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Bayesian Analysis of Electron Spectroscopic SEM Images

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The novel ultra-low voltage SEM Delta [1,2] allows electron spectroscopic imaging of both secondary (SE) and backscattered (BSE) electrons with a primary energy down to 50eV and a resolution better than 1nm. To recover the true sample spectra, we use Bayesian inference, a tool applying forward simulations. This statistical approach is especially suited to deal with the stochastic nature of the measurement process and provides physically motivated error estimates.

The DELTA consists of complex electron optics: A magnetic beam splitter together with an electrostatic energy filter and the detection chain. To determine local electron spectra and quantitative material composition, especially of surfaces, with high spatial resolution, we need to take into account in particular the complicated energy filter response, and improve its energy resolution numerically. This is not only demanding due to the microscope response but also because shot noise and electron-sample interaction are random processes. As a consequence, to deduce material properties (e.g. spectra and material composition) with high spatial resolution it is important to deal with high signal noise and to estimate the errors. We suggest to apply Bayesian inference and to model the stochastic behavior of the system *purely* in physical terms. After formulating additional previous knowledge about the sample in form of a prior, Monte Carlo sampling [4] allows to obtain the quantitative estimates of the desired properties, including error estimates.

Preliminary results for inferring the SE spectrum of Aluminum (Fig. 1) have been deduced by considering Poisson distributed shot noise, arbitrary random electron-sample interaction - with the restricting assumption that the detected electrons are pairwise statistically uncorrelated - and a preliminary characterization of the detection chain. In order to test the model, the data in fig. 1 has been collected under high signal-to-noise ratio leading to a narrow a-posteriori distribution (not shown). Fig 1 left shows deviations between the measured data (black) and the green line – the median of the distribution of the expectation values of measurements of the Monte Carlo sampled spectra. These systematic deviations indicate that the applied model does not perfectly describe the recorded data.

The ability to deduce quantitative material composition is demonstrated by applying the previously described preliminary model to simulate a spectral signal (recorded for varying grid potential from -10V to 5V in 1V steps) of a mixture of 3 materials. Each material is assumed to have a total SE yield of 0.7. However, their spectra differ by the position of their maximum (1.5eV, 1.75eV, 2eV). Though the energy filter itself has a resolution of about 5 eV, the Bayesian approach can be used to deduce the correct quantitative material composition under high dose. Under low dose the composition may be deduced only with a large error. These error estimates allow opzimizing the data acquisition protocol. The possibility to be quantitative and provide error estimates sets Bayesian inference apart from conventional, intensity-based [5] or qualitative approaches without error analysis [6,7].

We are working on improving our preliminary instrument model by characterization of the electron filter optics, the DELTA beam splitter and the detection chain [8].

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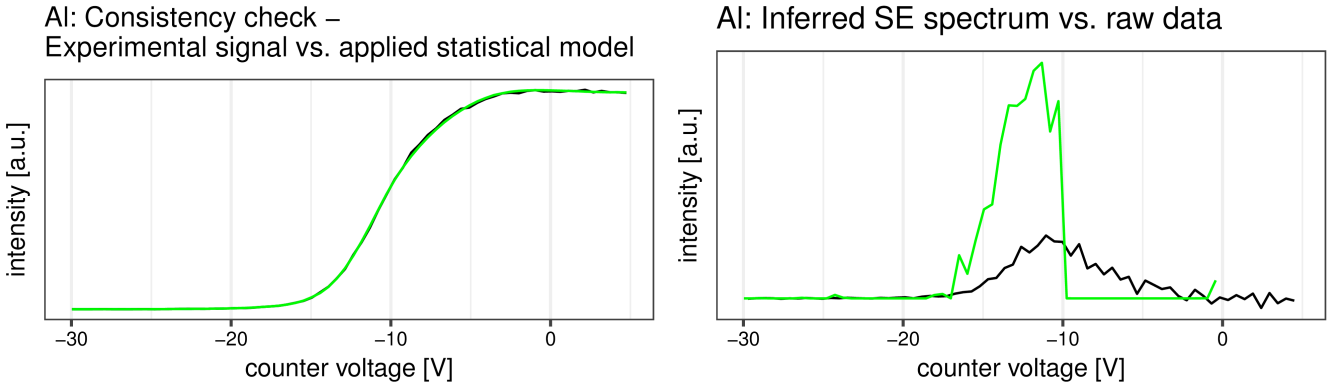

Figure 1. Deduction of Al SE spectra by inversion of microscope response using Bayesian inference and a preliminary statistical model. *Left:* consistency check indicates some problems with the preliminary model (for details cf. third paragraph) *Right:* differentiated raw spectrum (black) and median of a-posteriori distribution of sampled spectra (green)

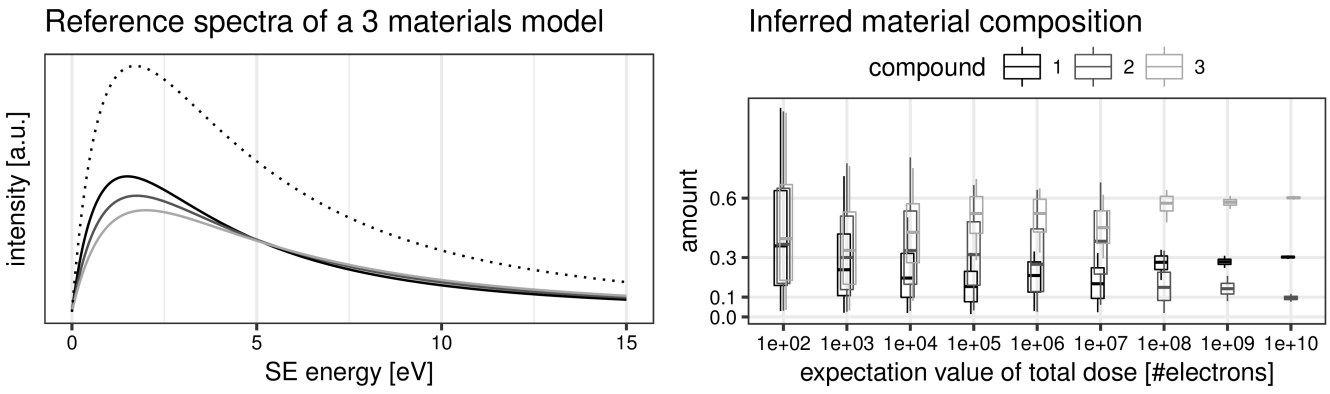

Figure 2. Demonstrating the ability to deduce material composition even under the condition that reference spectra of the corresponding materials are quite similar. Each gray level corresponds to one material. *Left:* solid lines – reference spectra of pure materials, dotted line: simulated spectrum of the mixture; *Right:* inferred material composition, for each total dose we infer the 5%, 25%, 50%, 75% and 95% quantiles of the a-posteriori distribution (ground truth: 30% compound 1, 10% compound 2, 60% compound 3). Note the perfect material decomposition at higher dose.

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