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# Measuring electric fields with 4D-STEM: Demonstration of pitfalls by the example of GaN and SiGe

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## Background

The development of fast pixel-based detectors in (scanning) transmission electron microscopy ((S)TEM) has resulted in 4D-STEM becoming almost a standard tool [1]. The computationally simplest analysis of 4D-STEM data is the calculation of the center of mass (COM) of the intensity in the diffraction pattern (the so-called COM or first-moment method) [2]. The COM corresponds to the expectation value of the net momentum transferred to a beam electron during the interaction with the sample. The momentum transfer is caused by a magnetic or electric field [3]. However, it is anything but easy to draw conclusions about an electric field in the sample from a measured COM.

In this contribution, we use the example of AlN/GaN as well as of SiGe/Si to demonstrate effects that influence the measured COM and which may lead to artifacts in the measured electric field. A knowledge of these effects is important for a correct interpretation of the COM measurement [4,5]. We focus primarily on two aims: (i) Deriving the difference of polarization induced fields in GaN and AlN and (ii) measuring the relative mean inner crystal potentials (MIPs) using the electric field at the interface between different materials.

## Methods

The investigations are performed by multislice simulations and by experimental 4D-STEM. In the experimental case, an FEI/Thermo Fisher Titan 80/300 and a Thermo Fisher Spectra 300 were used.

## Results

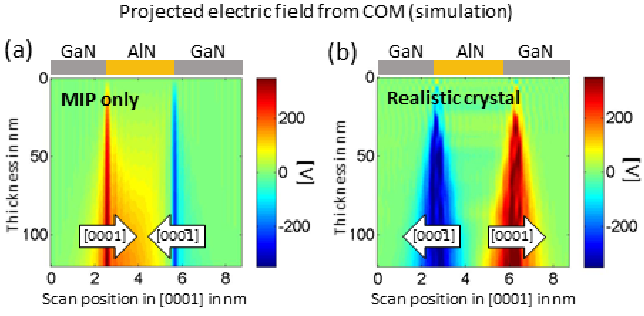
Figure 1a shows the projected electric field obtained from a simulated COM measurement [4] along a line profile of an unrealistic, non-atomistic supercell in which a layer with the MIP of AlN is embedded in a material with a MIP corresponding to that of GaN. The x-axis shows the line-scan position, the y-axis shows the simulated sample thickness.
Apparently, the beam electrons at both interfaces experience a momentum transfer towards GaN, i.e. towards the material with the higher MIP. This is

intuitively understandable, with the interpretation that an electric field exists - due to the (mean inner) potential difference - that deflects the electrons.
If one now considers the complex propagation and interaction of the beam electrons inside the specimen using an atom-based supercell, one gets a completely different picture shown in Figure 1b: the strength with which the beam electrons are deflected at the interface between GaN and AlN is not just higher - it points in the opposite direction. It can be shown that this simulation result agrees with experimental measurements.

In addition to this example, we will also address the influence of sample geometry (inclined surfaces) and examine what effect beam convergence has and how strongly nanobeam-electron diffraction (NBED) is influenced by it.

Conclusion
The interaction of the beam electrons in the STEM with the sample is strongly influenced, for example, by dynamic scattering. Thus, there are also effects on the measured COM of the diffracted intensity in 4D-STEM image series. Caution is therefore advised when interpreting these COM results (e.g. for quantifying electric fields). For complex and especially small-scale structures, comparison with simulations is a must.

**Graphic:**




Projected electric field for a simulated 4D-STEM line profile along the [0001] direction. **(a)** For an unrealistic, non-atomistic supercell in which a layer with the mean inner potential (MIP) of AlN is embedded in a material with a MIP corresponding to that of GaN. **(b)** For a realistic, atom-based supercell in which a layer of AlN is embedded in GaN.

**Keywords:**

4D-STEM, COM, electric fields

**Reference:**

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