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EFTEM assistant: A tool to understand the limitations of EFTEM

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Abstract

The first version of a free tool for Gatan's Digital Micrograph^{TM} is presented which aims to aid the energy-filtered TEM (EFTEM) community by predicting and correcting the most common sources of degradation. The software allows selection of either Krivanek's or Egerton's approach to account for the spatial resolution degradation caused by the electron optical aberrations. The effects of aberrations and signal 'delocalization' are combined to simulate the blurring caused in EFTEM elemental maps. Two microstructural features with ideal geometry are used to illustrate use of the software: spherical particles and parallel sided interfaces. The software also allows the simulation of the effects of the noise and drift in the final elemental map, independently or in combination. It can be easily demonstrated that when the dimensions of the feature of interest are comparable in scale to the image degradation factors, the effects of the latter should not be neglected. More importantly, the software can deconvolute the effects of the degradation factors, revealing the true dimensions and signal intensity of the feature of interest.
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1. Introduction

Energy filtered TEM (EFTEM) has become a widely used technique in recent years. Modern microscopes are capable of acquiring EF images very easily and more complex acquisitions, such as jump-ratio images, three-window maps and EFTEM series of images, are readily implemented in the image acquisition software. The spatial resolution achieved by recent measurements is approaching the sub-nanometre scale [1], and further consideration of the interpretation of results is needed. When the features of interest have dimensions of the same order of magnitude as the expected image degradation and/or the recorded drift, a good understanding of these effects is needed. In addition, EFTEM images are noisy in nature due to the limited electron collection from core-losses and the extra noise added by the background extrapolation. With the present version of the software, two kinds of features can be simulated: a spherical particle and an interface/layer of given size, mean signal intensity and image noise. The software has been found to be very useful for estimating the real size and composition of particles and interfaces/layers of dimensions comparable to the spatial degradation. It will also be shown that it is possible to estimate the true size of the features and their real signal intensity once the effects of the degradation have been deconvoluted by the software.

Drift is assessed in two different ways: by direct simulation and through correction by deconvolution. Cross-correlation of consecutively recorded images allows the estimation of the magnitude and direction of drift during the acquisition. Using real drift data, the effects of linear drift during acquisition on the shape and signal of the selected feature are simulated for each image. The resultant images are cross-correlated and integrated to simulate the global effect of drift in the EFTEM elemental

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map. Deconvolution includes the possibility of restoring images that have been acquired under severe drift conditions.

All the above-mentioned facilities are presented in an easy-to-use script for Gatan's digital micrograph^{TM} (DM) with a graphics user interface (GUI).

2. Software description

The "EFTEM assistant" (EA) software has been written as a script for Gatan's DM^{TM} 3.8.1 and will be made freely available through the DM Script Database from the Graz University of Technology [2]. DM is by far the most commonly used EELS acquisition and analysis software platform interfaced to modern transmission electron microscopes (TEMs). "EA" has a GUI which appears in the form of an extra window in DM, which can be used in conjunction with other routines or acquisitions. The main EA window is divided into five tabs: "Experimental", "Predict", "Errors", "Correct" and "Drift" each of which is described in the following sections. Only the "Experimental" tab will be described in detail, as it contains all the information about the acquisition and feature of interest.

The "Experimental" tab, shown in Fig. 1, is used to input data for the experimental conditions used for the EFTEM acquisition: energy of electron beam (E_o), energy loss (E_{loss}), collection semiangle (Beta), chromatic aberration coefficient (C_c) and spherical aberration coefficient (C_s). These data are used to estimate the image blurring by following three approaches reported in the literature, by Krivanek [3], and by Egerton for both thin and thick samples [4–6]. The blurring is represented as the diameter of the simulated blurred disc image of an ideal point object.

Since Egerton's approach describes the point spread function (PSF) as a Lorentzian, the user is required to select the percentage of electrons (% electrons) for calculating the total blurring diameter. Thus, a selected percentage value of "50" means that blurring diameter returned by the calculation is the diameter within which lies only 50% of the total electron intensity. An analytical expression has been derived for calculating these values from the different PSFs as a function of chromatic aberration, spherical aberration and diffraction by the objective aperture. This has considerably minimized the computational time and enables realistic times for multiple calculations. For all the three approaches, individual contributions from the spherical and chromatic aberration, diffraction by the objective aperture and delocalization from the inelastic interaction of the electrons with the nuclei [3,7] are calculated and added in quadrature. Any of the parameters can be changed and the effect of any change is reflected automatically in the three blurring values displayed in the window.

In the "Sample info" section, the data used for generating the artificial EFTEM maps can be input. The current version of the software can simulate the signal from two microstructural features: totally embedded spherical objects (precipitates, bubbles, etc.) and parallel sided, planar layers (grain boundary segregation, multilayered samples, etc.). The information requested is: the diameter of the sphere or the interface width, the intensity of the signal in the surrounding area (B), the intensity of the signal coming from the feature in the elemental map (I) and the standard deviation of the signal (σ) or "noise amplitude" (see Fig. 2). In the case of a totally embedded spherical object, the signal is defined as the difference between the matrix and the feature intensity. This intensity can be negative if the elemental map reveals it as a depletion in the signal (e.g. when the feature does not contain one of the main elements of the matrix). The signal intensity and the noise amplitude inputs are used to calculate the signal to noise ratio (SNR) defined as: SNR = signal intensity/σ. Finally, the software offers the possibility of producing 2D plots using the different approaches, in which the total delocalization is plotted vs. one of the parameters (beta angle (β), energy-slit width

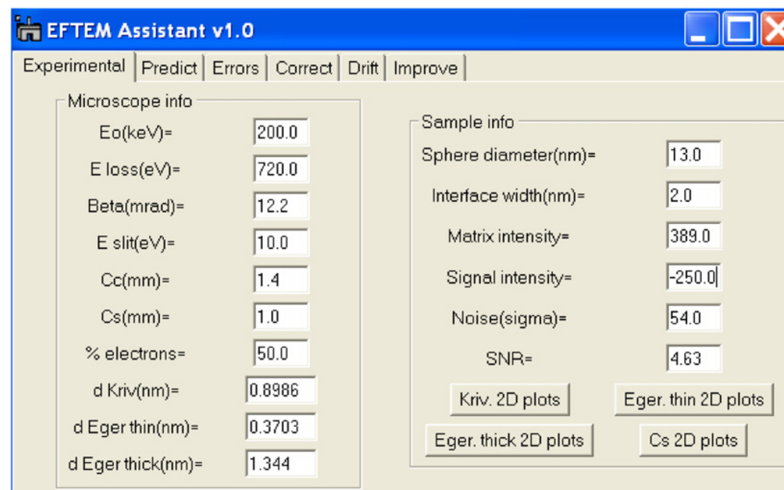

Fig. 1. EFTEM assistant GUI, showing an example of selected acquisition and experimental conditions.

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