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Measurement of Atomic Electric Fields by Scanning Transmission Electron Microscopy (STEM) Employing Ultrafast Detectors.

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Contemporary aberration-corrected STEM enables to probe materials at a resolution of 50pm. This renders the mapping of electric fields at the subatomic scale possible which can give insight to charge densities, ionicity or polarization fields. Differential phase contrast (DPC) STEM as an established method to detect the field-induced angular deflection of the electron beam commonly employs segmented ring detectors [1,2] to record portions of the Ronchigram. This is usually assumed to be homogeneously filled and shifted as a whole in the presence of electric fields, causing characteristic signal differences in opposite segments. By multislice simulations for GaN the validity of these assumptions was checked [3]. With an aberration-corrected probe scanned over the Ga-N region as shown in Fig.1a, the Ronchigrams in Fig.1b have been obtained at 1.3nm specimen thickness. The dominant effect of atomic electric fields is hence a complex redistribution of intensity inside the Ronchigrams making segmented detector data difficult to quantify as to the deflection of the probe.

By basic quantum mechanical arguments we take the complex intensity distribution in the Ronchigram into account. The diffraction plane shows the Fourier transform of the specimen exit wave, which corresponds to a transition from real to momentum space. The local diffracted intensity I(**p**) is hence proportional to the probability for the lateral momentum transfer vector **p** to occur. Consequently, the expectation value for the momentum transfer <**p**> is calculated by a centre-of-gravity-type summation. This condenses the rich details of the Ronchigram to a single vector with fundamental physical meaning [3]. Fig.1c shows the vector field <**p**> resulting from scanning over the GaN patch in Fig.1a, exhibiting atomic sites as sinks of momentum transfer whose magnitudes depend on the atomic number.

To relate the electric field in the specimen to the observed momentum transfer, Ehrenfest's theorem is applied. For thin specimens, <**p**> is found to be proportional to the projection of the electric field along the optical axis, convolved with the intensity distribution of the incident STEM probe [3]. We demonstrate the potential of this approach in both simulation and experiment. For the GaN simulation in Fig.1c, we find the electric field depicted in Fig.1d. Atomic sites appear as sources of the field which has a magnitude of up to 1.5V/pm. As only the convolution of the true field with the probe intensity can be measured, the field strength decreases in the direct vicinity of atomic sites. In a first experiment, 20x20 Ronchigrams of $SrTiO_3$ with a thickness of 2.5nm have been recorded on a conventional charge-coupled device (CCD), yielding momentum transfers and the electric field in Figs.2a,b.

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Our contribution closes with prospects regarding the mapping of charge- and electron densities by employing Maxwell's equations, and by considering practical aspects. In particular, we report on pilot experiments with the ultrafast *pnCCD* camera [4] which was operated at read-out rates of up to 4kHz. For example, Fig.2c shows the momentum transfers recorded at a MoS_2 mono/bilayer interface, demonstrating that fast detectors are the key for atomic-scale materials analyses at a reasonable field of view.

