

Supporting Information for

Atomic structure of defects and interfaces in TiO₂-B and Ca:TiO₂-B (CaTi₅O₁₁) films grown on SrTiO₃

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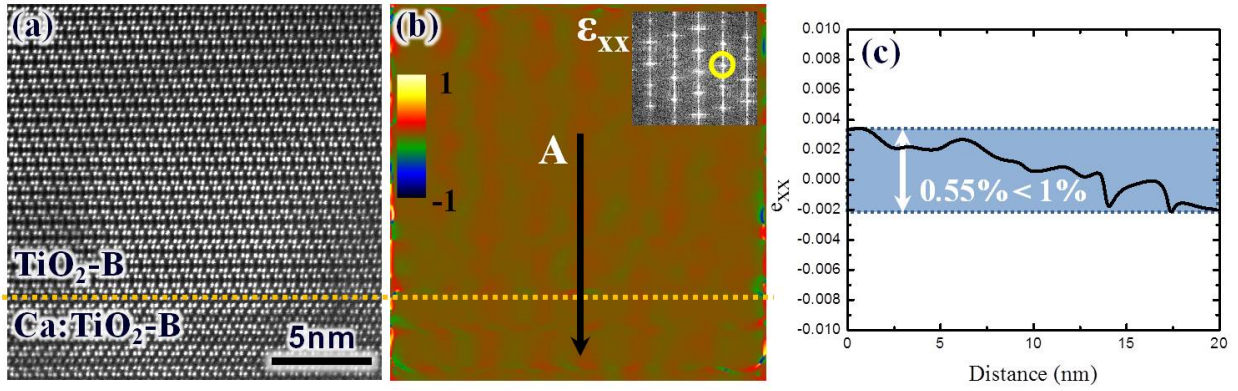


Fig. s1 Misfit strain analysis of $\text{TiO}_2\text{-B}$ and $\text{Ca:TiO}_2\text{-B}$ using geometric phase analysis. (a) An actual HR-STEM image, (b) a strain (ϵ_{xx}) map of an image, and (c) a strain profile from the line-scan A.

