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MS-12-O-3053 Imaging polarisation around charged antiphase boundaries in doped bismuth ferrite

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Doping BiFeO₃ with Ti and Nb can suppress electrical conductivity as well as altering both ferroelectric and ferromagnetic orderings [1]. Higher doping levels of 10% Ti also result in the formation of novel, negatively-charged antiphase boundaries (APBs) that polarise the surrounding perovskite matrix [2]. In this study, we investigate the polarisation and electric fields further using high-resolution STEM (HRSTEM) imaging, high resolution TEM (HRTEM) using negative Cs imaging (NCSI), differential phase contrast (DPC) STEM, and scanned diffraction.

Quantitative determination of the atomic structure using HRSTEM or HRTEM/NCSI is compared in Figure 1. The structures are qualitatively similar, but with significant quantitative differences. Specifically, the deviation of oxygen atoms from the positions in an unpolarised material is reduced in HRTEM as compared to HRSTEM. This results in reduced polarisation measured for the HRTEM, as also shown in Figure 1. The discrepancy probably arises from differences in the sample thickness, since for HRSTEM the sample was about 16 nm thick whereas the HRTEM data was taken from an area about 4 nm thick. For very thin samples, the polarisation is expected to be reduced by surface effects and by some of the electric field escaping the specimen as stray fields.

DPC STEM shows a clear signal when scanning across one of these APBs, as shown in Figure 2, peaking strongly to either side and flipping sign at the APB, consistent with the polarisation of Figure 1. Scanning diffraction, however, shows no shift of the diffraction discs, as would be suggested by simplistic interpretations of DPC data in terms of Lorentz deflections from an E-field. In fact, the data in Figure 2 forces us to adopt an alternative interpretation of the DPC signal in terms of the redistribution of intensity due to dynamical scattering in a non-centrosymmetric structure, together with almost perfect screening of the E-field by the polarisation. This is found to accord perfectly with the expectations of dielectric theory for ferroelectric and polar-ordered materials.

This investigation shows that explicit consideration of electrostatics in the sample is required when interpreting atomic or nano-resolved studies of polar-ordered materials.

[1] K. Kalantari et al., *Adv. Func. Mater.* 21, 3737 (2011).

[2] I. MacLaren et al., *APL Materials* 1, 021102 (2013).

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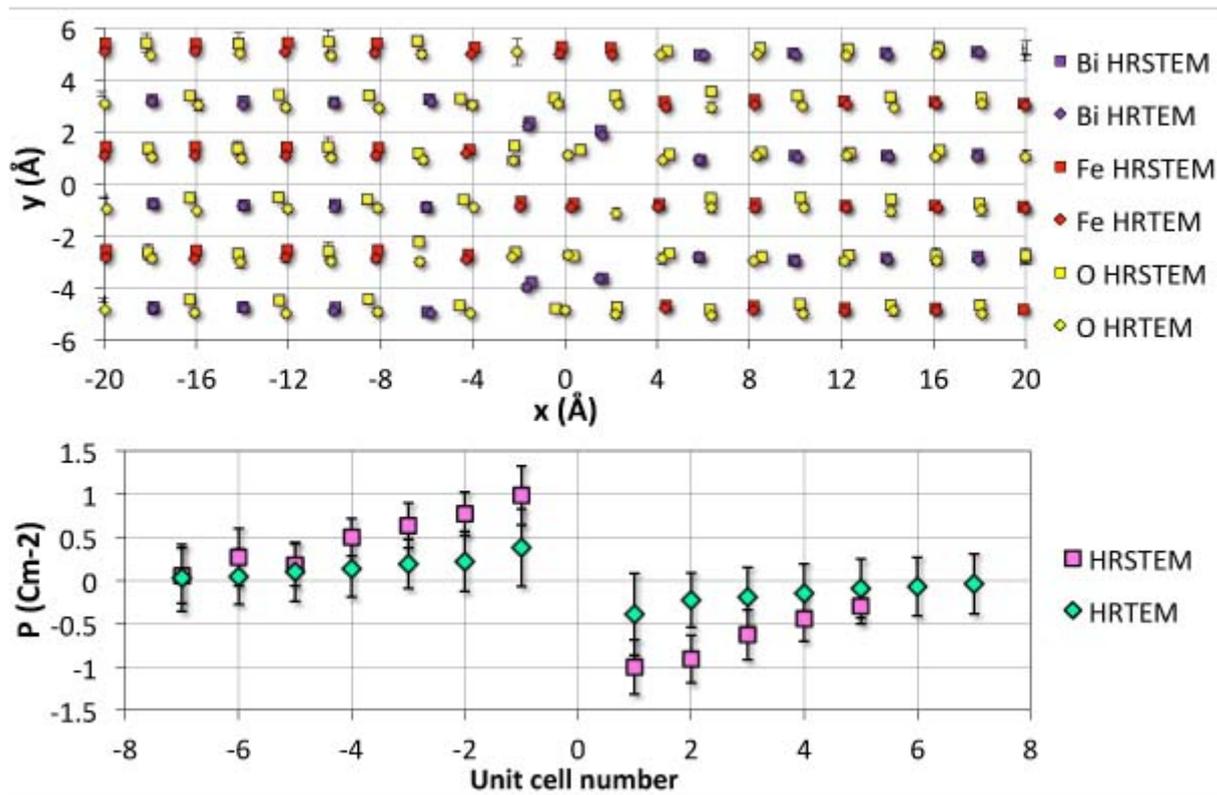


