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Finding Optimal Imaging Parameters for Measuring Long-Range Electric Fields with 4DSTEM by Utilizing STEM Multislice Simulations

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Built-in nano-scale electric fields are inherent to many of today's electronic devices like solar cells, transistors and batteries, accordingly their quantification is highly desired. Scanning transmission electron microscopy (STEM) combined with fast pixelated detectors (4DSTEM) is a promising means to measure those fields directly [1, 2]. This is the case, because a shift in the center of mass (COM) of the electron diffraction pattern is approximately proportional to the electric field which induces the shift [3].

In experiment, the COM signals of built-in electric fields and the ones of atoms superimpose each other. So, one challenge in measuring long-range built-in electric fields is to determine them from these superimposed signals. Two possible approaches are to either disentangle the two signals during post-processing or to minimize the influence of the atoms during measurement.
Retrieving the fields during post-processing has been done successfully for HR-STEM parameters at high convergence angles [1]. This was done by averaging over suitable regions in real space.
The second approach, i.e. minimizing the influence of atoms already during the measurement, can be achieved by tuning parameters in a way that the probe size is increased intentionally until single atoms cannot be resolved anymore. This results in a real-space averaging already during the measurement. There are several experimental parameters which can be used to achieve this in principle, e.g. lens aberrations, gun brightness, defocus and diffraction limit. Tuning the diffraction limit can be done by using different sizes of apertures and hence is a comparably easy-to-tune parameter.

This study investigates the optimum imaging parameters to measure long-range electric fields with 4DSTEM. In order to investigate this, long-range electric fields are included in STEM multislice simulations [4, 5]. A GaAs p-n junction serves as a first model system, at whose depletion region an electric field is formed due to the different doping levels on both sides [6] (see Figure 1). The built-in field of the p-n junction is included in simulations by adding the corresponding electric potential to the atomic potentials. Since in simulations single parameters can be tuned individually, this is a well-suited approach to investigate the influence of the imaging parameters, e.g. different convergence angles.

Figure 2 shows results of simulation studies for different semi-convergence angles. One clearly sees that with decreasing convergence angle, the influence of atoms gets smaller according to the diffraction limit. However, the long-range electric field which one wants to measure becomes more apparent. Moreover, the shape of the COM-shift gets more and more similar to the shape expected from the electric built-in field which is shown in the right-most image in Figure 2.

This study also includes an investigation on the influence of the choice of angular range within the electron diffraction pattern from which the COM-shift is determined and how this depends on the chosen semi-convergence angle. It is revealed that this is very crucial.

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