Electronic Supplementary Information

Creating High Quality Ca:TiO_2-B ($CaTi_5O_{11}$) and TiO_2-B Epitaxial Thin Films by Pulsed Laser Deposition

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Table S1. Lattice structures of the phases and substrates involved in this study.

Phase	Crystal system	Lattice parameters
Ca:TiO_2-B	orthorhombic	a=12.1702 Å, b=3.8013 Å, c=17.9841 Å
TiO_2-B	monoclinic	a=12.1787 Å, b=3.7412 Å, c=6.5249 Å, β=107.054°
TiO_2-anatase	tetragonal	a=b=3.7820 Å, c=9.5150 Å
TiO_2-rutile	tetragonal	a=b=4.5900 Å, c=2.9600 Å
$CaTiO_3$	pseudocubic	a=3.8917 Å
$SrTiO_3$	cubic	a=3.9051 Å
LSAT [a]	cubic	a=3.8680 Å
$LaAlO_3$	pseudocubic	a=3.7913 Å
YSZ [b]	cubic	a=5.1420 Å
MgO	cubic	a=4.2130 Å
Al_2O_3	hexagonal	a=4.7580 Å, c=12.9910 Å

[a] ($LaAlO_3)_{0.3}(Sr_2AlTaO_6)_{0.7}$; [b] yttria-stabilized zirconia

Table S2. In-plane mismatch (calculated on a diagonal basis) between difference phases and the substrate surfaces. The preferred phase eventually adopted by the film deposited from a (80% TiO_2 + 20% CaO) target on each specific substrate is set in bold.

Substrate surface	Ca:TiO_2-B (001)	TiO_2-anatase (001)	TiO_2-rutile (001)	$CaTiO_3$ (001)	TiO_2-B (001)
$SrTiO_3$ (001)	**3.25%**	-3.15%	17.5%	-0.343%	3.17% [a]
LSAT (001)	**4.24%**	**-2.22%**	18.7%	0.613%	4.16% [a]
$LaAlO_3$ (001)	**6.35%**	**-0.245%**	21.1%	2.65%	6.27% [a]
YSZ (100)	14.7%	10.3%	**-10.7%**	13.5%	13.9% [a]
MgO (100)	-4.30%	-10.2%	8.95%	**-7.63%**	-4.37% [a]
α-Al_2O_3 (0001)	-22.6%	-11.1%	**7.95%**	-8.48%	-22.6% [a]
Ca:TiO_2-B (001)	0	-6.20%	13.8%	-3.48%	**-0.075%**

[a] For comparison only. TiO_2-B does not grow directly on these substrates in this study.

