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# Analytical model for the bremsstrahlung spectrum in the 0.25–20 keV photon energy range

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**Abstract**

A model for the bremsstrahlung spectrum is presented in order to cover photon energies below 1.5 keV, since no reliable description for this energy range allows one to take advantage of the information generated by ultra-thin window Si(Li) detectors. Starting from Kramers formula and assessing a large set of experimental spectra, an analytical expression was fitted as a function of atomic number, incidence energy and photon energy. The expression obtained describes properly the bremsstrahlung spectrum for photon energies ranging from 0.25 to 20 keV and atomic numbers between 4 and 83, at beam energies ranging from 5 to 38 keV. Finally, the proposed model is compared to different expressions for the continuum available in the literature.


*Keywords:* Bremsstrahlung; Electron probe microanalysis; Low photon energies; Ultra-thin window detector

## 1. Introduction

In electron probe microanalysis (EPMA), the characteristic X-ray spectrum is superimposed on a continuum spectrum originating from bremsstrahlung due to the deceleration of electrons within the sample. The dependence of the bremsstrahlung spectrum on sample composition and the experimental conditions was approximately predicted by Kramers in 1923 [1]; since then, different attempts have been made to improve that description [2–6].

In previous work [7], an analytical expression was derived by fitting 52 experimental spectra and taking Kramers formula as the starting point, the resulting model describing adequately bremsstrahlung spectra for photon energies greater than 1.5 keV. The need of extending the prediction to lower energies arises from the increasing availability of windowless detectors, which allow the detection of lower energy peaks (down to boron Kα line). Particularly, a good description for bremsstrahlung at low energies is of great interest for the application of quantification algorithms based on peak-to-background ratios [8].

As a different alternative a method of parameter optimisation in EPMA has recently been developed by minimising the quadratic differences between the experimental spectrum and an analytical expression [9]. In order to use this method for any of its several applications (standardless quantitation, detector characterisation, optimisation of atomic parameters, etc.), it is necessary to rely on a proper prediction for the continuum spectrum.

## 2. Experimental

The expression for the bremsstrahlung spectrum presented in this work was obtained by fitting a set of 82 experimental spectra measured with different instruments from standard samples irradiated at different incidence energies. In all cases, the take-off angle was 40° and the spectra were registered with Si(Li) detectors attached to energy dispersive systems. One of them is a conventional detector, with a beryllium window with a gold contact, whilst the other one has an ultra-thin

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Table 1
Spectra used to fit the function for bremsstrahlung (Fitting) and to validate the obtained expression (Checking)

| Number of spectra | Equipment | $Z$ range | $E_o$ range (keV) | Used for |
|---|---|---|---|---|
| 6 | JSM-840 (SEM) | 6.129 | 5.2–30 | Fitting + Checking |
| 49 | JEOL-JXA 733 | 12–83 | 10–38 | Fitting + Checking |
| 27 | JEOL-JXA 733 Ultra-thin window detector | 10.645–76 | 5–30 | Fitting + Checking |
| 6 | JEOL-JXA 733 Ultra-thin window detector | 4–47 | 9.7–20 | Checking |
| 18 | JSM-840 (SEM) | 10.41–37.34 | 15–20 | Checking |
| 26 | JEOL-JXA 733 | 14–82 | 13–38 | Checking |

formvar window with an aluminium contact. An additional set of 50 spectra from standard samples was used to evaluate the performance of the obtained function. In Table 1, the most important features of the considered spectra are presented.

## 3. Data processing

According to the analytical expression obtained in previous work [7], when a pure sample with atomic number $Z$ is irradiated with electrons of energy $E_o$, during a live time $t$ with a beam current $i$, the generated bremsstrahlung intensity for photons of energy $E$ is given by:

$$I = \alpha\ i\ t\ g(Z,E_o,E) \tag{1}$$

where $\alpha$ is a factor involving the detection geometry and

$$g(Z,E_o,E) = \sqrt{Z}\frac{E_o - E}{E}\left(-54.86 - 1.072E + 0.2835E_o + 30.4\ln Z + \frac{875}{Z^2 E_o^{0.08}}\right). \tag{2}$$

This expression was now used as a starting point in order to extend the continuum description to lower energies. For this purpose, 27 spectra acquired with an ultra-thin window detector were used, along with 55 spectra measured with conventional detectors (see Table 1). Channels corresponding to peaks (characteristic, escape and due to internal fluorescence) were excluded from each of the 82 spectra used to perform the fitting. For those spectra recorded with the conventional detectors, channels below 1 keV were disregarded, due to their very low efficiencies. With the aim of accurately determining the value of $E_o$, a careful calibration was performed on each spectrum to obtain the Duane-Hunt limit, i.e. the energy value for which the continuum intensity falls to zero.

