



Numerical method for external Bremsstrahlung cross sections in compounds

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Received 8 March 2006; received in revised form 19 October 2006; accepted 30 October 2006

Abstract

A numerical method is used to evaluate External Bremsstrahlung (EB) cross section in compounds such as NaI, SiLi, and GeLi first time using tabulated data given for elements. Modified atomic number defined for compound is used to evaluate cross section. This evaluated theoretical data may be useful for the analysis of experimental spectrum and yield of EB in thick target compounds.

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Keywords: External Bremsstrahlung; Radiation; Cross section; Compounds

1. Introduction

When a beta particle passes through the Coulomb field of the target nucleus, it accelerates and emits out external Bremsstrahlung (EB). Accurate theory for EB is developed by Tseng et al. (1977) using the self-consistent coulomb field wave function. A similar approach of Tseng et al. is followed by Seltzer and Berger (1986) to extend it to the field of an atomic electron. Chapman (1967) evaluated the theoretical attenuation coefficient of gamma ray for germanium at different photon energies ranging from 0.05 to 15 MeV based on the attenuation coefficients of five elements tabulated by Grodstein (1957) whose atomic numbers are adjacent to the atomic number of germanium, using the following Lagrange interpolation method as described in detail by Sokolnikoff and Redheffer (1958):

$$X_{Z'} = \sum X_z \left\{ \prod_{Z' \neq Z} (Z' - Z) / \prod_{z \neq Z} (z - Z) \right\}, \quad (1)$$

where z is the atomic number of the element of known attenuation coefficient, X_z adjacent to the atomic number Z' of the element whose attenuation coefficient $x_{Z'}$ is desired and Z are atomic numbers of other elements of known attenuation coefficients adjacent to Z' .

The Lagrange interpolation method is general one which can be used not only for attenuation coefficient of gamma ray for elements but also for EB cross section which is evaluated for compounds in the present study.

Classical Kramer's law has been used extensively for the prediction of the Bremsstrahlung intensity (I) for elements

$$I = \text{const.} (\Delta E/E_\nu) Z(E_0 - E_\nu), \quad (2)$$

where E_ν and E_0 are emitted photon energy and incident electron energy, respectively, Z is the atomic number of the target element. Some authors (Ware and Reed, 1973; Reed, 1975; Statham, 1976; Lifshin, 1976; Sherry and Vander Sande, 1977; Statham, 1979; Smith and Reed, 1981; Vander Wood et al., 1983) have reported that this derivation ignores the back scattering of the electron which may in heavy elements eliminates a large fraction of high energy electrons from the target. In order to improve the agreement between the experimental results and the theoretical predictions, various empirical modified versions of Kramer's expression have been proposed (Statham, 1976; Lifshin, 1976; Sherry and Vander Sande, 1977; Smith and Reed, 1981). For a set of compound samples Vander Wood et al. (1983) found definite discrepancies between the measured Bremsstrahlung intensities and the values predicted via Kramer's law when weighted mean atomic number ($Z_{\text{mean}} = \sum W_i Z_i$, where W_i and Z_i are weight fraction and atomic number of i th element, respectively) of the element present in the compound was used as Z in (1). As one possible explanation

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for these discrepancies, they suggested that Kramer's law may not be adequate description for the Bremsstrahlung radiation emitted by compound samples.

Markowicz and VanGriken (1984) proposed a new expression to take into account the self-absorption of Bremsstrahlung and electron back scattering and to obtain the accurate description of the Bremsstrahlung process

$$I = \text{const.} (\Delta E/E_v) Z_{\text{mod}}(E_0 - E_v)[1 - f]. \quad (3)$$

Here

$$Z_{\text{mod}} = \frac{\sum_i^I \frac{W_i Z_i^2}{A_i}}{\sum_i^I \frac{W_i Z_i}{A_i}} \quad (4)$$

A_i is mass number of the i th element, f is a function of E_0 , E_v and composition. For pure elements (3) simplifies to (2). The atomic number Z_{mod} defined for compound is more accurate one than Z_{mean} . The new Markowicz formula derived in a more rigorous way gives theoretical results for composite samples which are in better agreement with experimental values than those predicted by Kramer's law. From the known atomic numbers of elements and measured Bremsstrahlung yields for various elements and compounds, Shivaramu (1990) evaluated the effective atomic number (Z_{eff}) of the compound from the interpolation method. He reported that Z_{eff} agrees fairly well with Z_{mod} than Z_{mean} .

