

Electronic Supplementary Information

Orientation-Controlled BaTiO₃ Thin Films Fabricated by Chemical Solution Deposition

Tadasu Hosokura,* Akira Ando, and Takehiro Konoike

Murata Manufacturing Co., Ltd.

10-1, Higashikotari, 1-chome, Nagaokakyo-shi, Kyoto 617-8555 Japan

*e-mail address: hosokura@murata.com

characterizations.

Crystal characterizations were performed by X-ray diffraction (XRD) (Model RINT-KI, Rigaku, Tokyo, Japan). The orientation of the film along the axis parallel to the substrate was characterized by X-ray pole figure measurement (Model Smart Lab, Rigaku, Tokyo, Japan). Cross-sectional images of the obtained film were taken by a field emission-scanning electron microscope (FE-SEM) (Model S-5000, Hitachi, Tokyo, Japan). Cross-section images of the obtained films and selected area electron diffraction (SAED) patterns were taken by transmission electron microscope (TEM) (Model EM-002B, TOPCON, Tokyo, Japan). Cross-section images of the obtained film were also taken by spherical aberration corrected scanning transmission electron microscopy (Cs-STEM) (ARM-200F, JEOL, Tokyo, Japan). Polarization-electric field (P-E) hysteresis loops were measured using a ferroelectric tester (Precision Premier II, Radiant Technologies, Albuquerque, New Mexico, USA). Small signal AC (100 mV, 1 kHz) capacitance and dielectric constant temperature dependence were measured by using an LCR meter (HP 4284A, Hewlett-Packard, Palo Alto, California, USA). DC resistivities were measured by using an Electrometer (Model 6517A, Keithley Instruments, Cleveland, Ohio, USA).

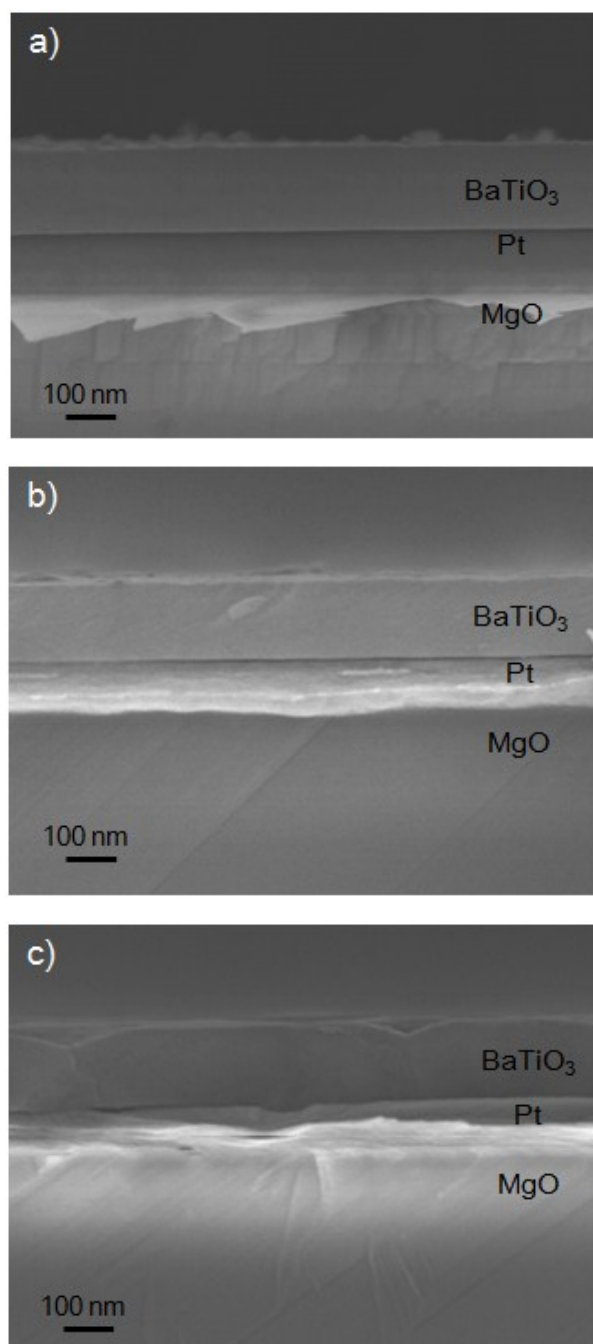


Fig. S1 Cross-sectional FE-SEM image of (a) BaTiO₃(100) film on a Pt(100)/MgO(100) substrate, (b) BaTiO₃(110) film on a Pt(110)/MgO(110) substrate, and (c) BaTiO₃(111) on a Pt(111)/MgO(111) substrate.