The mathematical procedure used to obtain the bremsstrahlung involves a least square fitting in the spectral regions free of peaks. This procedure consists of minimising the normalised quadratic differences $\chi^2$ between the proposed function $y'$ and the experimental data $y$, by varying the $P$ parameters to optimise:

$$\chi^2 = \frac{1}{N-P}\sum_{i=1}^{N}\frac{(y_i - y_i')^2}{y_i},$$

where $N$ is the number of the spectral channels involved in the fitting. A numerical algorithm is necessary to achieve the set of parameters which minimises this expression. Among the different possibilities available, the 'downhill simplex' algorithm [10] was chosen, due to its good performance and to the fact that it does not require evaluation of derivatives.

In order to perform the fitting, the right hand side of Eq. (2) was multiplied by a factor $1 + f(Z,E_o,E)$, where the function $f$ rapidly becomes zero for energies above 1.5 keV. Thus, the strategy consisted of seeking a new function, coincident with the old one in the region of intermediate and high energies, and also capable to describe properly the continuum spectrum for lower energies, down to 0.25 keV. Spectra acquired with an ultra-thin window detector were included in the set of spectra to fulfil the second condition (see Table 1). After several attempts, the function $f$ was found to have the following behaviour:

$$f(Z,E_o,E) = (a + bE_o)\frac{Z}{E}, \tag{3}$$

where $a$ and $b$ are parameters to fit.

The last term in Eq. (2) is significant only for low atomic numbers and low energies; in spite of this fact, it did not help to describe adequately this region of the set of data, as observed during the fitting process. Therefore, it was necessary to optimise the exponent of $Z$ in this last term; nevertheless, with a function $f$ such as that given by Eq. (3), the exponent was found to be

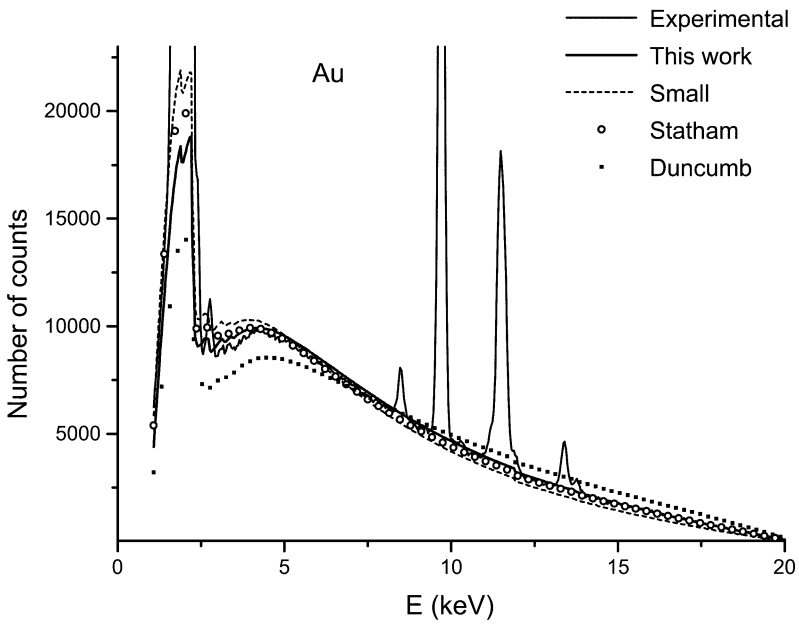


Fig. 1. Measured spectrum from Au at 20 keV. Bremsstrahlung predicted by the models of Small et al. [5], Statham [4], Duncumb et al. [6], and that described in this work are also displayed.

close to unity. In addition, the coefficient for $E_o$ in the third term of Eq. (2) was negligible. Hence, the expression proposed for the generated bremsstrahlung spectrum becomes:

$$g(Z,E_o,E)=\sqrt{Z}\frac{E_o-E}{E}\left(a_1+a_2E+a_3\ln Z+a_4\frac{E_o^{a_5}}{Z}\right)\times\left[1+(a_6+a_7E_o)\frac{Z}{E}\right], \quad (4)$$

where $a_i$ are the parameters to fit. Eq. (4) was corrected for the absorption within the sample, the effect due to the backscattered electrons and detection efficiency [7], in order to fit experimental data. This expression, proposed for pure elements was averaged for multielemental samples taking the atomic fractions as weights:

$$I=\frac{\sum C_i\frac{Z_i}{A_i}I_i}{\sum C_i\frac{Z_i}{A_i}},$$

where $C$ and $A$ denote mass concentration and atomic weight, respectively, and the index $i$ stands for each element composing the sample.