Llovet et al. (2003) and Salvat et al. (2006) developed Monte Carlo algorithm to simulate the Bremsstrahlung emission by electron impact only for elements. However, Salvat has suggested an additivity rule to extend from elements to compounds.

2. Present work

In the present work, we have evaluated Z_{mod} using Markowicz's equation (4). The estimated Z_{mod} for NaI, GeLi and SiLi are 45.780, 29.517 and 12.058, respectively. The six elements whose atomic numbers adjacent to that of NaI chosen are Te, Ru, Rh, Pd, Ag and Cd and their Z values are 43,44,45,46,47,48, respectively. Similarly, six adjacent elements are considered for other two compounds. We have evaluated Bremsstrahlung cross sections for various compounds by extending Lagrange's interpolation technique, theoretical EB cross sectional data given by Seltzer et al. for elements and the above evaluated results of Z_{mod} . Seltzer et al. has tabulated the total scaled energy weighted EB cross section for elements. We have converted this into the actual EB cross section for the elements using a factor as suggested by them and then we have evaluated for EB cross section

($\sigma_{Z'}$) for compounds using the following expression:

$$\sigma_{Z'} = \sum \sigma_z \left\{ \frac{\prod_{Z' \neq Z} (Z' - Z)}{\prod_{z \neq Z} (z - Z)} \right\}, \quad (5)$$

where z is the atomic number of the element of known EB cross section, σ_z adjacent to the modified atomic number Z' (here Z' is treated as Z_{mod}) of the compound whose EB cross section $\sigma_{Z'}$ is desired and Z are atomic numbers of other elements of known EB cross section adjacent to Z' . Here Eq. (5) is deduced from Eq. (1) by replacing attenuation coefficient into EB cross section. The detailed calculations made to evaluate $\sigma_{Z'}$ for NaI is as follows:

$$\begin{aligned} \sigma_{Z'} = & \sigma_{43} \left[\frac{(45.78 - 44)(45.78 - 45)(45.78 - 46)(45.78 - 47)(45.78 - 48)}{(43 - 44)(43 - 45)(43 - 46)(43 - 47)(43 - 48)} \right] \\ & + \sigma_{44} \left[\frac{(45.78 - 43)(45.78 - 45)(45.78 - 46)(45.78 - 47)(45.78 - 48)}{(44 - 43)(44 - 45)(44 - 46)(44 - 47)(44 - 48)} \right] \\ & + \sigma_{45} \left[\frac{(45.78 - 43)(45.78 - 44)(45.78 - 46)(45.78 - 47)(45.78 - 48)}{(45 - 43)(45 - 44)(45 - 46)(45 - 47)(45 - 48)} \right] \\ & + \sigma_{46} \left[\frac{(45.78 - 44)(45.78 - 45)(45.78 - 47)(45.78 - 48)(45.78 - 43)}{(46 - 43)(46 - 44)(46 - 45)(46 - 47)(46 - 48)} \right] \\ & + \sigma_{47} \left[\frac{(45.78 - 43)(45.78 - 44)(45.78 - 45)(45.78 - 46)(45.78 - 48)}{(47 - 43)(47 - 44)(47 - 45)(47 - 46)(47 - 48)} \right] \\ & + \sigma_{48} \left[\frac{(45.78 - 43)(45.78 - 44)(45.78 - 45)(45.78 - 46)(45.78 - 47)}{(48 - 43)(48 - 44)(48 - 45)(48 - 46)(48 - 47)} \right]. \end{aligned}$$

Thorough literature survey reveals that none of the workers have attempted so far to make use of this additivity rule to work out Bremsstrahlung cross section for compounds. Z_{eq} of compound used in additivity rule is based on classical Kramer's law. Hence Z_{eq} may be considered less accurate one than Z_{mod} .