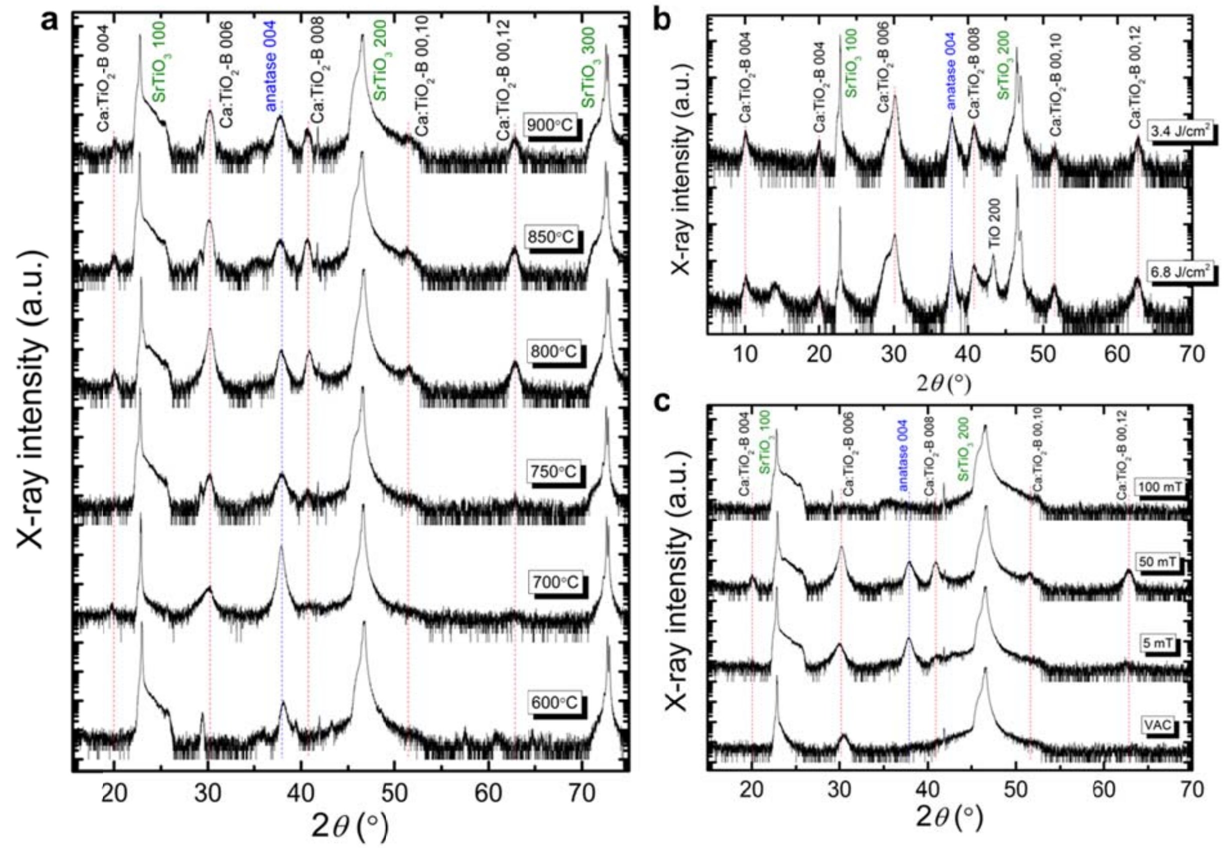

Figure S1. XRD patterns of the films deposited from a 10% CaO target on (001) $SrTiO_3$ substrates under different conditions: a) growth temperatures from 600 to 900 °C; b) laser fluence from 3.4 to 6.8 J cm^{-2}; c) O_2 partial pressure from vacuum to 100 mTorr. Substrates peaks are labeled in green, anatase peaks in blue. Vertical dashed lines are drawn to mark peak positions for comparison.

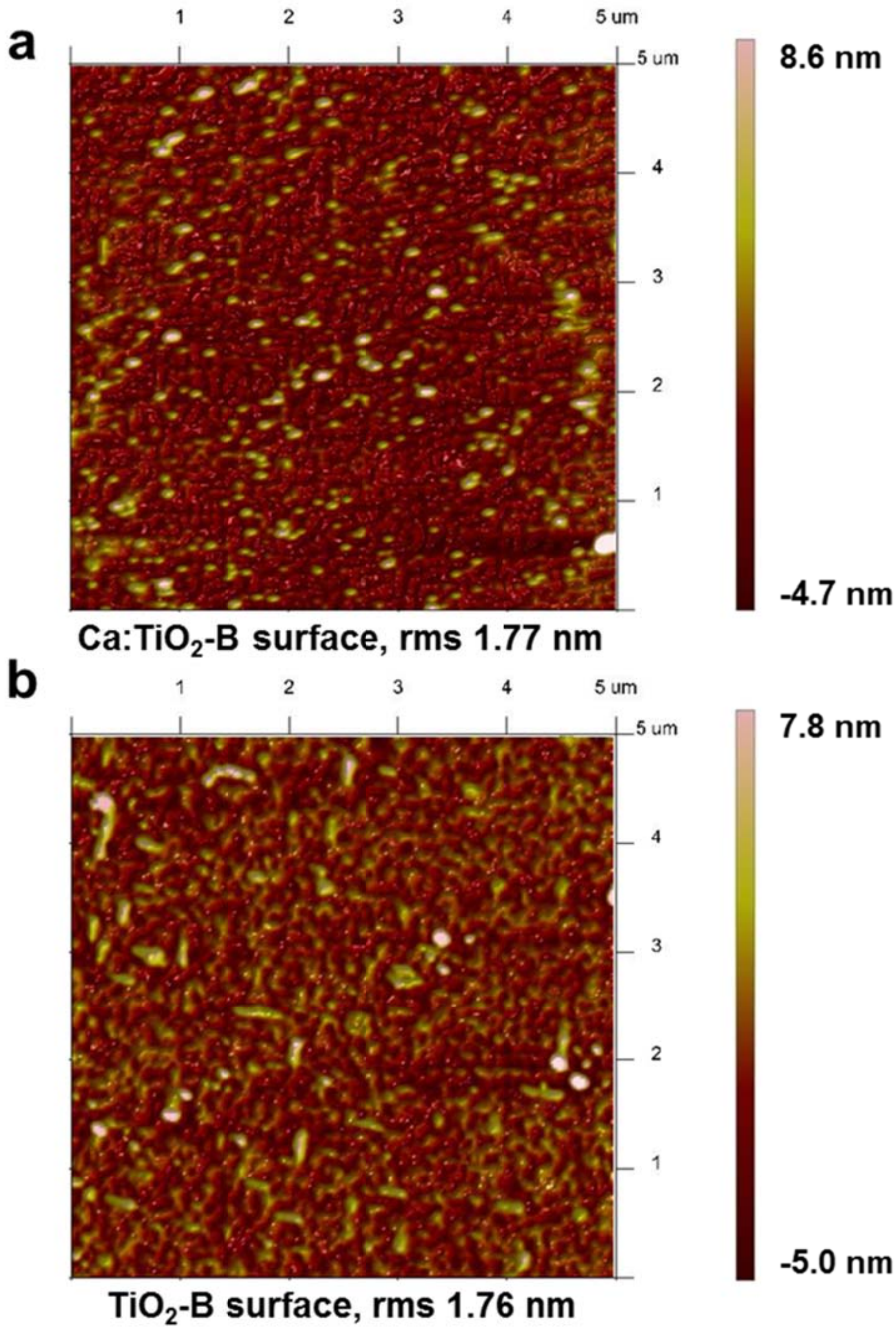

Figure S2. AFM images (tapping mode) showing the surfaces of a) a (001) Ca:TiO_2-B film and b) a (001) TiO_2-B film, respectively. Scan area is 5 μm × 5 μm for both.