For certain particular spectra, the overall scale factor ($\alpha\ i\ t$) was not properly matched. This effect is due to uncertainties in the beam current and the detection live time. In order to solve this problem, a specific scale factor was fitted for each spectrum. Finally, the analytical expression obtained for the bremsstrahlung spectrum generated within the sample was:

$$g(Z,E_o,E)=\sqrt{Z}\frac{E_o-E}{E}\left(-73.90-1.2446E+36.502\ln Z+\frac{148.5E_o^{0.1293}}{Z}\right)\times\left[1+(-0.006624+0.0002906E_o)\frac{Z}{E}\right], \quad (5)$$

where the overall scale factor must be fitted when beam current, live time or detection solid angle are inaccurately known.

Regarding the uncertainties underlying the characteristic detector thicknesses, a careful analysis of their influence was previously performed for the conventional detector [7]. In the case of the ultra-thin window detector, a test of sensitivity was carried out, allowing concluding that the dead layer and the aluminium contact are much less influential than the formvar thickness. In order, to assess the sensitivity to this parameter, the bremsstrahlung intensity was calculated by means of Eq. (5) in the region ranging from 0.46 to 0.60 keV, corresponding to the O-Kα peak, for a silicon pure sample excited with 10 keV electrons. When the formvar thickness is largely varied by 20%, a difference of only 5% was obtained for the calculated intensity. Therefore, a quite reasonable estimate of the detector

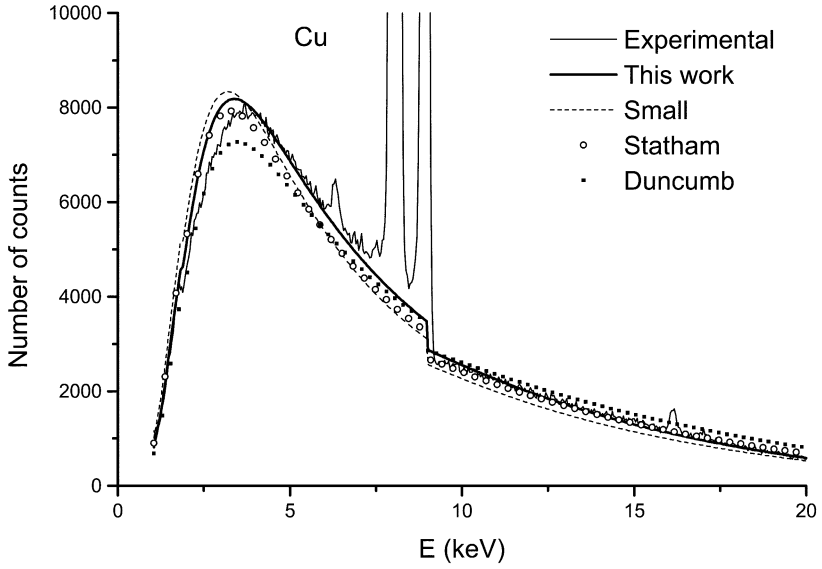


Fig. 2. Measured spectrum from Cu at 30 keV. Bremsstrahlung predicted by the models of Small et al. [5], Statham [4], Duncumb et al. [6], and that described in this work are also displayed.

thicknesses, as the available one, is enough to predict the continuous spectrum adequately.

## 4. Results and discussion

The new expression given in Eq. (5), was assessed with a larger set of data, adding 50 spectra to those used to perform the fitting (see Table 1). The normalised sum of quadratic differences between Eq. (5) and the experimental spectra is $\chi^2=5.9$. Bearing in mind the great heterogeneity of the set of spectra, this value for $\chi^2$ suggests a very good performance to describe experimental data.