Similarly $\sigma_{Z'}$ is evaluated for other two compounds using the above method. The estimated $\sigma_{Z'}$ is expressed in barn per MeV per atom. It is tabulated in Tables 1–3 for various kinetic energy of the incident electron (T_1) and fractional EB photon energy (k/T_1). Here, k is the EB photon energy. The variation of $\sigma_{Z'}$ with (k/T_1) as well as with T_1 is shown in Figs. 1–3.

Table 1
EB cross sections of NaI (barn/MeV per atom)

T_1	k/T_1									
	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
0.01	277 920	142 320	95 210	70 940	56 400	46 740	39 890	34 750	30 810	27 764
0.05	19 785	9390	5920	4210	3190	2540	2080	1760	1510	1310
0.1	6290	2850	1720	1180	880	694	550	457	380	320
0.5	539	223	125	79	54	39	28	21.2	15	12
1	232	94	52	32	21.8	15.1	10.4	7.6	5.3	3.7
2	111	45.6	25.2	15.9	10.7	7.4	5.2	3.6	2.4	1.4
10	26.6	9.83	5.78	3.79	2.69	1.99	1.49	1.111	0.732	0.224
100	2.30	1.048	0.639	0.444	0.334	0.265	0.218	0.184	0.149	0.020
1000	0.232	0.106	0.311	0.045	0.0348	0.028	0.023	0.025	0.0194	0.002
10 000	0.023	0.0106	0.0065	0.0046	0.003	0.0028	0.0024	0.002	0.0019	0.0002

k and T_1 are out going EB photon energy and incident electron energy in MeV.

Table 2
EB cross sections of GeLi (barn/MeV per atom)

T_1	k/T_1									
	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
0.01	140 995	70 420	46 190	33 910	26 580	21 690	18 240	15 660	13 690	12 174
0.05	8860	4140	2549	1767	1322	1042	850	708	597	509
0.1	2681	1189	707	478	348	266	210	171	141	131
0.5	222	90	49.5	31	21	14.5	10.3	7.44	5.30	3.89
1	96.8	38.5	20.98	13	8.5	5.8	4.026	2.77	1.84	1.170
2	47.2	19.06	10.46	6.52	4.34	2.98	2.057	1.401	0.891	0.466
10	10.02	4.34	2.524	1.658	1.165	0.852	0.634	0.46	0.30	0.0760
100	1.025	0.465	0.283	0.197	0.148	0.1174	0.0968	0.081	0.065	0.007
1000	0.1032	0.047	0.029	0.020	0.0154	0.0125	0.0106	0.0093	0.0084	0.0006
10 000	0.0103	0.0047	0.0029	0.0020	0.0015	0.0012	0.0010	0.00095	0.00080	0.00006

k and T_1 are out going EB photon energy and incident electron energy in MeV.

Table 3
EB cross sections of SiLi (barn/MeV per atom)

T_1	k/T_1									
	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
0.01	30 516	14 699	9312	6596	5040	4010	3295	2776	2387	2088
0.05	1639	3602	423	283	204	153	119	94	76	64
0.1	471	200	109	74	51	37	28	24	16	13
0.5	37	7.4	7.9	4.8	3.1	2.12	1.44	0.97	0.63	0.34
1	15	6.08	3.23	1.96	1.271	0.84	0.56	0.41	0.22	0.096
2	8.41	3.28	1.76	1.08	0.71	0.47	0.323	0.211	0.124	0.041
10	1.86	0.79	0.45	0.29	0.20	0.15	0.11	0.08	0.05	0.007
100	0.194	0.087	0.053	0.037	0.027	0.021	0.018	0.015	0.0118	0.00068
1000	0.0196	0.089	0.005	0.0038	0.0029	0.0023	0.0020	0.0017	0.0015	0.00006
10 000	0.0019	0.00089	0.00055	0.00038	0.00029	0.00023	0.0002	0.00018	0.00016	0.00006

k and T_1 are out going EB photon energy and incident electron energy in MeV.

