Supplementary materials for Structural and photoelectric properties of tensile strained $BiFeO_3$

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I NDSCO$_3$ STRUCTURE

Figure S1 shows the two possible distinct pseudocubic $\langle 100 \rangle_{PC}$ zone axes (i.e. viewing the crystal normal to the $\{100\}_{PC}$ lattice planes) for the $NdScO_3$ (NSO) structure. The most obvious distintion between the two orientations is that the orthorhombic $\langle 110 \rangle_O$ type axes show a 'zig-zag' in the Nd lattice (up and down shifts in Fig. S1(b)). This feature can then be used to easily work out the orientation of the substrate relative to the $BiFeO_3$ (BFO) film. This is important as, due to the differences in the surface for the different directions, the BFO films will experience different strain.

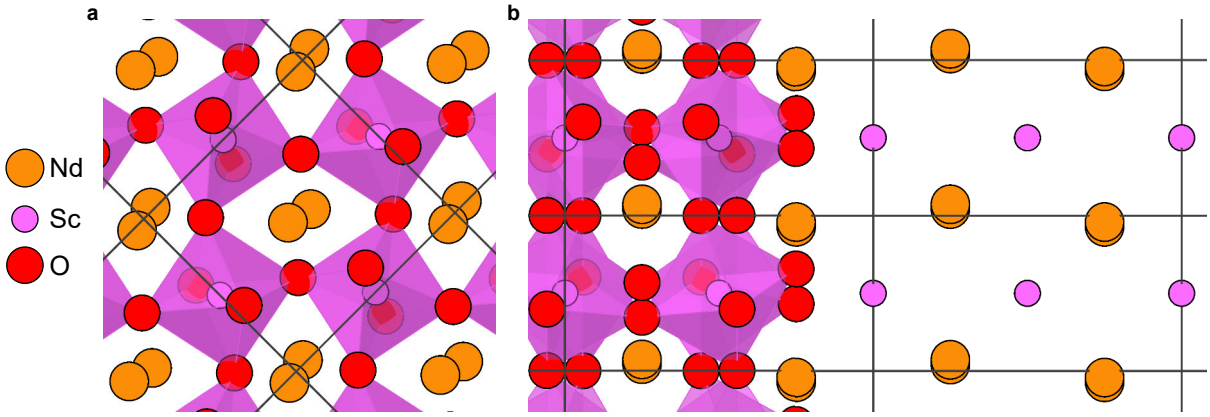

Figure S1: The NSO structure as viewed along the two distinct pseudocubic $\langle 100 \rangle_{PC}$ zone axes. (a) shows the orthorhombic $\langle 001 \rangle_O$ zone axis and (b) shows the $\langle 110 \rangle_O$ zone axis. The left and right sides of (b) show the structure with and without oxygen atoms, respectively, for clarity.

II TRANSMISSION ELECTRON MICROSCOPY

Figure S2(a) shows a selected area electron diffraction pattern (SAED) taken from both the BFO and NSO structures. The in-plane 010_{PC} type peaks show no splitting, showing the BFO is fully strained to the NSO. The out-of-plane 001_{PC} type peaks show some splitting from the different out-of-plane lattice parameters. $00{+}\frac{1}{2}{}_{PC}$ peaks are also visible due to the 'zig-zag' structure of the NSO. Figure S2(b)d shows a dark field image showing domains over a large area, where the good periodicity of the domains can be seem.

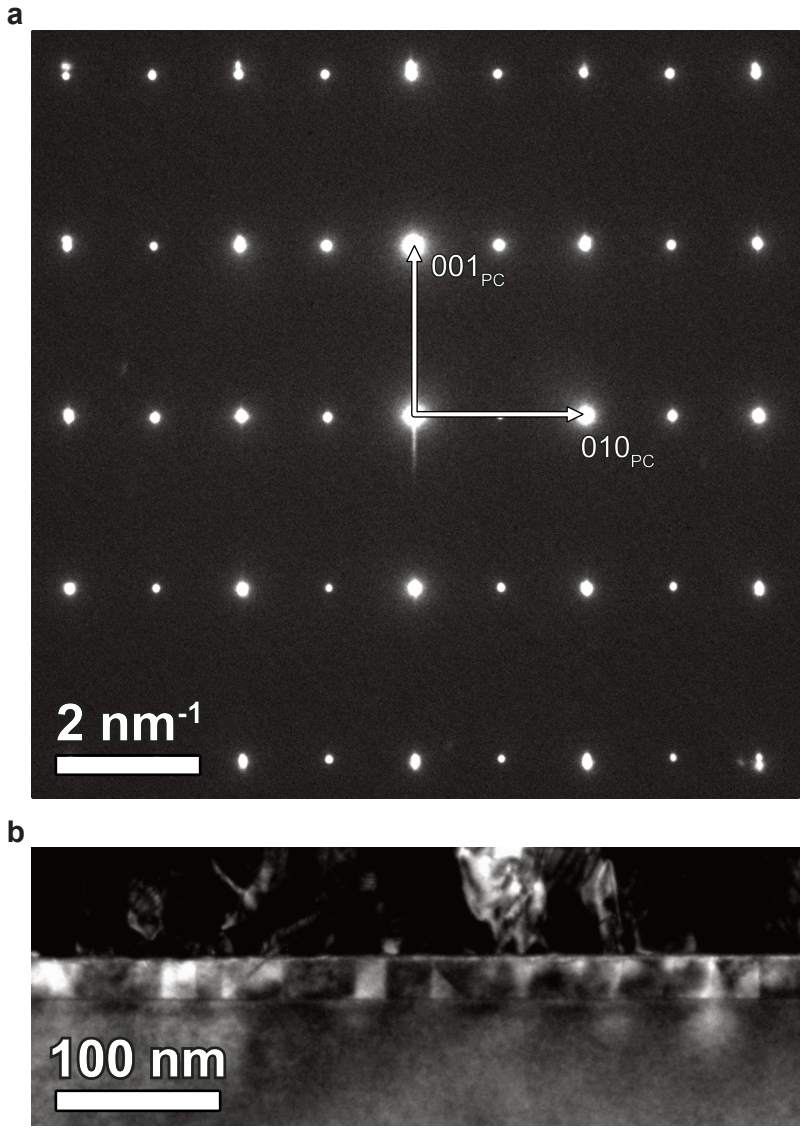

Figure S2: (a) Selected are diffraction pattern including contributions from both the NSO and BFO. (b) Dark field image showing the domain structure over a wide area.