The results given by Eq. (5) were compared to those obtained by using other three models available in the literature. The expression given by Statham [4]:

$$g_{\mathrm{St}}(Z,E_o,E)=Z\frac{E_o-E}{E^{1+c}}, \tag{6}$$

with the constant $c$ fitted by the authors only for five elements (Al, Ti, Mn, Cu and Au); the analytical

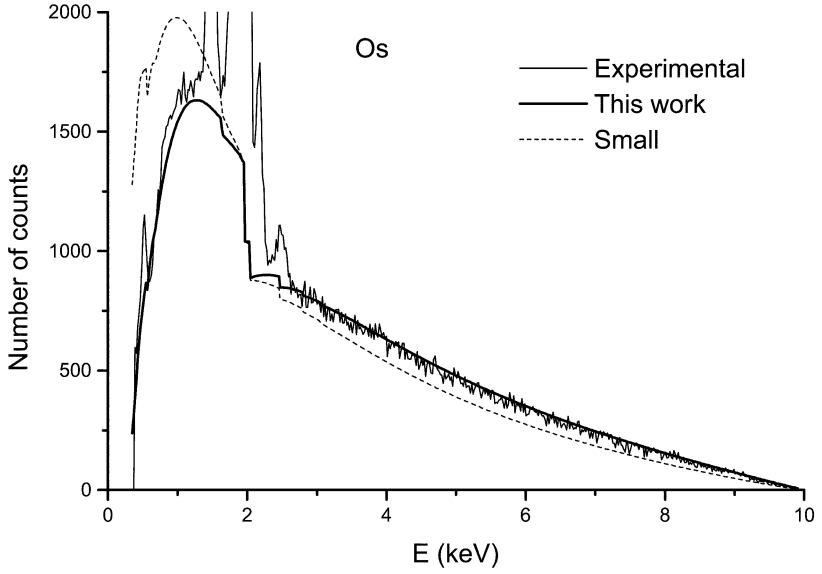


Fig. 3. Measured spectrum from Os at 10 keV. Bremsstrahlung predicted by the model of Small et al. [5] and that described in this work are also displayed.

Table 2
Normalised sum of quadratic differences ($\chi^2$) between experimental bremsstrahlung and prediction given by different models using a set of 132 spectra for the expression proposed in this work and the one given by Small et al. The sets of data used to assess the models given by Statham et al. and Duncumb et al. involve 24 and 7 spectra, respectively

| | This work | Statham [4] | Small et al. [5] | Duncumb et al. [6] |
|---|---|---|---|---|
| $\chi^2$ | 5.9 | 13 | 29 | 73 |

expression given by Small et al. [5]:

$$g_{\mathrm{Sm}}(Z,E_o,E)=\left(Z\frac{E_o-E}{E}\right)^M e^B, \tag{7}$$

with $M=0.00599\ E_o+1.05$ and $B=-0.0322\ E_o$; and a function proposed more recently by Duncumb et al. [6]:

$$g_{\mathrm{Du}}(Z,E_o,E)=F\ Z\left(\frac{E_o-E}{E}\right)^P. \tag{8}$$

The coefficients $F$ and $P$ were assessed only for three elements and four particular $E_o$ values. Parameters $B$, in Eq. (7) and $F$, in Eq. (8) are not important for the present treatment of data, since, as mentioned above, an overall scale factor was fitted to each spectrum, according to the model for bremsstrahlung used.

The correction for backscattered electrons was accounted for by the model given by Statham [11], and absorption was corrected according to Riveros et al. [12], since this model, developed for characteristic radiation, has produced good results also for bremsstrahlung; particularly, the function proposed by Small et al. [5] achieves a better performance with this absorption correction instead of that used originally by the authors [7]. It is worth mentioning that, according to Duncumb et al. [6], the choice for the correction models does 'not appear to be critical to the final result' and for this reason they used simplified methods. The values for $\chi^2$ obtained with the different models assessed are shown in Table 2.

As can be seen, the model presented here achieves the best agreement with the experimental values. It must be borne in mind that among the expressions considered in this paper, only the model given by Small et al. and Eq. (5) correspond to general analytical expressions, while the other two were optimised for particular situations. For this reason, the sets of data used to assess these last two models were reduced to include only the particular cases for which they were implemented by the authors. The poor performance of the model given by Duncumb et al. is probably due to the low statistics in their set of data: the number of counts in the spectra used to obtain Eq. (5) is approximately 10 times larger for silicon, 1.5 or 60 times for copper (depending on the spectrum) and 100 times for gold.

