Monte Carlo modelling of the low-loss electron signal in scanning electron microscopy and comparison with the BSE signal

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Abstract. Nanotechnology places increasing demands on techniques for sample characterisation on the sub-100 nm length scale, and the low-loss electron (LLE) signal may provide one possible way of addressing this need. Simulations of the LLE signal from a line-scan across a semiconductor superlattice structure have been performed using two different Monte Carlo models in order to assess their effectiveness in predicting spatial resolution for compositional imaging. Additionally, experimental measurements of LLE data using a detector added to a scanning electron microscope were made to investigate compositional contrast.

1. Introduction

The growth of nanotechnology in recent years has placed increasing demands on the techniques for the characterization of nanostructures in both a scientific and industrial context. The latter, in particular, often imposes the additional requirement that the technique should be both non-destructive and have a reasonable turn-around time. An area which still poses challenges is the compositional analysis of nanostructures, i.e. providing compositional information from features on a sub-100 nm length scale.

Scanning electron microscopy (SEM) provides fast turn-around and a sub-100 nm probe is easily formed. Imaging using the secondary-electron (SE) signal provides high-resolution topographic imaging but whilst the SE signal is affected by sample composition, the SE contrast mechanism is complex and may be influenced by factors which are not easily controlled. Traditionally, X-ray microanalysis has been used for compositional analysis in the SEM, however the large interaction volume for X-ray generation makes its application to nanostructured samples at best challenging.

The backscattered electron (BSE) signal carries Z-contrast information, however this signal originates from a volume of similar size to that associated with the X-ray signal; thus the spatial resolution of the compositional information available from the BSE signal must be questioned. The low-loss electron (LLE) signal is that part of the BSE signal in which the electrons have lost no more than a certain energy, $E_{\text{loss}}$, during their passage through the sample, i.e. they leave the sample with energies from the primary beam energy $E_P$ to $E_P - E_{\text{loss}}$, as shown in Fig. 1. The volume from which the LLE signal originates is restricted by virtue of this limit placed on the maximum energy loss. The original experimental work on the LLE signal by Wells [1] concentrated on improving the imaging resolution of the BSE signal; subsequent work has examined the dependence of the LLE yield on composition of bulk specimens under ultra-high vacuum [2,3] and high-vacuum [4] conditions.
provide useful information on nanoscale sample composition, it is important to be able to reliably model the LLE signal. In this paper we discuss the effectiveness of Monte Carlo methods for modelling the spatial resolution attainable using the LLE signal for compositional imaging. We further examine compositional contrast in the LLE signal using experimental data from a high-resolution field-emission gun SEM (FEGSEM).

2. Experiment & simulation

Experimental measurement of LLE images were made in an FEI Sirion XL30 FEGSEM (operated at $E_p = 5$ keV) which had been modified by the installation of a detector for recording the LLE signal. This detector was developed based on an existing design [2] and its energy-filtering action was based on the retarding-field principle. When the detector was operated with the loss energy set to $E_{\text{loss}}$, the recorded signal corresponded to those electrons within the shaded region of the spectrum shown in Fig. 1. The specimen used in this study was a Si/Si$_{0.85}$Ge$_{0.15}$ semiconductor superlattice structure which had been cleaved in order to permit its observation in cross-section in the SEM. A schematic indicating the form of this sample is shown in Fig. 2; the sample consisted of 12 alloy layers.

Monte Carlo simulations of the LLE and BSE yield were carried out using two different publicly-available codes. The NISTMonte2 code [5] used Mott cross-sections [6] and treated inelastic losses via the continuous slowing-down approximation (CSDA) using the Joy & Luo expression [7] for the stopping power. This approach neglected the effect of energy straggling. The other code used was PENELLOPE2006 [8] which similarly used partial-wave cross-sections [9] for $\sigma_{\text{el}}$ but in contrast implemented a discrete-loss model for inelastic scattering. To reduce computational demands the simulated signal was collected from a $2\pi$ solid angle. The aim of using these two different codes was to establish the significance of energy straggling on the LLE signal.

3. Results and discussion

3.1. Monte Carlo simulation of spatial resolution

In order to establish reliable figures for the periodicity and thickness, $d_1$, of the Si$_{0.15}$Ge$_{0.85}$ alloy layers in the sample, a thinned section cut from the superlattice wafer was examined in a transmission electron microscope (TEM). Analysis of the resulting TEM image resulted in a figure of $69.2 \pm 0.2$ nm for the periodicity and $d_1 = 11.5 \pm 0.4$ nm for the alloy layer thickness. These data were used to construct the geometrical models used in the Monte Carlo simulations. After checking for the influence of edge effects, simulations were run for line-scans across a single period of the superlattice structure, for reasons of computational efficiency.