Fig. 1: Figure 1: Quantitative comparison of averaged repeat units for the charged antiphase boundary from HRTEM (negative Cs imaging) and from HRSTEM (HAADF and BF combined); positions marked as Fe are either Fe or Ti. The lower graph shows the polarisation calculated from this atomic resolution data for both the HRSTEM and HRTEM data.

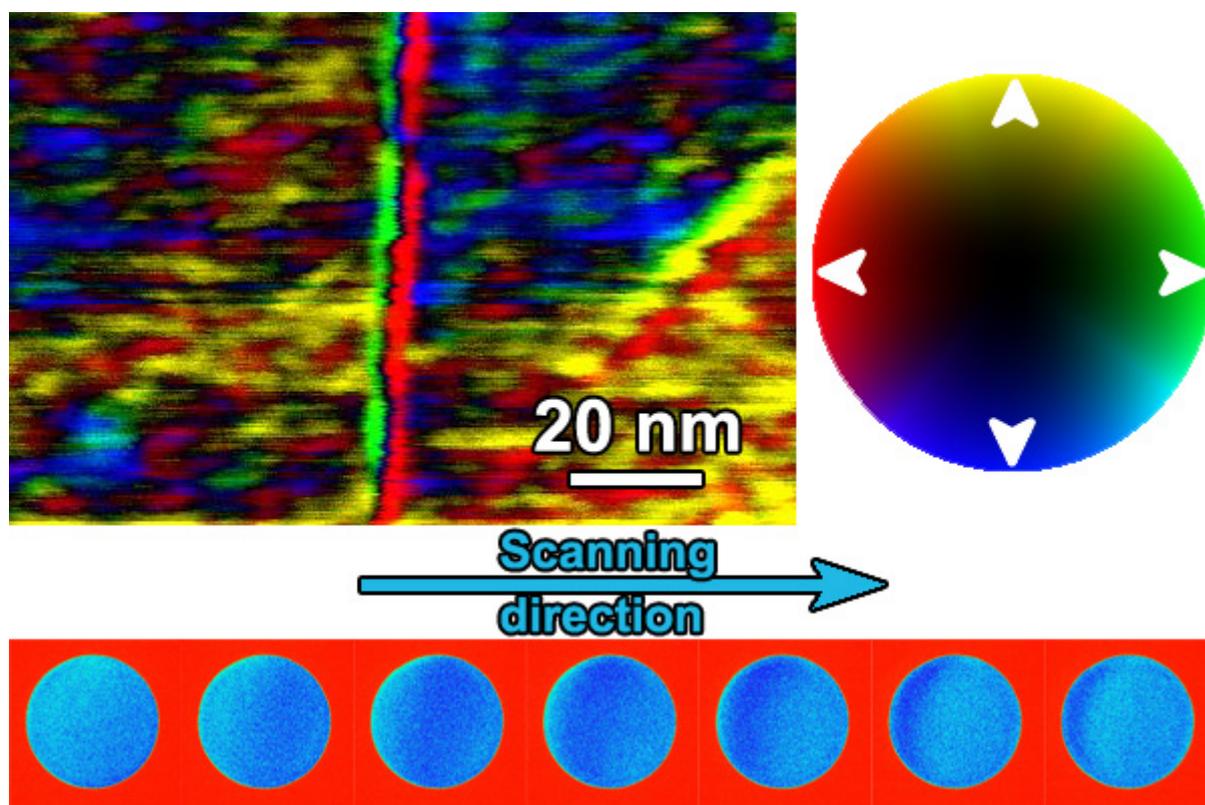


Fig. 2: Figure 2: Differential phase contrast STEM of a charged antiphase boundary in Ti, Nd co-doped BiFeO₃ (upper part, signal direction indicated in the colour wheel). Scanned diffraction in a line scan across one such boundary (lower part) showing a clear movement of intensity within the diffraction disc but no disc deflection.