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Probing point and planar defects in multiferroic $YFeO_3$ thin films

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The presence of point and planar defects, such as antisites and antiphase boundaries (APBs), can mediate the electronic and magnetic properties of thin film functional oxides. For example, antisite defects in $SrTiO_3$ can induce ferroelectric polarization [1] whereas the presence of APBs in magnetite (Fe_3O_4) leads to a reduction in spin polarization [2]. Understanding the presence, structure, and distribution of these defects is thus particularly critical when engineering multiferroic thin films, such as yttrium iron oxide, $YFeO_3$ [3]. Little is known, however, about the role of defects in these materials.

In this presentation, we report a study of defects in $YFeO_3$ thin films grown on Nb doped $SrTiO_3$ via pulsed laser deposition (PLD). Depending on film stoichiometry, we find antisite and planar defects. Antisite defects are identified using atomic resolution STEM-EDS mapping with signal denoising using non-local principal component analysis, Figure 1 [4]. Y_{Fe} antisites are distributed across the sample, shown in Figure 1b, inducing ferroelectric behavior in $YFeO_3$ thin films by breaking inversion symmetry, while Fe_Y antisites are found along APBs, Figure 1c. The APBs have a *c*/2 [001] translation on the pseudocubic {010} plane, and are vertical with respect to the substrate. While we find that the APBs are not readily apparent in annular dark field (ADF) images, strong, alternating intensity variation is observed in integrated differential phase contrast (iDPC) imaging, as in Figure 2. Quantifying the iDPC APB contrast, there is an 80% difference between Y atom columns along the boundary, whereas the contrast in ADF decreases to only 6%, Figure 2 c. We will show that the origin of the Y atom column contrast results from local distortions at the antiphase boundaries via STEM image simulations of DFT calculated structures. We will also discuss how the structure of these APBs favors the formation of Fe_Y antisites. Finally, we will discuss how these defects may provide additional routes to tune $YFeO_3$ properties [5].

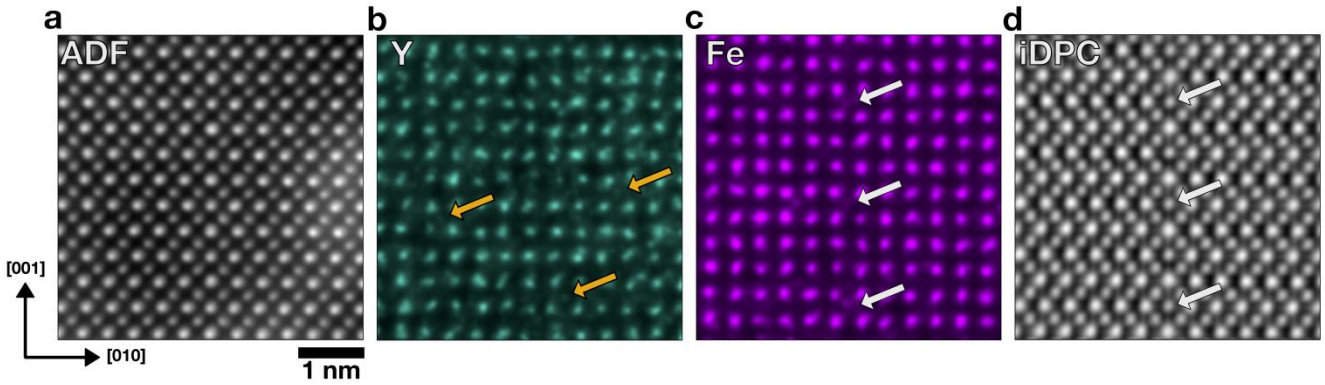

Figure 1. (a) ADF image, (b) Y, (c) Fe STEM-EDS elemental maps and (d) iDPC image from YFeO3 thin film. Orange arrows in Y elemental map highlight the location of YFe antisites while white arrows in Fe elemental map and iDPC image highlight the location of FeY antisites.

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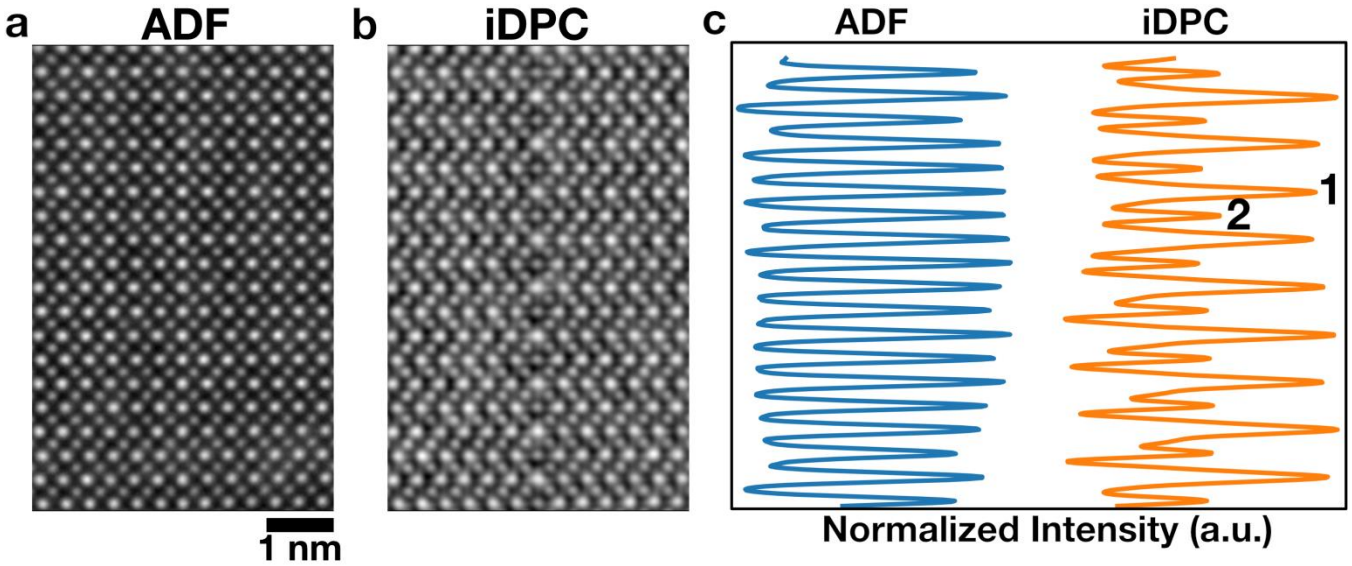

Figure 2. (a) ADF and (b) iDPC image of YFeO3 along pseudocubic [100] (c) normalized intensity of Y atom columns along antiphase boundaries in ADF and iDPC images.

References

[1] K. Klyukin and V. Alexandrov, Physical Review B **95** (2017) p. 035301
[2] K. P. McKenna et al., Nature Communications **5** (2014), p.5740.
[3] M. Shang et al., Materials Letters **175** (2016), p. 23
[4] J. Salmon et al., Journal of Mathematical Imaging and Vision **48** (2014) p. 279
[5] This material is based upon work supported by the National Science Foundation under MRSEC program, DMR 1419807.

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