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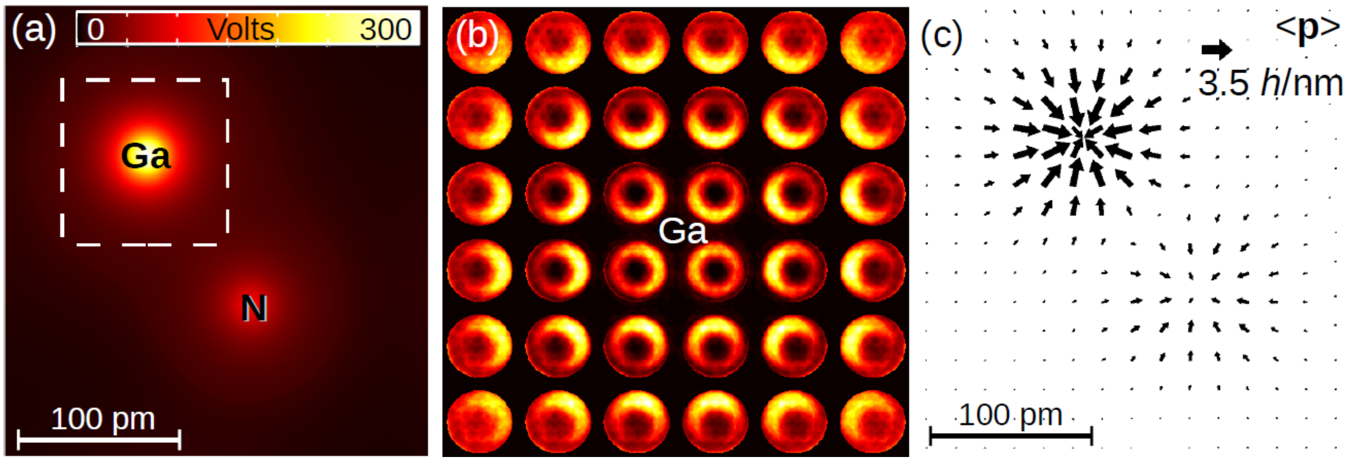

Figure 1. Simulation study of GaN. (a) Projected Potential used for the multislice. (b) Simulated Ronchigrams for rastering an aberration-corrected probe in the dashed region of (a), 1.3nm specimen thickness. (c) Momentum transfers for the region in (a).

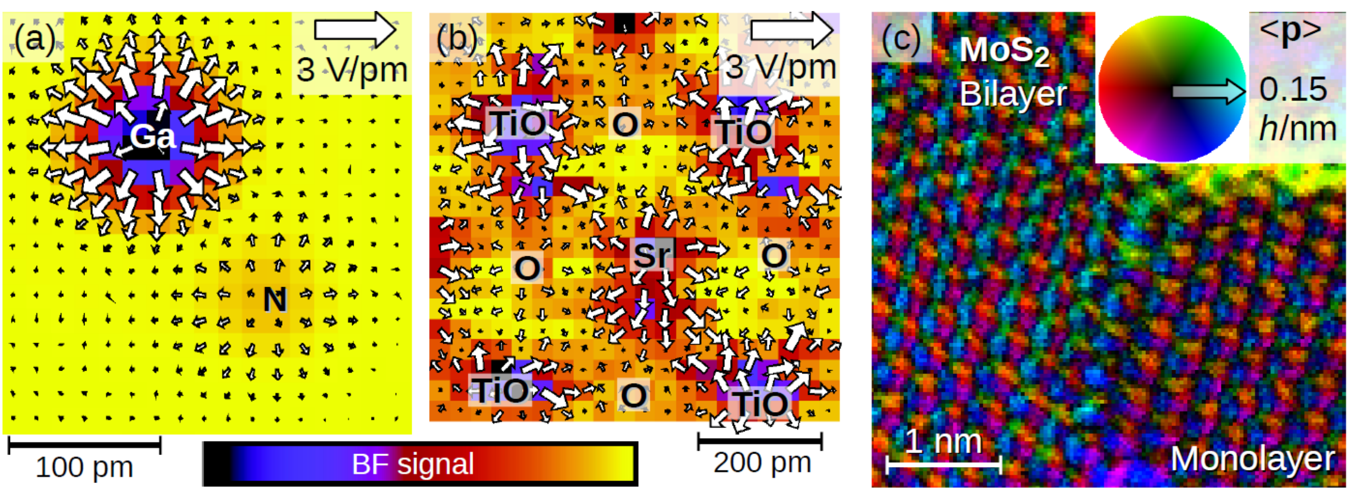

Figure 2. (a) Electric field for the GaN simulation determined from Fig. 1(c). (b) Electric field in a $SrTiO_3$ unit cell region measured experimentally on a 20x20 STEM raster. (a,b) contain the bright field (BF) signal as background. (c) Momentum transfers (direction hue-coded, magnitude saturation-coded) for a mono-/bilayer interface in MoS_2 on a 256x256 STEM raster.

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