

Supporting information for

Atomic scale investigation of enhanced ferroelectricity in (Ba,Ca)TiO₃

Xiao Na Zhu, Xing Chen, He Tian[†], Xiang Ming Chen[†]

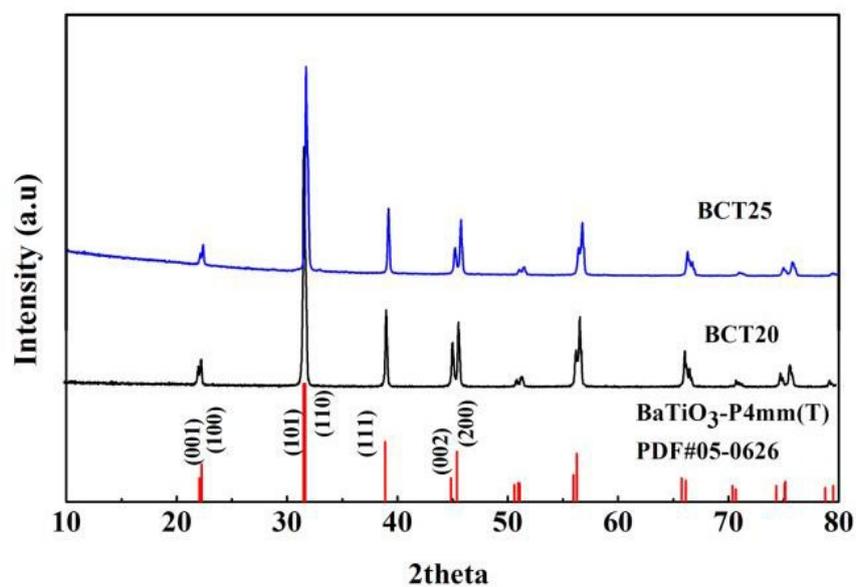


Figure S1, XRD pattern of $x=0.2$, $x=0.25$ and phase diagram of (Ba,Ca)TiO₃ system.