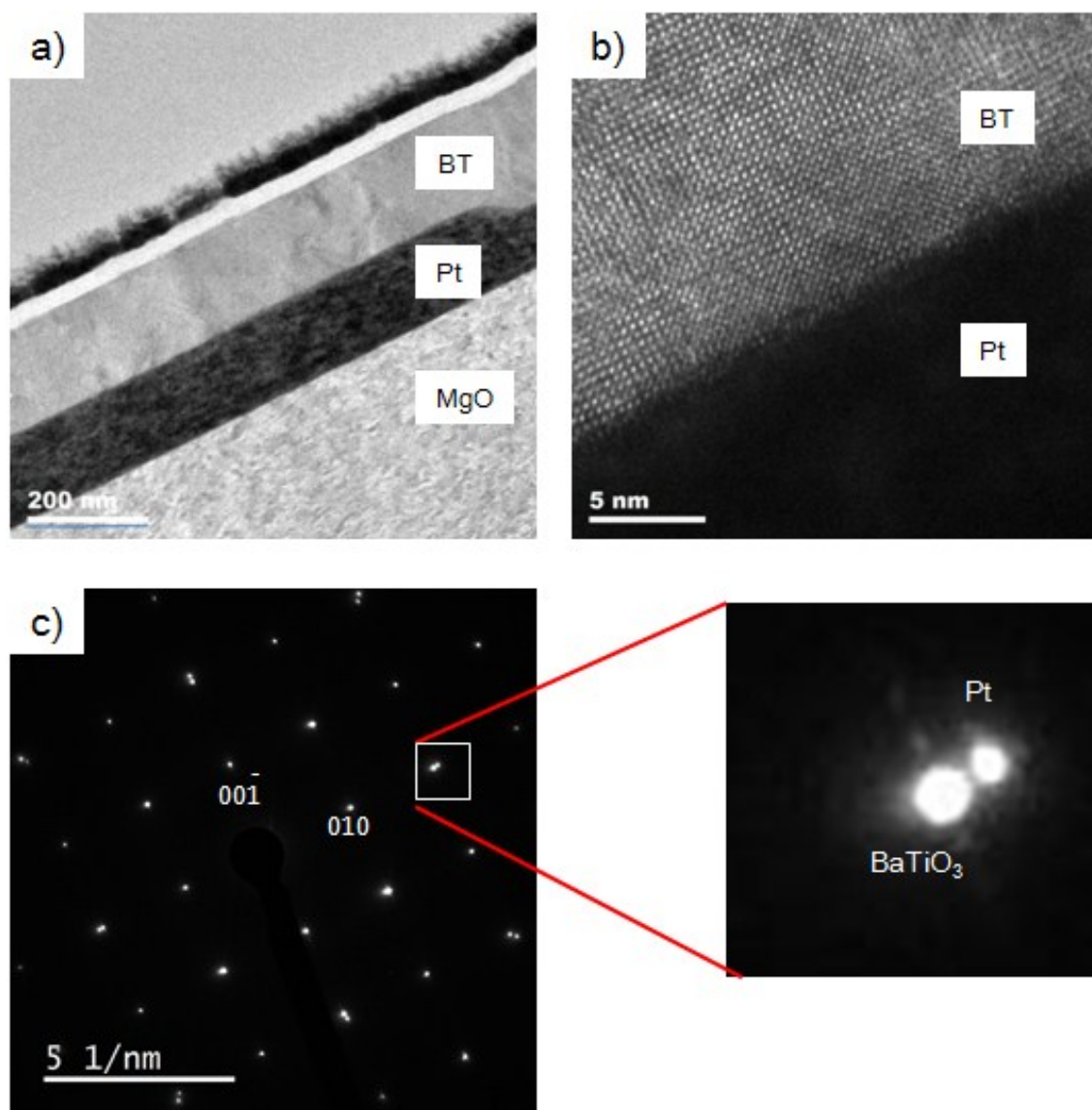


Fig. S2 (a) Cross-sectional TEM images of the BaTiO₃(100) film on Pt(100)/MgO(100), (b) boundary of the BaTiO₃(100) film and Pt(100) film, and (c) SAED of boundary of the BaTiO₃(100) film and Pt(100) film.