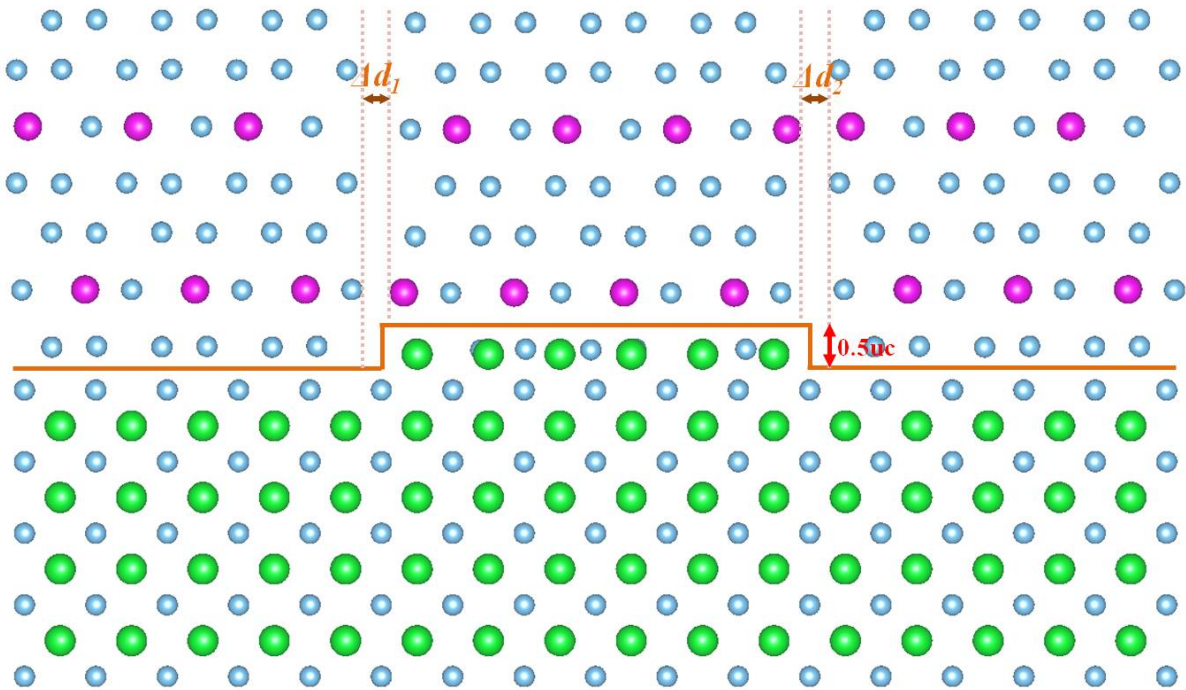


Fig. s2 (a) Schematic illustration of a surface step terrace (= 0.5 unit cell (u.c.)), or SST, at the interface between STO and Ca:TiO₂-B. Unit cells of Ca:TiO₂-B cannot fulfill epitaxy everywhere along the surface where there are gaps (equivalent of Δd_1 and Δd_2 in the diagram) due to the step. However, during growth, each gap is filled with another vertical row of atoms.

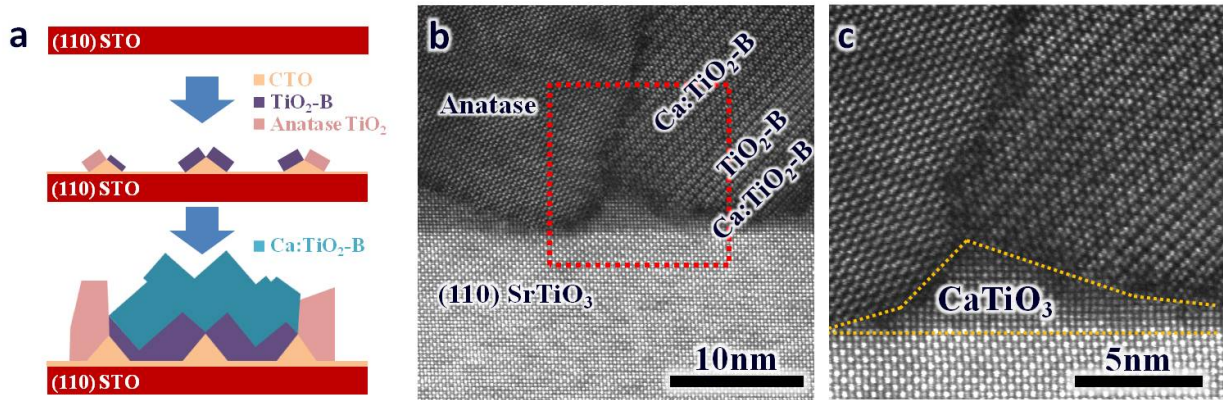


Fig. s3 (a) Schematic of sequential growth of TiO₂-B + Ca:TiO₂-B mixture phase and another titania polymorph, anatase, grown on (110) STO, (b) high-resolution STEM images showing the presence of CaTiO₃ layer for tilted growth of the mixture phase. (c) an interphase boundary formed between anatase and TiO₂-B grains.

