

## SD-WDS Second Order Bremsstrahlung and Peak to Background Ratios

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With the advent of the wavelength dispersive spectrometer WDS detecting X-rays with an incorporated high resolution silicon drift detector (SDD), referred to as SD-WDS [1-3], it is now possible to simultaneously measure the bremsstrahlung at the peak intensity by measuring the second order diffraction peak and applying an algorithm to calculate the equivalent background under the first order peak. This calculation is not necessarily available for every element in the spectrometer, but can be used along with the EDS background to calculate, reasonably accurately, the background under the peak. One of the biggest time consuming measures when using the WDS, is measuring the backgrounds by moving the spectrometers to both sides of the WDS peak. For trace elements this means at least double the collection time of the peak count. This talk discusses where a calculated background is possible and how it can be achieved. The SD-WDS spectra are taken from four different SD-WDS spectrometers using the crystals LIF, PET, TAP and STE at 20keV on a carbon coated Cu sample.

If the peak to background ratio (P/B) is high enough, there is little need to measure the background for analysis (SD-WDS improves all P/B ratios). For example, if the P/B is 1000 then, if the peak is 10,000cps and the analysis is for 100sec, then the background is close to 1,000. The one standard deviation error in measuring the peak is the same as ignoring the background, i.e. 0.1%. If we estimate the background and get it wrong by 10% then the bias error is 0.01%. This approximation can work down to the level of accuracy required, where it can be determined if it is necessary to perform background measurements for an element. Once the peak is below this level, the background can be determined by the bremsstrahlung function. Historically this function has been represented by Kramer (1923) as [4]:

$$Nc(E) = aZ(E_0 - E)/E \quad \text{Equation 1}$$

Where,  $Nc(E)$  is the intensity in photons per second per unit energy per incident electron,  $a$  is a constant,  $Z$  is atomic number,  $E_0$  is the initial energy of the electron and  $E$  is the energy of the excited photon. There are other more accurate modifications to Kramer's equation [4], but for simplicity equation 1 is suitable for energies above 2 keV. In this case, bremsstrahlung is dominated by the term  $(E_0 - E)/E$  with all other terms constant for any given sample. In this copper sample, the ratio that should be seen at a particular wavelength, in this case Cu background (Fig 1) is a ratio of 6.1 (Fig 2). Since the actual ratio is 29 (Fig 3), then the efficiency ( $\epsilon$ ) of second order reflection for LIF at Cu is  $29/6.1$  or  $\epsilon = 4.8$ . For PET at Mn, the ratio is  $62.1/3.41$  or  $\epsilon = 18.2$ . For TAP at Si, the ratio is  $39.25/\sim 1$  or  $\epsilon \sim 39$ . For Carbon the continuum seen at the second order is much higher due to lower absorption in the sample. The sample surface also contains carbon from the coating and contamination. Even with this, the combined ratio is  $< 10$ , making the STE crystal the best possibility to measure continuum.

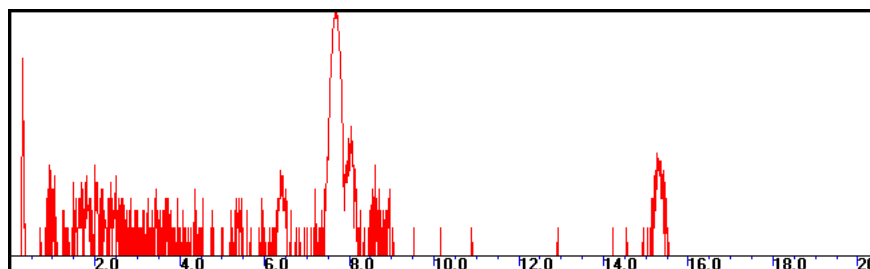
The following is a list of conditions for which the second order bremsstrahlung can be used for first order background determination from the SD-WDS spectrum: 1) The SD-WDS first order can only be used up to the wavelength representing  $E_0/2$ , because the second order line needs to be well below  $E_0$  to

have any statistical significance. 2) There cannot be an element line present at this energy. 3) If the primary diffraction line is too intense, pulse pile up of the primary peak needs to be taken into account, making the calculation difficult. 4) The second order reflection is much less than the primary reflection, especially for energies above 2 keV, due to equation 1 and shown by Fig 2, making them statistically too poor to use on their own. The use of more than one spectrometer to calculate the background can improve this. Using all information to calculate the density of the material and using an algorithm for bremsstrahlung, is the best option. Simple calculations can be utilised by ratioing the measured background to the second order peaks and then applying this ratio.

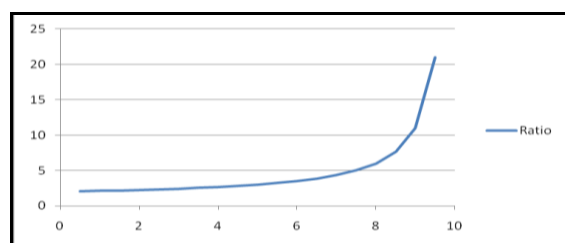
When performing SD-WDS X-ray maps at low concentration levels, it is very important to apply some form of background correction. Currently the images after applying background correction, although more correct, do not look much different to the uncorrected ones. Where it becomes important is when quantifying these maps. Correcting for background removes the background error.

## References

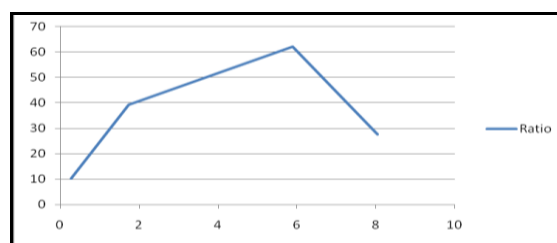
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**Figure 1.** Log scale of EDS spectrum measured at high angle background, showing bremsstrahlung from first and second order diffractions on a sample of Cu.



**Figure 2.** Theoretical ratio of the first order to the second order line versus first order energy calculated from Kramer [4]. The lower this ratio, the more likely that it can be used for calculating bremsstrahlung. Below 2 keV, this ratio drops below 1 due to sample absorption.



**Figure 3.** Actual ratio of the first order to the second order line versus first order energy calculated from Cu, Mn, Si and C on LIF, PET, TAP and STE, respectively. The lower this ratio, the more likely it can be used for calculating bremsstrahlung.