.0	0.007	0.029	0.033	1.589±0.006	-0.020	1.583

comparison between the convoluted renormalized free atom (RFA) [10] (column 7) and experimental (column 5) profiles for 662 keV (with and without incorporating the BS background mentioned in column 6), shows that besides in the low-momentum region, the BS correction also leads to a relatively better agreement between the experimental and theoretical profiles in the high-momentum region. It is worth mentioning here that the remaining significant differences between the convoluted theory and the experiment (at 662 keV) in the low-momentum region are due to a simple nature of RFA profiles used here [10].

It is clear from the above discussion that the BS background correction enhances the reliability of the data analysis and the precision of the experimental Compton data.

4. Conclusion

In the case of Compton measurements using high-energy (like 200 keV) synchrotron radiation sources, it is seen that the contribution of K-shell and the Compton electrons falls abruptly in the Compton profile region and it gives a significant non-linear background contribution. To avoid the non-linear background in synchrotron-based experiments one should carefully tune the incident energy in such experiments, taking care of glitches. It is further concluded that for a high-precision Compton profile of heavy materials, measured using high incident energy like that from ^{137}Cs source, one should apply the bremsstrahlung background correction to the Compton profile along with other usual corrections.

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