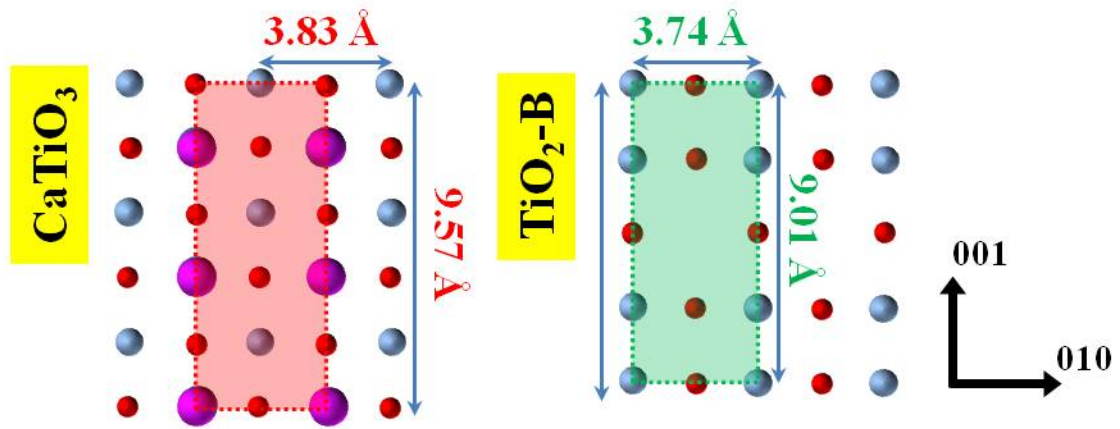


Fig. s4 Comparison of atomic configuration between (100) planes of CaTiO_3 and $\text{TiO}_2\text{-B}$.

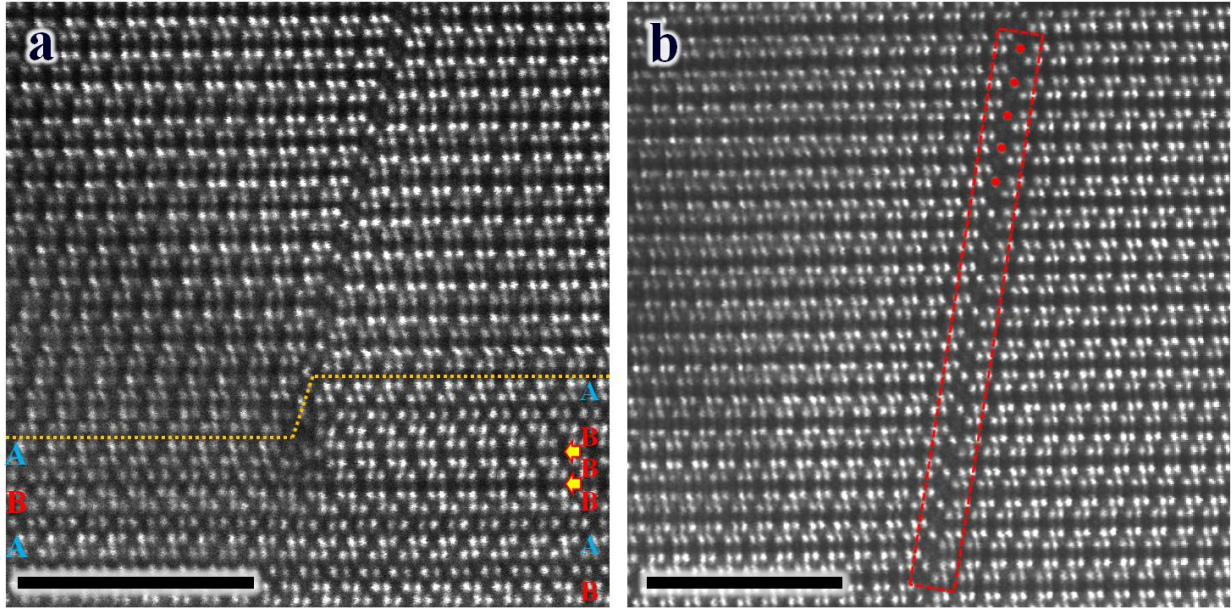


Fig. s5 (a) High-resolution STEM images of defects at the interface between $\text{TiO}_2\text{-B}$ and $\text{Ca}:\text{TiO}_2\text{-B}$ with two missing Ca-modified layers that generate the two adjacent $\text{TiO}_2\text{-B}$ grains oriented same direction. (b) This generates the long-range boundary condition throughout the boundary with possible occupancy sites for Ti atoms from either left or right-side $\text{TiO}_2\text{-B}$ grain.