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Background Modelling for Quantitative Analysis in Vibrational EELS

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Vibrational peaks in electron energy loss spectroscopy (EELS) are typically located on a rapidly falling background, arising from both the tail of the zero-loss peak, and non-characteristic phonon losses. The signal-to-background ratio is often quite small (~10–20%), which makes accurate background modelling and peak fitting essential for revealing subtle differences in characteristic peak shapes and intensities.

Here, we evaluate the effectiveness of different functions for background modelling for vibrational EELS. Background models tested include the exponential, and power-law functions, which have traditionally been used for background subtraction in EELS [1]. We hypothesized that functions used to model spectral peaks might be effective background models, and we therefore also tested the pseudo-Voigt function (a Gaussian plus Lorentzian), which has previously been used for zero-loss peak removal [2], and the Pearson VII function (essentially a Lorentzian raised to a power) [3]. Vibrational EEL spectra acquired under different experimental conditions, were used to test the background models. Figure 1 shows background fits and background subtracted spectra acquired from silicon [4]. Background fitting windows were placed immediately before, and immediately after the vibrational peaks of interest, and are shown by the blue and green rectangles on the Figures. A reduced χ^2 value was used to evaluate the quality of the background fit within the fitting windows. The pseudo-Voigt, Pearson VII, and power-law fits all produced qualitatively similar background subtracted spectra, with the pseudo-Voigt function yielding the smallest reduced χ^2 value, and hence the best fit quality. Figure 2 shows background fits and background subtracted spectra acquired from samples of SiO_2 [4] and graphitic carbon nitride [5]. In these examples, obtaining a high quality fit is challenging, because the region of interpolation between the fitting windows is relatively large, and the width of the zero-loss peak is a factor of ~2 greater than for the data in Figure 1, resulting in a steeper background. Again, the pseudo-Voigt, Pearson VII, and power-law fits all produced qualitatively similar background subtracted spectra, with the pseudo-Voigt function yielding the best fit quality.

These results are encouraging, and suggest that the pseudo-Voigt function in particular may be more suitable for background modelling and quantitative analysis in vibrational EELS than traditional functions such as the power-law. Future efforts will focus on evaluating the performance of these functions on more complex experimental spectra, for example at interfaces between different materials.

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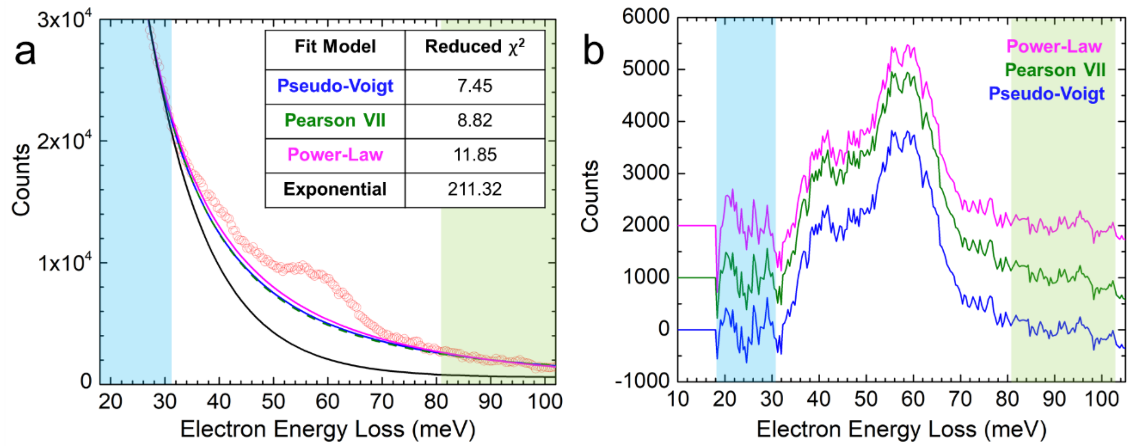

Figure 1. **a** Vibrational EEL spectrum acquired from silicon (red circles) with different background fits (colored lines). The table inset shows estimated reduced χ^2 values used to evaluate fit quality. **b** Background subtracted spectra obtained from data in (a) using different background models. The light blue and green rectangles show the positions of the background fitting windows.