Line-scans generated using the CSDA-based NISTMonte code are shown in Fig. 3. Qualitatively, improved spatial resolution can be seen in the LLE signal compared to the BSE signal and resolution improves further as $E_{\text{loss}}$ is decreased. At $E_{\text{loss}} \leq 250$ eV the LLE signal reproduces the composition profile quite closely. Line-scans from the PENELLOPE code which uses a discrete-loss inelastic model
are shown in Fig. 4. The resolution follows a similar trend to the CSDA case, however using this model the composition profile would appear to be not faithfully reproduced until $E_{\text{loss}} \leq 100$ eV.

To make a quantitative comparison of the resolution predicted by the two approaches, measures of resolution $d_P$ were used which measured the distance in $x$ over which the signal rose from $P\%$ to $(100 - P)\%$ of $\Delta I$ above $I_{\text{min}}$ where $\Delta I = I_{\text{max}} - I_{\text{min}}$. Here $I_{\text{max}}$ and $I_{\text{min}}$ are the minimum and maximum signal respectively. Two specific cases of this resolution measure were used, namely $d_{25}$ and $d_{10}$.

The variation of spatial resolution with $E_{\text{loss}}$ using the two different metrics is shown in Fig. 5. A decrease in resolution with increasing $E_{\text{loss}}$ is observed, with the discrete-loss model showing a generally poorer resolution than the CSDA results, indicating that in reality, energy resolution is degraded relative to that predicted by a CSDA-based simulation. The influence of $E_{\text{loss}}$ on the spatial resolution is also much weaker in the case of $d_{25}$ than in the case of $d_{10}$. For compositional imaging, it is important that the resolution is such that the measured signal reflects the composition profile of the sample, rather than simply being sufficient that two closely-spaced features are resolved. For this reason, $d_{10}$ is a more relevant measure of resolution for the purpose of compositional imaging and the strong variation of $d_{10}$ with $E_{\text{loss}}$ indicates the significance of the latter in this imaging mode.

It can also be seen from Fig. 5 that $d_{10}$ shows the greatest differences between the CSDA-based and discrete-loss simulations of the resolution, suggesting that energy-straggling is an important effect in compositional imaging. The greatest differences in the values of $d_{10}$ are actually found at around 250 eV loss, indicating that the effect is most significant in the low-loss regime. Presumably the influence of energy straggling has a lesser effect in the BSE signal since the electrons contributing to this signal have undergone a significant number of discrete loss processes.

Figure 3. Simulated line-scans across the cross-sectioned superlattice sample generated by the NISTMonte code. (a) BSE signal; (b-d) LLE signal with losses of 500, 250 and 100 eV respectively.

Figure 4. Simulated line-scans across the cross-sectioned superlattice sample generated by the PENELLOPE code. (a) BSE signal; (b-d) LLE signal with losses of 500, 250 and 100 eV respectively.

3.2. Contrast in LLE and BSE imaging

The SEM equipped with the LLE detector described earlier was used to collect a series of images of the superlattice sample at a variety of loss energies $E_{\text{loss}}$. In order to permit their analysis with good signal-to-noise ratio, each of these LLE images was projected onto the $y$-axis to form a line-scan across the superlattice structure. These line-scans were analysed to establish how the contrast between the Si and $\text{Si}_{0.85}\text{Ge}_{0.15}$ layers varied with $E_{\text{loss}}$. The results of this analysis are illustrated in Fig. 6 which shows a consistent increase in the contrast as the loss energy is decreased, corresponding to a reduction of the volume from which the detected signal electrons emerge. This demonstrates that, in
addition to any benefit associated with improved spatial resolution, the LLE signal can be used as a way of increasing compositional contrast compared with the BSE signal when performing compositional imaging on nanostructured materials. Although the data in Fig. 6 suggest that the gains in contrast begin to slow as $E_{\text{loss}}$ drops below 100 eV, the influence of sample contamination on this experimental finding must be taken into account. It is suspected that the extreme surface sensitivity of the LLE signal at $E_{\text{loss}} \leq 100$ eV could reduce the measured contrast in the poor vacuum environment of a conventional SEM to below the maximum theoretically possible.

4. Conclusions
Monte Carlo simulation showed that the LLE image offers greater spatial resolution for compositional imaging than the BSE image, however, energy straggling means that the achievable resolution is always less than that predicted by simulations based on the CSDA. The $d_{10}$ measure of resolution is more suitable than $d_{25}$ for compositional imaging and the former shows greater differences between the resolutions predicted by CSDA-based simulations and those based on a discrete-loss model. Consideration of the $d_{10}$ parameter has shown that the influence of energy-straggling on spatial resolution is particularly significant in the low-loss regime. Although a SEM with a very small probe size is needed to appreciate the resolution improvement offered by the LLE signal, the LLE image also shows increased contrast in comparison to the BSE image when imaging nanostructures.

Acknowledgements
The authors are grateful for the use of the computational facilities of the White Rose Grid. Financial support of the Engineering and Physical Sciences Research Council (EPSRC) is acknowledged.

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