3. Results and discussions

The method we have discussed in the present study is a general one and first of its kind which can be extended to any of the compounds. The cross section data given in Tables 1–3 for

NaI, SiLi, and GeLi can be used further to evaluate theoretical EB spectrum of thick target compounds which in turn may be used to compare with the measured EB spectrum. As these three compounds are mainly used in detectors to detect radiation, there is a possibility of production of secondary EB in the

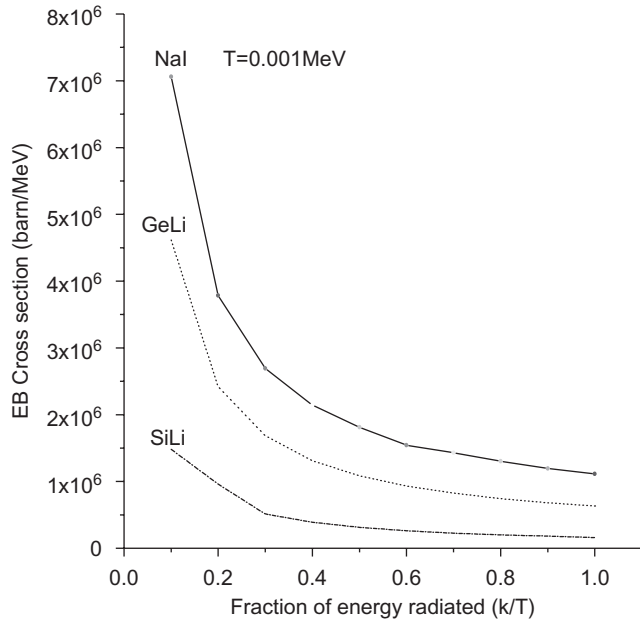


Fig. 1. Variation of EB cross section of compound ($\sigma_{Z'}$) with fraction of energy radiated at $T_1 = 0.001$ MeV.

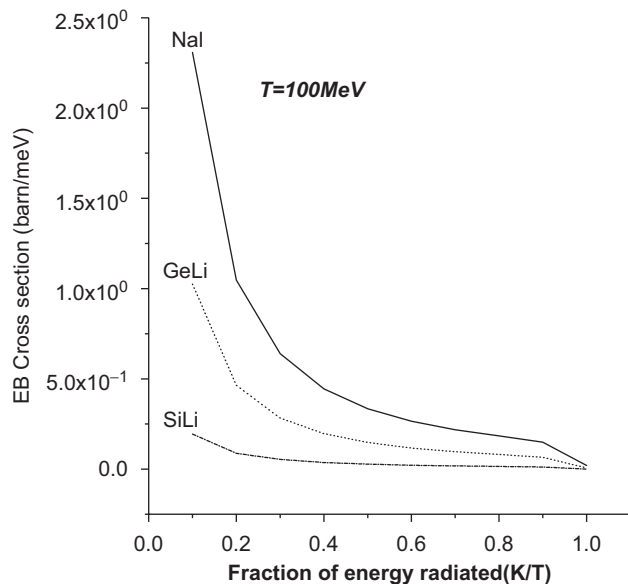


Fig. 2. Variation of EB cross section of compound ($\sigma_{Z'}$) with fraction of energy radiated at $T_1 = 100$ MeV.

detector itself whenever beta passes through these detectors. This component is normally neglected while carrying out the regular experiment on measurement of primary EB of same or other compound which are normally kept between beta source and the detector. Hence our data may be useful to apply corrections, in case the theoretical spectrum mismatch with measured one. Our method is an accurate one as this is based on the accurate Lagrange's interpolation method and Markowicz equation and we claim our data is more accurate one as it is obtained from Seltzer et al. data. We find, Salvat's additivity

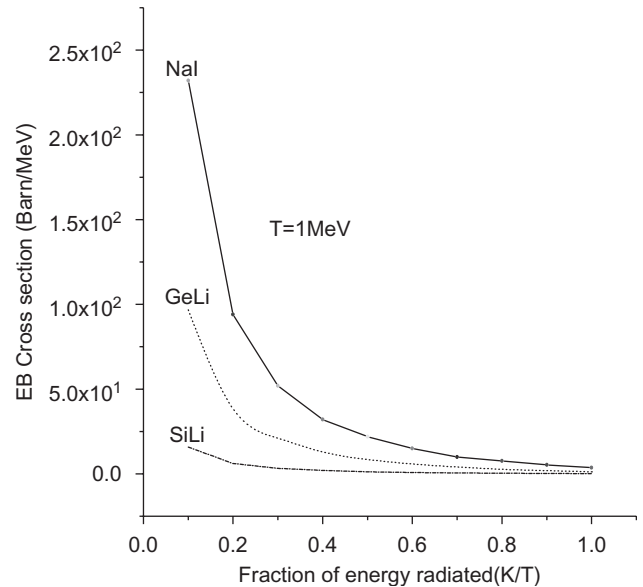


Fig. 3. Variation of EB cross section of compound ($\sigma_{Z'}$) with fraction of energy radiated at $T_1 = 1$ MeV.

