

Controlling polarization through defects in Si-integrated BaTiO₃

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Abstract : BaTiO₃ (BTO), a uniaxial ferroelectric, finds wide application in memory device or electro optic modulator in integrated photonics (depending on the orientation of c axis with respect to the substrate). In our earlier work¹, we have shown that it is possible to directly grow epitaxial BaTiO₃ with precise orientation control. From the room and high temperature XRD analysis we have concluded that the origin of an out of plane orientation in BaTiO₃/TiN/Si, is anti-site like defect mediated. Here we further present the structure and chemistry of these Si integrated BTO systems through aberration corrected STEM.

Results and discussion:

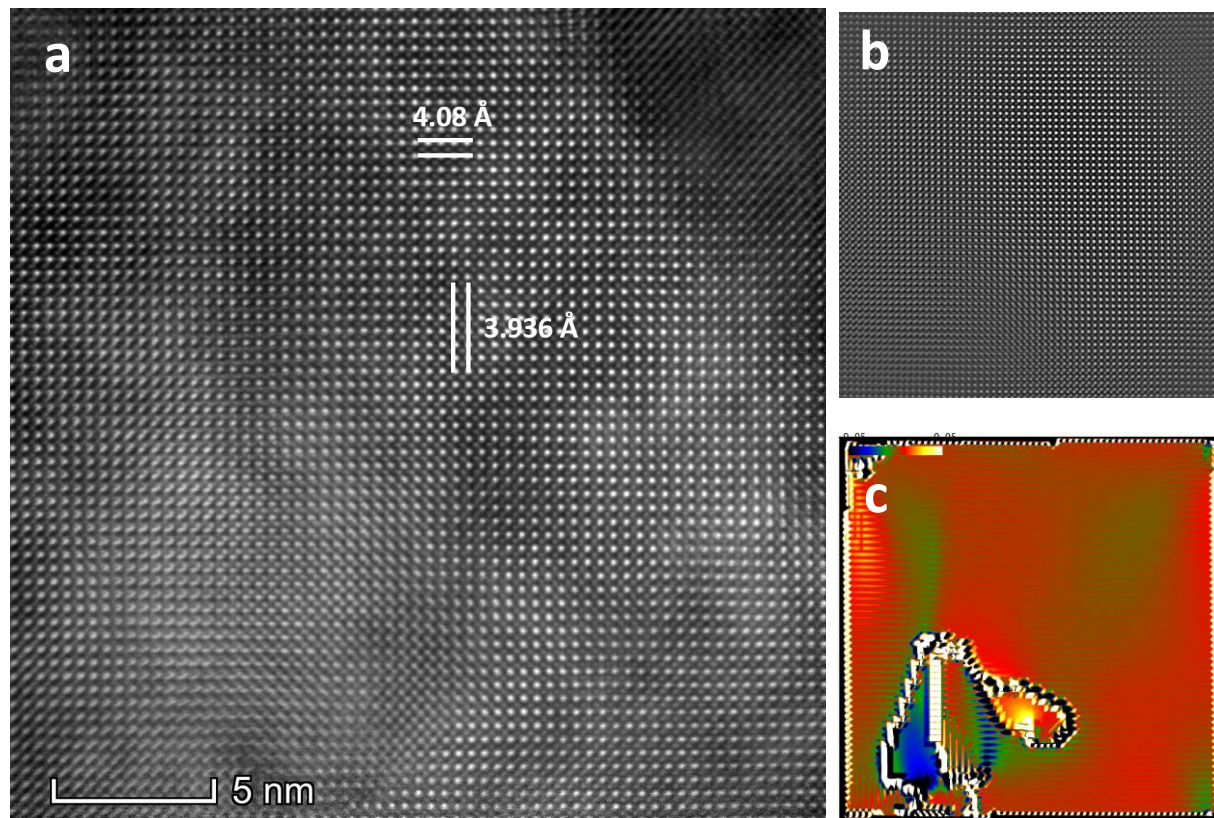


Figure:1: HAADF-STEM image of BaTiO₃ film along [001] zone axis, reveals that our samples are Ba rich, (b) represents the same image, with a Bragg filtering, where antisite positions can be identified clearly.(c) reveals x-component of strain(e_{xx})- Peak pair analysis performed on these images, revealed an average domain size of $\sim 3-4$ nm, with inhomogeneous strain gradients, possibly arising from the antisite defects.

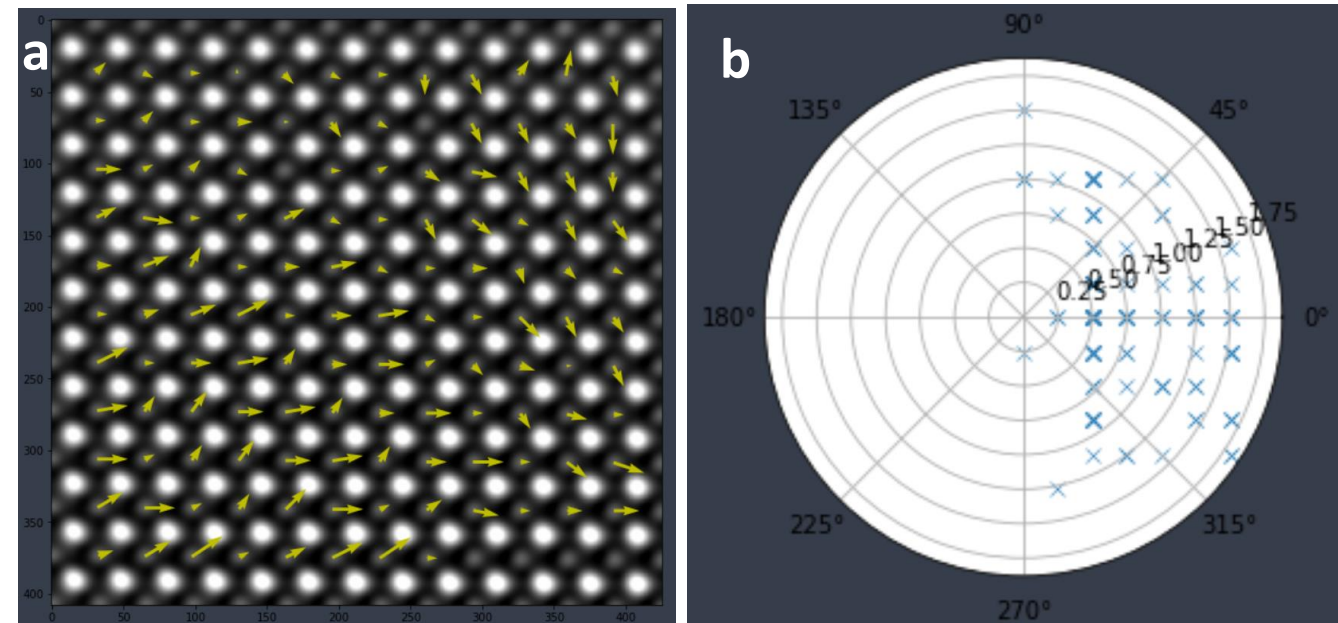


Figure:2: (a) Displacements of Ti atoms mapped using a home-built algorithm- the magnitude of displacement lies within ~ 50 pm, (b) corresponding polar plot, which is symmetric about 0 degree.

Conclusion:

- Although the tetragonality is out of plane, the Ti displacement is more or less in plane. This suggests we have less symmetric structure than tetragonal, due to defects.
- The microstructural inhomogeneity in composition (contrast), strain as supported by PPA analysis and polarization maps bolster our hypothesis of defect mediated polarization engineering.