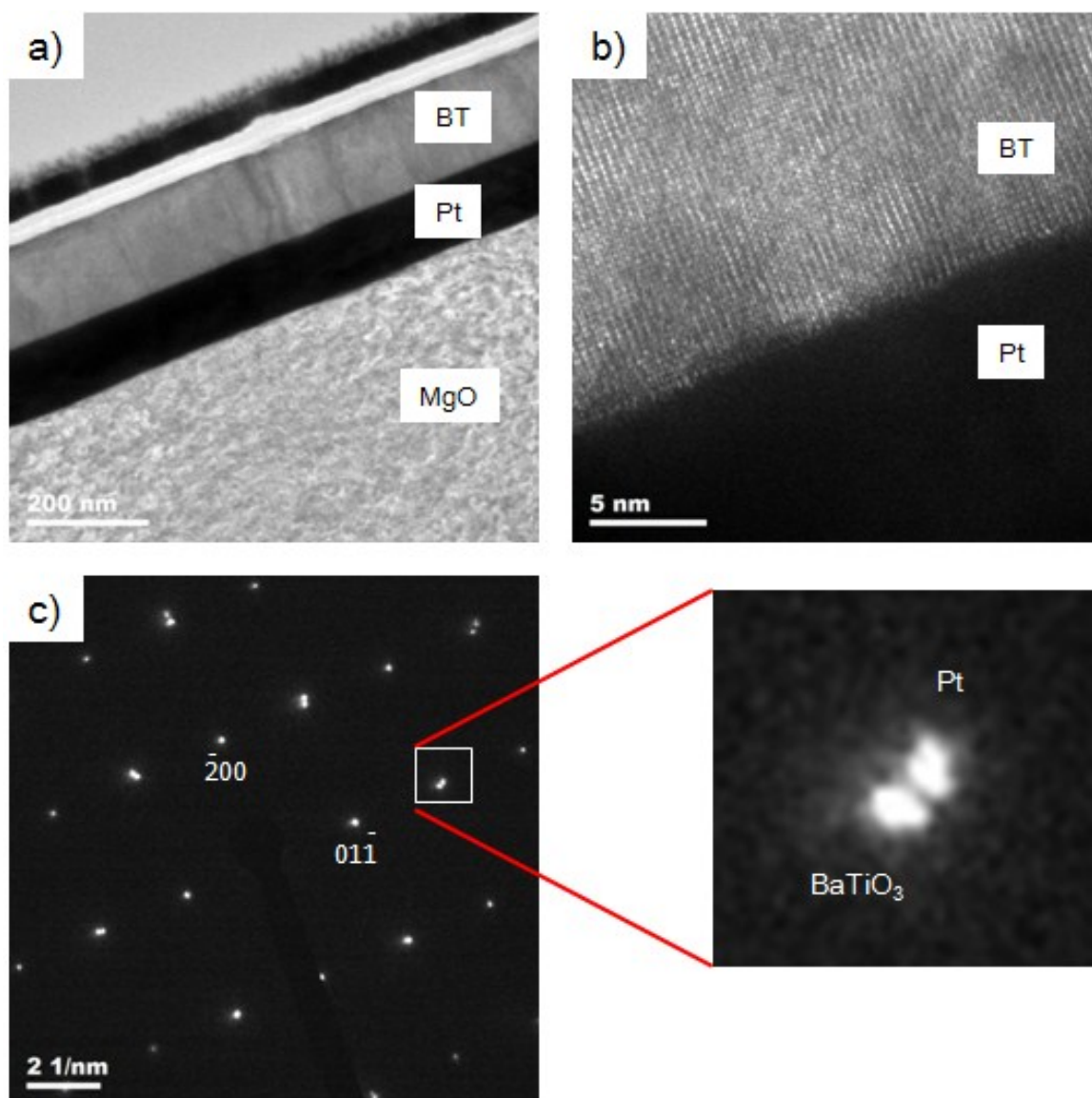


Fig. S3 (a) Cross-sectional TEM images of the BaTiO₃(110) film on Pt(110)/MgO(110), (b) boundary of the BaTiO₃(110) film and Pt(110) film, and (c) SAED of boundary of the BaTiO₃(110) film and Pt(110) film.

