Necessity and application of the transmission cross-coefficient for simulation of low-voltage HRTEM images

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The correct interpretation of the experimental high-resolution transmission electron microscopy (HRTEM) image contrast requires quantitative comparison with simulated images. Conventional models for HRTEM image calculation consider only elastic scattering. The interaction between the incident electron wave and the sample is usually modelled by a multi-slice algorithm. The propagation of the outgoing waves is described by a convolution between the waves and the contrast transfer function (CTF), which includes the geometric aberrations, and envelope functions in order to account for the finite lateral and temporal coherence of the source as well as instabilities of the microscope [1]. However, the convolution of the scattered electron wave with the envelope function is only applicable for weak phase objects. In this case the non-scattered part of the electron wave dominates the scattered part. As a result, interferences between the diffracted partial waves can be neglected. This assumption holds true for most thin low-*Z* materials imaged at accelerating voltages above 200kV. However, for low accelerating voltages in the range between 20-80kV as applied in the SALVE (Sub-Angstrom Low-Voltage Electron microscopy) instrument [2], the conventional envelope function procedure is not applicable. Instead, a consistent image- simulation procedure must be employed which accounts for the interference between all constituent waves. Such a procedure based on the incorporation of the transmission cross-coefficient (TCC) has been established [3].

In our work, the range of validity of the envelope-function method has been explored for both the Cs-corrected (at 80kV) and the Cc/Cs-corrected microscope (40kV and 80kV). The envelope function method has been compared with the precise model using the TCC procedure and with the experiments on $MoTe_2$. As shown in Fig. 1, the images calculated with the TCC model match with the experiments and the images calculated with the conventional model using envelope functions show lower contrast than the experimental images.

The results of our calculation show that the discrepancy between the simulated images employing (a) the envelope-function model and (b) the TTC model increases with decreasing accelerating voltage, increasing thickness of the sample, and increasing atomic number *Z*. To summarize: The conventional image model using the envelope function fails at the accelerating voltage of 80kV already for a monolayer of $MoTe_2$, thus it is necessary to apply the computationally more demanding TCC model.

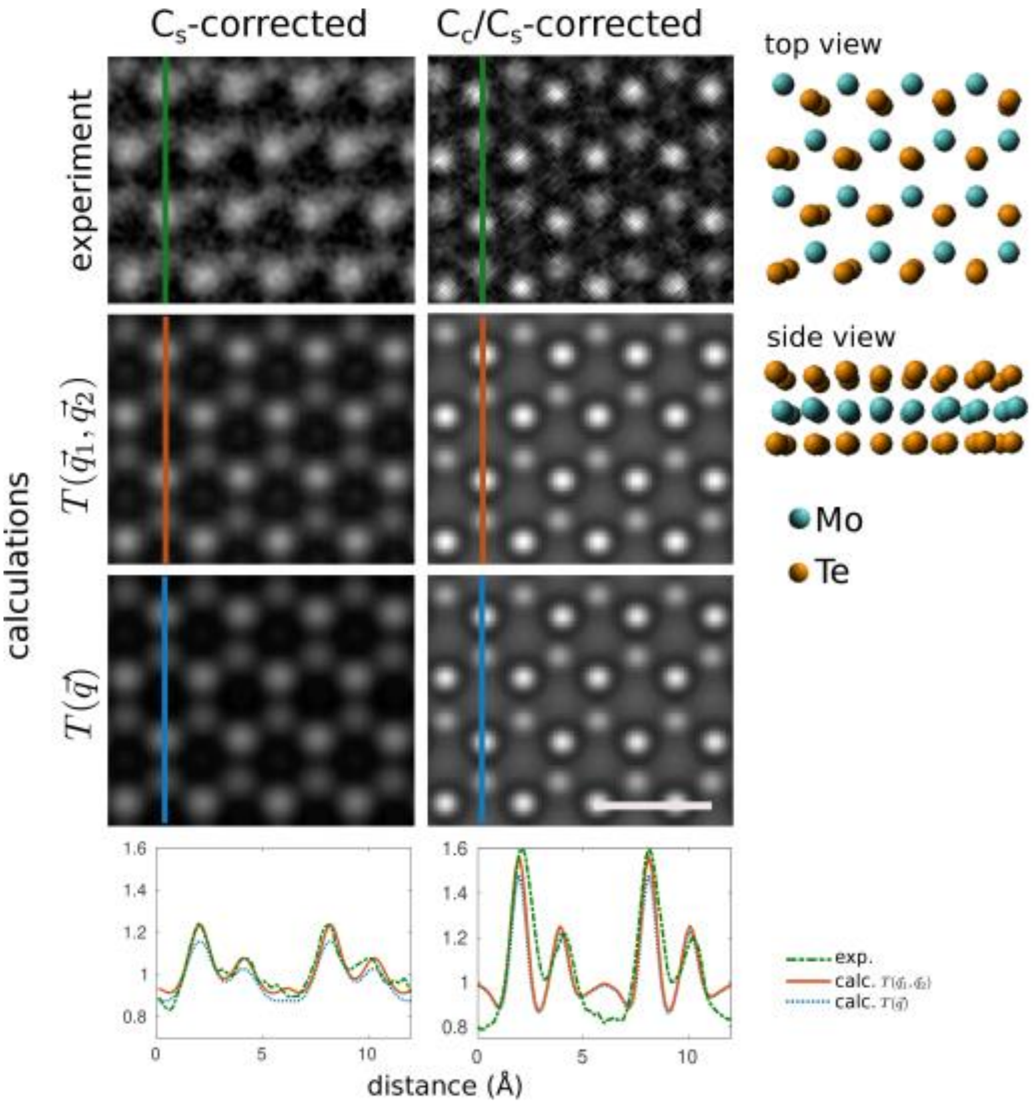

Figure 1: Comparison between experimental and calculated images of $MoTe_2$ at 80kV. The 1st and 2nd columns correspond to the images for the Cs-corrected microscope and the Cc/Cs-corrected microscope, respectively. The last column displays the structure of $MoTe_2$ from two perspectives. The 1st row shows the experimental images. The 2nd and the 3rd rows show the calculated images using the TCC and the conventional transfer function, respectively. All microscope parameters are the same for the calculations in the same column. The last row displays the line profiles marked in the images from the same column. Scale bar: 5Å.

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