

Methodology for the Quantification of Hyperspectral Cathodoluminescence

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Recent advances in hardware and software associated with cathodoluminescence (CL) detection have resulted in better system stability, faster data collection, improved sensitivities, spectra analysis and hyperspectral data collection¹. The recent development of a luminescence database has provided the means for identification of intrinsic and extrinsic peaks². Using the identified peaks spectra can be analysed for both major and minor peaks more rigorously, leading to improved CL spectra fitting, resulting in more accurate speciation. With independent measurement of elemental abundances using, for example x-rays or laser induced inductively coupled mass spectrometry, the CL fitted peaks can be calibrated which allows for the quantification of hyper-spectral cathodoluminescence datasets.

However, in order to be quantitative we need to be assured that the CL spectra will behave with a linear response. To determine the maximum beam-power-density (BPD) to which the cathodoluminescence generation process has a linear response, we collect a series of spectra, from the material being investigated, over the same region with increasing BPD levels until the onset of non-linear CL response is observed. Based upon these tests we select a conservative maximum BPD for collection.

To determine the optimum peak fitting parameters we have developed software, OpticalFit, to deconvolute a user definable number of Guassian and Lorentzian peaks. The software allows input of the peak position and width, in eV then performs a non-linear least squares fit on the spectra. Figure 1 shows baddeleyite, ZrO₂, spectra with three Guassian peaks fitting the spectra. A goodness of fit is shown by the residual plot. The peak intensity and full-width-half-maximum information is recorded in a table. To assist in the identification of peaks, the luminescence database includes spectra of some of the more common materials which can be downloaded and viewed using OpticalFit. This software is available from www.csiro.au/luminescence.

The scope of the CL database will grow with contributions from groups working in different research areas. Spectral response characteristics differ greatly between collection systems and this needs to be standardised, where possible, and fully documented so that contributions can be reproduced by other instrumentation. A range of standards for measuring CL detector wavelength calibration, spectral resolution and detector collector efficiency all need to be developed so that spectra collected on differing systems can be compared and spectra within a database can be documented. For example, a standard such as a ruby ball* (Al₂O₃) which contains Cr³⁺ is excellent for determining the spectral response of a detector in the 700 nm region, due to the doublet at 692 nm and 694 nm. Possible standards for measuring spectral response in the 550 nm and 370 nm region are Y₃Al₅O₁₂ (Ce) and YAlO₃ (Ce)**. Their associated spectral responses are given in Figure 2. These standards can be readily produced with similar doping levels and used routinely to check the performance of a detector.

