ATOMIC SCALE MAPPING OF THE ELECTRIC FIELD IN 1D AND 2D BN NANO-STRUCTURES BY 4D-STEM

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Variation at atomic scale of the electric field in 1D and 2D materials plays a key role in defining physical and chemical properties namely reactivity, interfaces effects and molecule rearrangement. However, the imaging of electric field fluctuations with single atom sensitivity still represents a challenge.

In this regard, four-dimensional scanning transmission electron microscopy imaging (4D-STEM) has recently appeared as a promising technique. In 4D-STEM experiments at every probe position a 2D convergent beam electron diffraction pattern is acquired, generating a 4D dataset. The displacements of the center of mass (COM) of the diffraction pattern is linked to the interaction between the electron beam and the electrostatic field as it propagates through the material. In case of weak phase objects, this technique is in principle quantitative providing space variation down to the atomic scale. This method has been successfully employed in the study of perfect and defective 2D materials but up to now only qualitative results have been presented without a precise estimation of the electric fields.

In this work, we present 4D-STEM analysis performed on several boron nitride (BN) based 1D and 2D structures, going from single and multi-walled nanotubes to mono and few layers h-BN crystals. We measure the electric field at sub-atomic scale, and we study its dependence as a function of the number of layers in few layers h-BN and curvatures effects in BN nanotubes. Furthermore, we investigate field modulations in presence of defects such as vacancies, adatoms and flake edges. These experimental results show an excellent agreement with theoretical estimation obtained from first principle simulations.

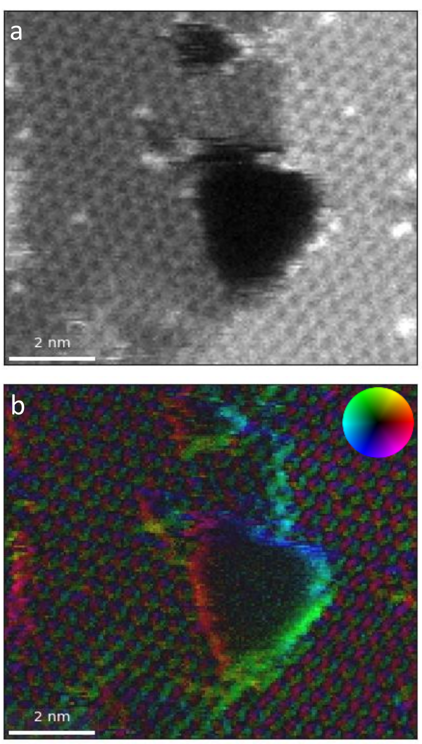

Figure 1: (a) ADF and (b) electric field orientation map images large defects and adatoms in a multi-layer h-BN.

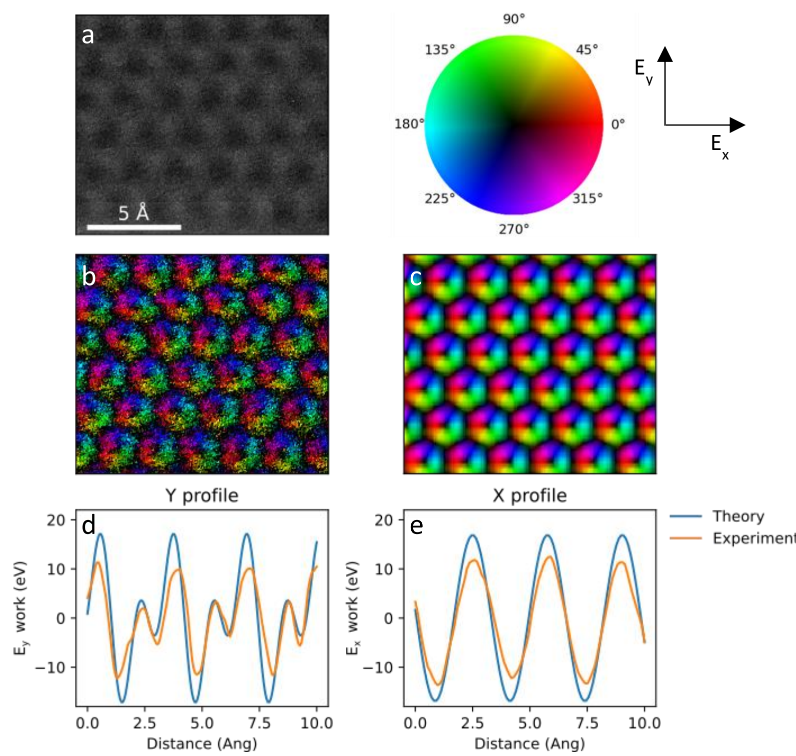

Figure 2: (a) ADF image and (b) electric field orientation map of h-BN monolayer compared with the electric field obtained by DFT integrated over the direction of propagation of the electrons (c). (d,e) Profiles of the electrical field intensity extracted along x and y direction.

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