Supplementary Material for the manuscript

Mapping octahedral tilts and polarization across a domain wall in BiFeO$_3$ from Z-contrast STEM image atomic column shape analysis

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Thickness dependence of the diagonal distortion of the column shapes analyzed by PCA
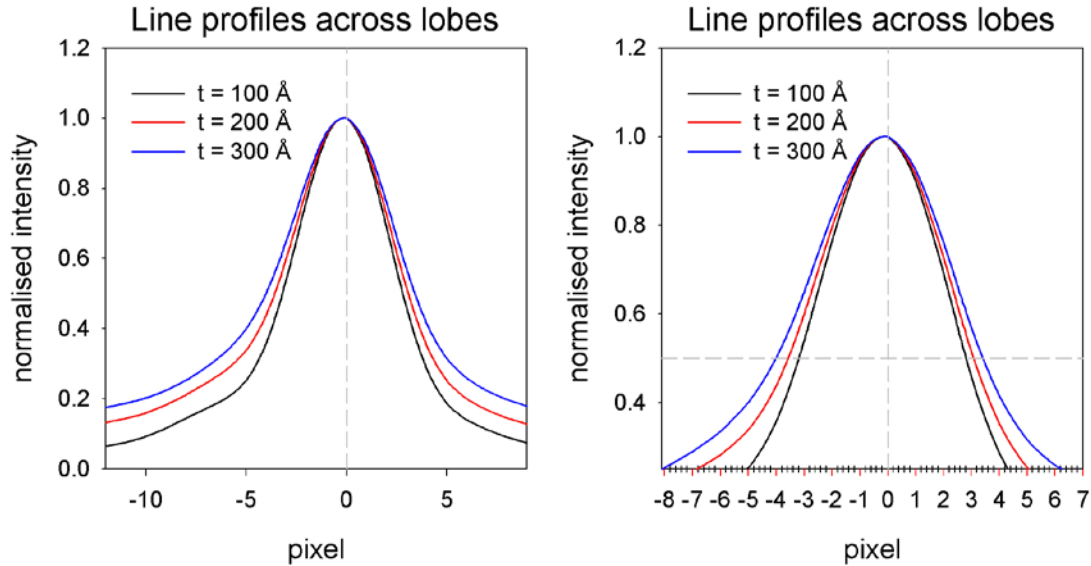
Here are two graphs made from measuring the line profiles across the simulated "lobes" in BFO using a line width of 3 pixels for the thicknesses of 100, 200 and 300 Å. The vertical line represents the location of the maxima (normalized to one for comparison. The plot on the right is the same as the one on the left except the minimum of the intensity axis is set to 0.25 in order to measure the widths either side of the maxima.

The raw data is

Pixel	t = 100	t = 200	t = 300
-12.0000	0.0649	0.1331	0.1759
-11.0000	0.0762	0.1442	0.1874
-10.0000	0.0930	0.1601	0.2027
-9.0000	0.1164	0.1827	0.2241
-8.0000	0.1445	0.2117	0.2531
-7.0000	0.1719	0.2445	0.2896
-6.0000	0.2014	0.2823	0.3352
-5.0000	0.2524	0.3386	0.4002
-4.0000	0.3588	0.4391	0.5018
-3.0000	0.5401	0.6001	0.6500
-2.0000	0.7647	0.7955	0.8223
-1.0000	0.9474	0.9542	0.9597
0.0000	1.0000	1.0000	1.0000
1.0000	0.8999	0.9126	0.9247
2.0000	0.6900	0.7259	0.7604
3.0000	0.4594	0.5158	0.5699
4.0000	0.2861	0.3520	0.4152
5.0000	0.1876	0.2529	0.3158
6.0000	0.1400	0.2000	0.2588
7.0000	0.1125	0.1686	0.2235
8.0000	0.0911	0.1454	0.1981
9.0000	0.0745	0.1283	0.1797

From the plots on the right we have the following measure of the "lobe distortion". I have used the ratio of the intercept of one quarter intensity of the left/right side. The results are as follows

thickness	ratio
100	1.16
200	1.36
300	1.32

In summary, for these simulations, the lobe is small for thicknesses of less than 10 nm, becomes maximized at around 20 nm and then the increasing background in the ADF signal means there is little subsequent change in the lobe distortion.
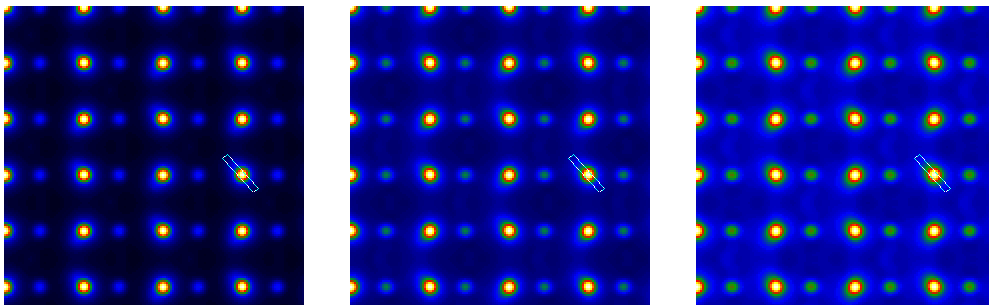
The positions of the line scans are shown on the images above 10 nm (left), 20 nm (middle) and 30 nm (right). The image minima are set to zero so the build up of the background is obvious.