rule for compound is less accurate one than our method as Z_{eq} used there is less accurate than Z_{mod} of our method, for the reason discussed earlier.

The thorough literature survey reveals that Z_{mod} (Z_{eff} or Z_{mean} or Z) is independent of Bremsstrahlung energy. EB cross sectional data given in Tables 1–3 are available only for specified EB photon and electron energies. However, they can be read for all EB photon and electron energies as evident from Figs. 1–3. EB cross section is found to be higher for a compound of higher Z_{mod} for a given EB photon and electron energies and it decreases with increase of EB energy for a given compound and electron energy.

References

- Chapman, G.T., 1967. Gamma ray attenuation coefficients for germanium. Nucl. Instrum. Methods 52, 101.
- Grodstein, G.W., 1957. X-ray attenuation coefficients from 10 keV to 100 MeV. NBS-583.
- Lifshin, L., 1976. Quantitative microprobe analysis with energy dispersive detectors. Adv. X-ray Anal. 19, 113–152.
- Llovet, X., Sober, L., Campos, C.S., Acosta, E., Salvat, F., 2003. Monte Carlo simulation of X-ray spectra generated by kilo-electron volt electrons. Radiat. Phys. Chem. 93(1), 3844–3852.
- Markowicz, A.A., VanGriken, R.E., 1984. Composition dependence of Bremsstrahlung background in electron-probe X-ray microanalysis. Annu. Chem. 56, 2049.
- Reed, S.J.B., 1975. The shape of the continuous X-ray spectrum and background corrections for energy dispersive electron microprobe analysis. X-ray Spectrom. 4, 14–17.
- Salvat, F., Fernandez-varea, J.M., Sampau, J., Llovet, X., 2006. Monte Carlo simulation of Bremsstrahlung emission by electrons. 75, 1201–1219.
- Sherry, W.M., Vander Sande, J.B., 1977. A background correction for energy dispersive X-ray analysis of thin sections. X-ray Spectrom. 6, 154–160.
- Shivaramu, 1990. Modified Kramer's law for Bremsstrahlung produced by complete beta particle absorption in thick targets and compounds. J. Appl. Phys. 68 (1), 1225–1228.

- Smith, D.G.W., Reed, S.J.B., 1981. The calculation of background in wavelength dispersive in electron microprobe analysis. *X-ray Spectrom.* 10, 198–202.
- Sokolnikoff, I.S., Redheffer, R.M., 1958. *Mathematics of Physics and Modern Engineering*, McGraw-Hill, Newyork, p. 699.
- Statham, P.J., 1976. The generation absorption and anisotropy of thick target Bremsstrahlung and implications for quantitative energy dispersive analysis. *X-ray Spectrom.* 5, 154–168.
- Statham, P.J., 1979. *Mikrochim. Acta* 8 (Suppl.) 229–242.
- Seltzer, S.M., Berger, M.J., 1986. Bremsstrahlung energy spectra from electrons with kinetic energy 1 keV–10 GeV incident on screened nuclei and orbital electrons of neutral atoms with $Z = 1–100$. *At. Data Nucl. Data Tables* 35, 345–418.
- Tseng, H.K., Pratt, R.H., Lee, C.M., Kissel, L., MacCallum, C., Riley, M., 1977. *At. Data Nucl. Data Tables* 20, 175–209.
- Vander Wood, T.B., Pearson, J.G., Buseck, P.R., 1983. *Proceedings of Annual Conference—Microbeam Analysis Society* 18, 85–88.
- Ware, N.G., Reed, S.J.B., 1973. Background corrections for quantitative electron microprobe analysis using a lithium drifted silicon X-ray detector. *J. Phys. E* 6, 286–288.