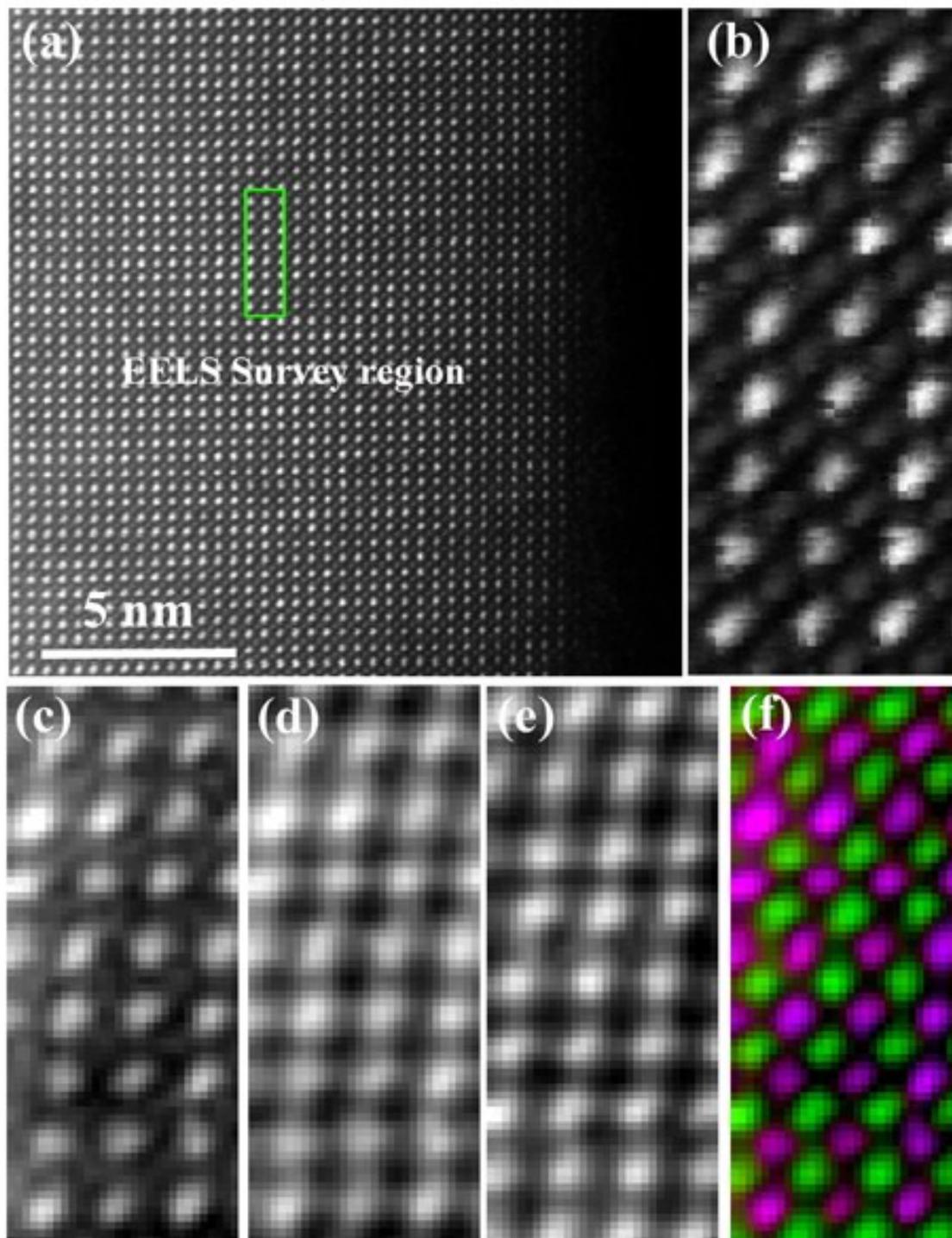


Figure S2 (a) HAADF STEM image of $\text{Ba}_{0.80}\text{Ca}_{0.20}\text{TiO}_3$ ceramics including the survey region 3D EELS data is acquired from the region indicated by the green rectangle. (b) HAADF image of the survey region acquired simultaneously with EELS spectrum. The atomic resolution elemental maps of Ba (c), Ca (d) and Ti (e) are separately present. (f) Color map of the Ca (Red), Ti (Green) and Ba (Blue) from the survey region. The lattice distortion in STEM EELS (c-f) was induced by sample drafting during the acquirement of STEM EELS.

Table S1 Parameters for the Blochwave simulation of an STEM-EELS image of the BCTO sample using the STEM sim software.

Parameter	Unit	Value
Acceleration Voltage	kV	200
Total specimen thickness	nm	20
Defocus	nm	0
Spherical aberration C_s	mm	0.0405
Spherical aberration of 5th order C_5	mm	0
Zone axis	N/A	[111]
a-direction	N/A	[010]
Convergence angle	mrاد	21
Collection angle	mrاد	94
FWHM of the source image	Å	0.7

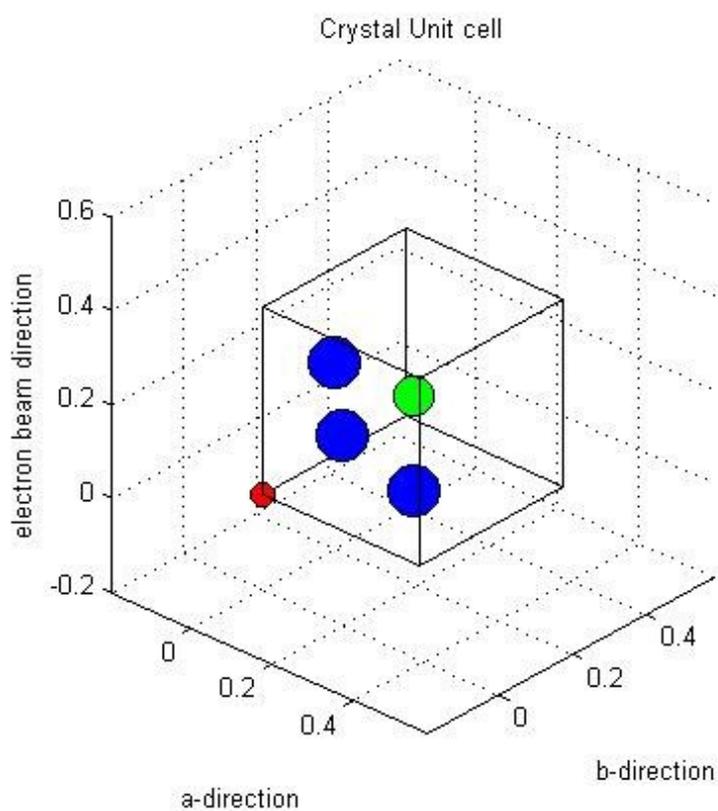


Figure S3 The input structure for the STEM simulation. A-direction: [010]. Axis unit: nm.