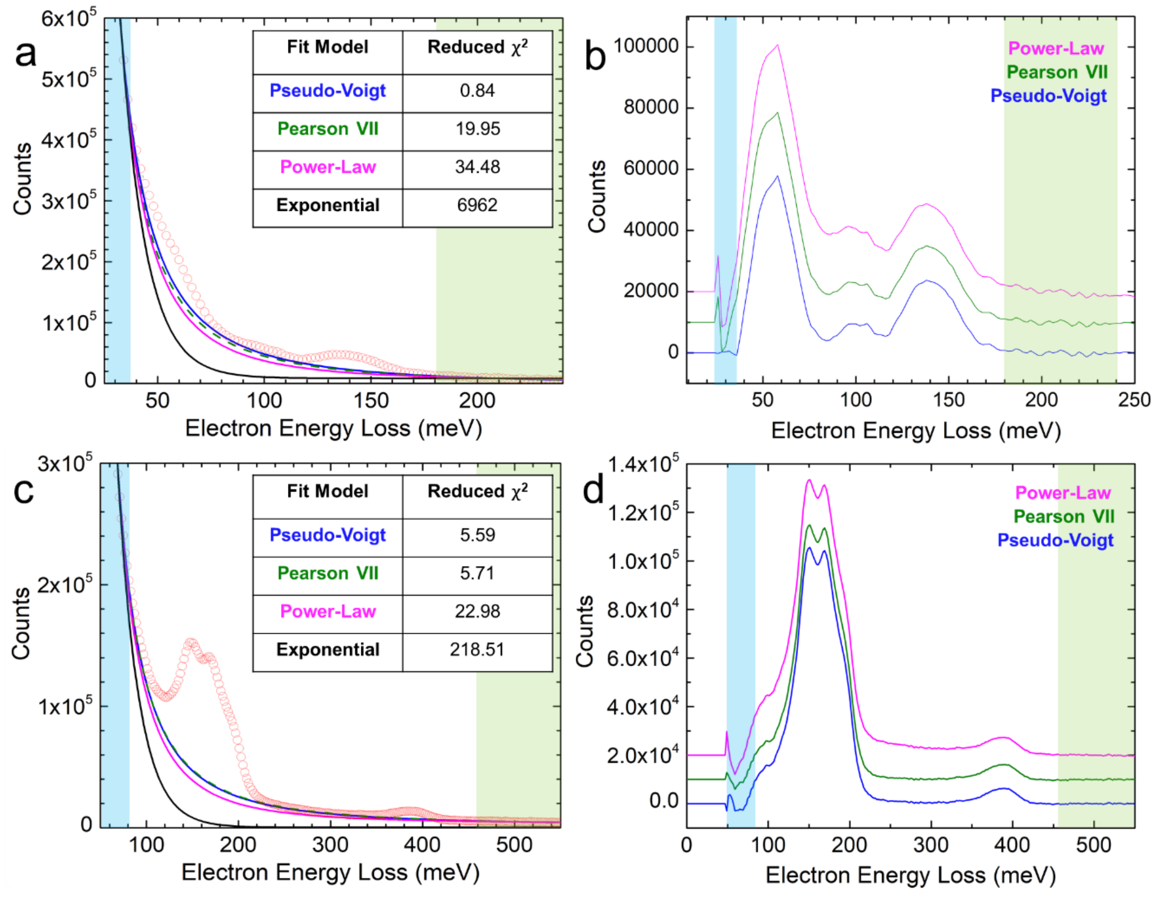

Figure 2. **a** Vibrational EEL spectrum acquired from SiO_2 (red circles) with different background fits (colored lines). **b** Background subtracted spectra obtained from data in (a) using different background models. **c** Vibrational EEL spectrum acquired from graphitic carbon nitride (red circles) with different background fits (colored lines). **d** Background subtracted spectra obtained from data in (c) using different background models. As in Figure 1, the table insets show estimated reduced χ^2 values used to evaluate fit quality, and the light blue and green rectangles show the positions of the background fitting windows.

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