EFTEM image calculation based on mutual coherence approach

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The SALVE (Sub-Angstrom Low-Voltage Electron microscope) project [1-2] aims for atomic resolution imaging of low-Z material with minimum radiation damage by employing voltages in the range between 20 and 80kV. In order to understand the image contrast, it is necessary to perform image calculations taking into account elastic and inelastic scattering. The conventional image simulations consider take elastic scattering, which suffices at medium voltages for most objects. However, because at 20kV all atoms are strong scatters [3], we must incorporate the effect of inelastic scattering in the image calculation.

For inelastic scattering, the sample states and the incident wave are coupled [4]. Therefore, we cannot ignore anymore excitations of the object as in the elastic case. Our approach is based on the mixed dynamic form factor and the light-optical concept of mutual coherence [5-7]. However, this procedure still poses a big challenge for the computer since it involves 4D Fourier transforms. Efforts have been made to look for suitable approximations to transform the 4D Fourier transform into 2D Fourier transforms [8-10].

In this work we will present a new approximation and calculated EFTEM images based on it for a voltage as low as 20kV. For mono-atomic layered structures, our approach takes one elastic scattering and one inelastic scattering into account; while it considers multiple elastic scattering and only one inelastic event for multi-layered structures. This approximation holds as long as the object thickness is smaller than the inelastic mean free path length. In accordance with our previous calculations [3], we employed the experimental EELS spectra [3] for the simulation of the EFTEM images. Fig. 1 shows the calculated images of graphene as typical example of a mono-layered structure. Both the zero-loss peak (Fig.1a) and the plasmon peak (Fig.1b) are normalized, which implies that the scale difference does not come from the different signal strength. Fig.1f shows convincingly the effect of inelastic and elastic double scattering at 20kV. However, in order to obtain the same S/N ratio as for the elastic image (Fig.1b), the dose must be 10^6 times higher.

Based on our calculations, we can draw the following conclusions:

1. The smaller the energy loss is, the more delocalized is the inelastic process and the lower is the blurring of the image formed by the doubly (elastically and inelastic) scattered electrons.
2. Energy filtered inelastic images are only visible when C_c is corrected.

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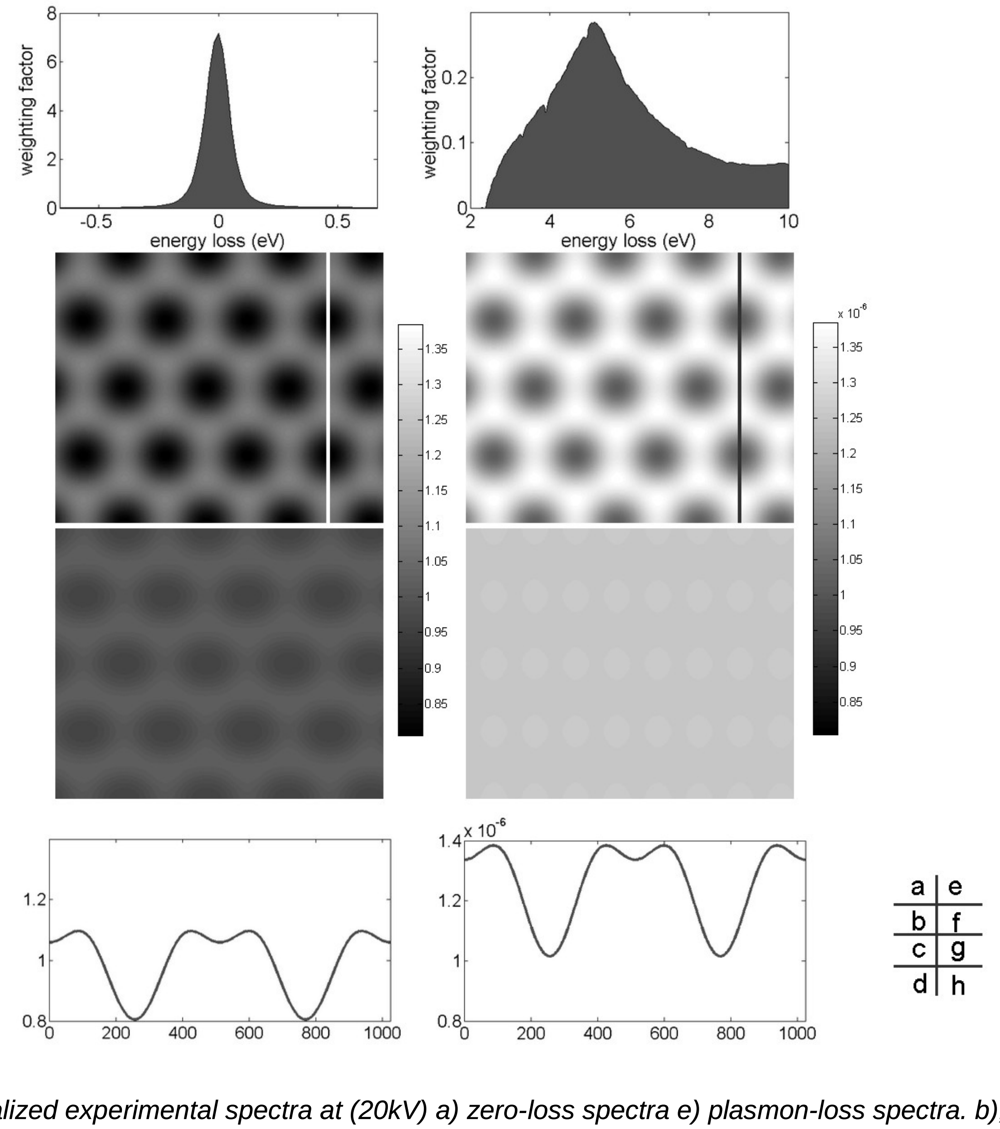

Figure 1. *Normalized experimental spectra at (20kV) a) zero-loss spectra e) plasmon-loss spectra. b),c),f),g) Calculated EFTEM images for graphene at 20kV (atoms are white) with the same geometric aberrations: Cs=-2µm and df=42Å. Zero-loss images with C_c=0 (b) and with C_c=1.26mm (c); plasmon-loss images with C_c=0 (d) and with C_c=1.26mm (g). d), h) Line profiles through the centre of the atoms corresponding to the line in b) resp. in f);.Please note the different scales in b),c) d) and f), g), h).*