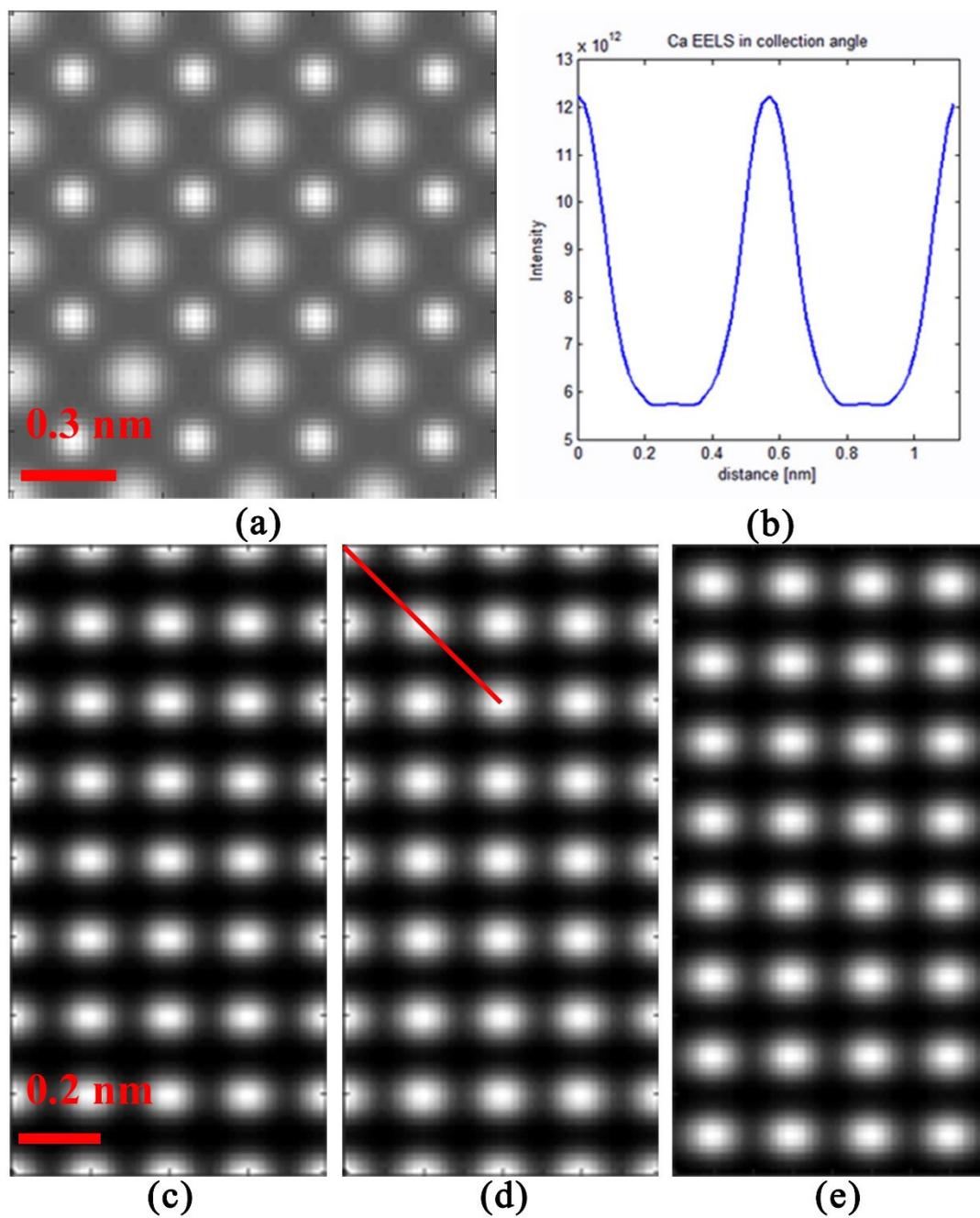


Figure S4 Simulated results for $\text{Ba}_{0.80}\text{Ca}_{0.20}\text{TiO}_3$ sample of (a) Atomic resolution HAADF STEM image viewed along [100] zone axis of BCTO. A-axis, [010]. (b) Intensity profile of the simulated EELS spectrum image of Ca along the indicated line in (d). Simulated STEM EELS image of (c) Ba (d) Ca (e) Ti with Gaussian Peak Filter of 0.07nm.