Figs. 1–5 show a comparison between the different models for the bremsstrahlung spectrum considered here and experimental data for different atomic number and incidence energy. The first two plots correspond to spectra acquired with a conventional detector, whilst the remainder three spectra were measured with an ultra-thin window detector. The examples considered show that the analytical function proposed in the present work describes adequately the continuum spectrum for low,

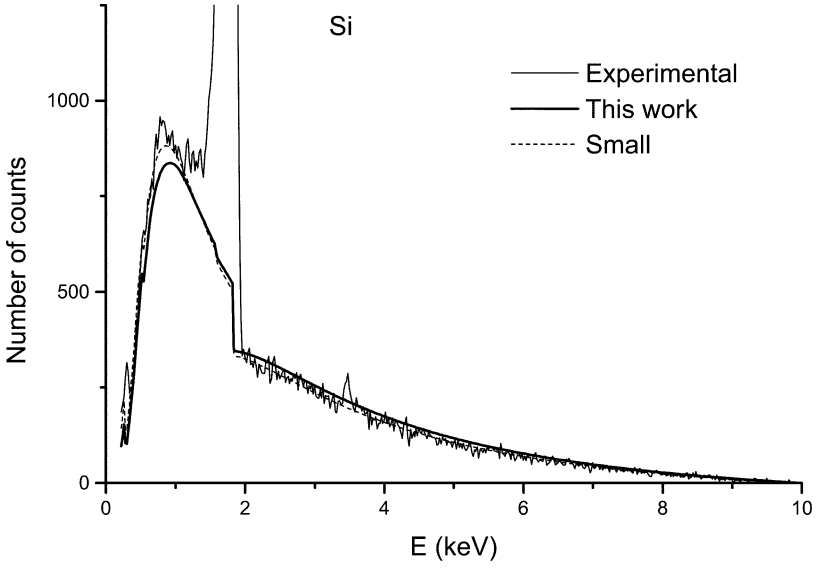


Fig. 4. Measured spectrum from Si at 10 keV. Bremsstrahlung predicted by the model of Small et al. [5] and that described in this work are also displayed.

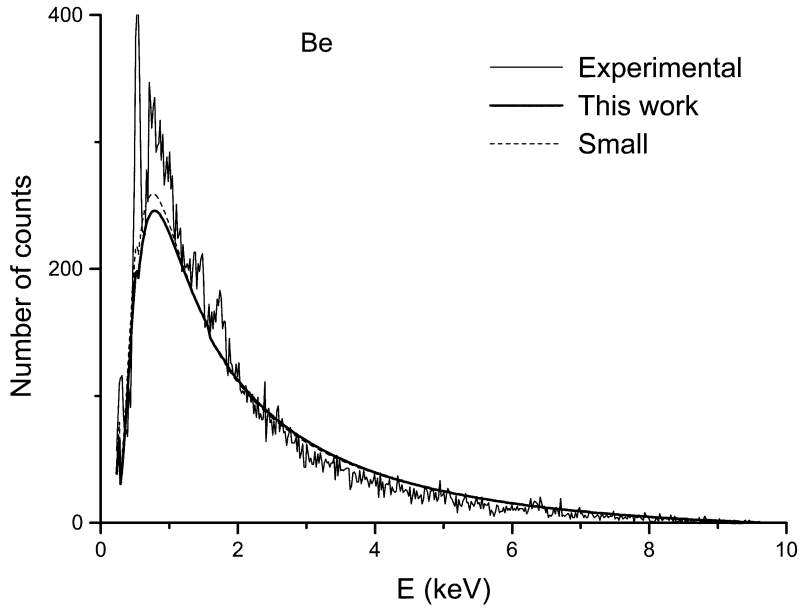


Fig. 5. Measured spectrum from Be at 10 keV. Bremsstrahlung predicted by the model of Small et al. [5] and that described in this work are also displayed.

intermediate and high atomic number; at different over voltages and in the whole photon energy range, down to approximately 0.25 keV (Figs. 3–5). The expression given by Small et al. also predicted bremsstrahlung reasonably well, with the exception of high atomic numbers at the low energy region. The formula proposed by Statham describes bremsstrahlung with a good performance, but is only valid for five elements. Finally, the model given by Duncumb et al. produces just a rough estimation of the continuum, although it was originally implemented for just three specific elements at four particular values for $E_o$.

## 5. Conclusion

The model developed for bremsstrahlung is expressed by a simple analytical function, which adequately describes the experimental data for $4<Z<83$ and $5<E_o<38$ keV. It must be emphasised that the expression proposed here has a good performance in the whole photon energy range of interest in EPMA; particularly at low energies (down to approx. 0.25 keV).

The good prediction achieved for the bremsstrahlung spectrum at the low energy range may become an important tool for the characterisation of environmental atmospheric pollutants, which usually contain low-$Z$ elements (C, N, O, etc.) at high concentrations, as well as intermediate-and high-$Z$ elements. Work is being done to implement the expression obtained here in reliable low-$Z$ matrix quantification by means of a peak-to-background algorithm.

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