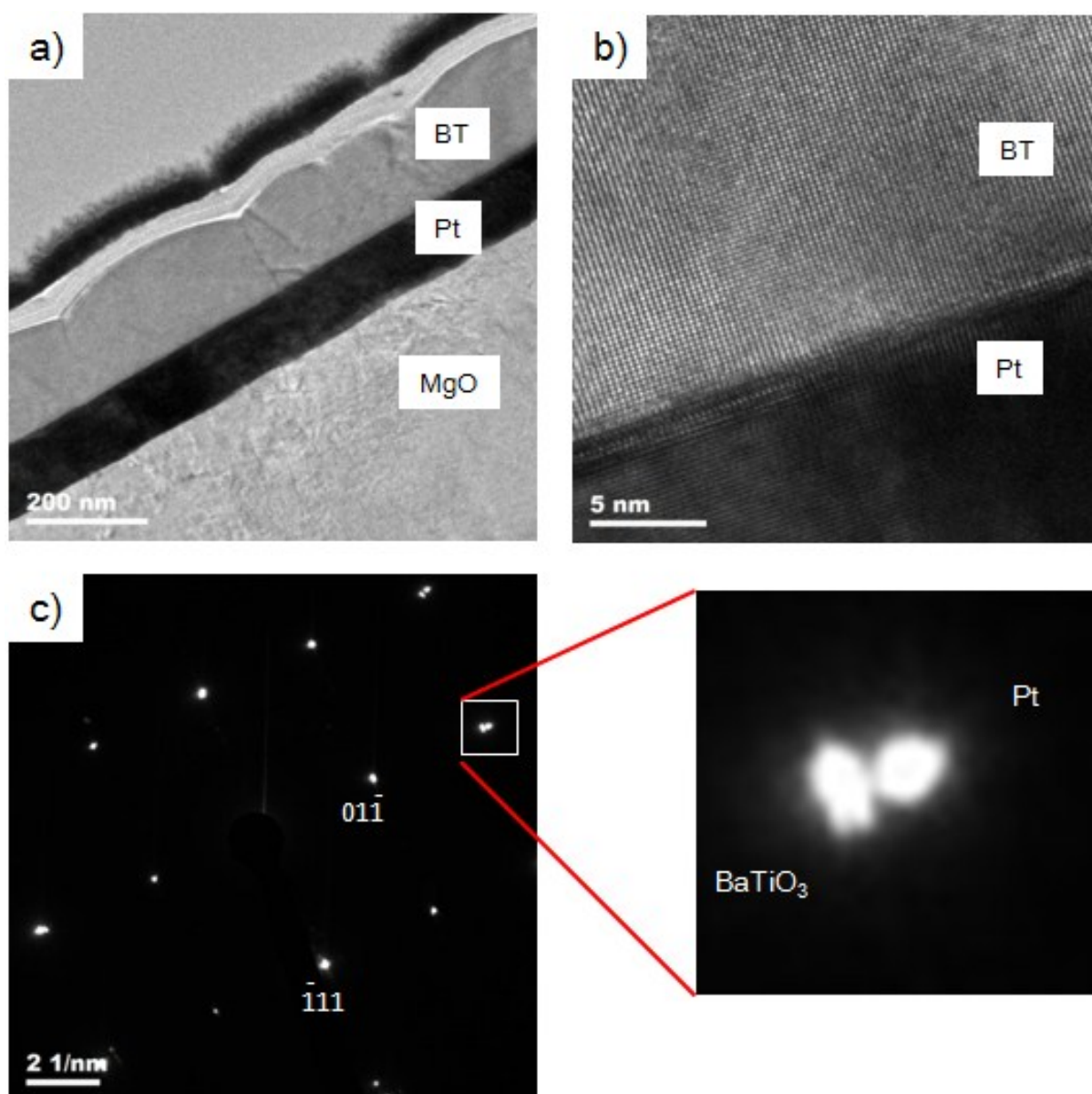


Fig. S4 (a) Cross-sectional TEM images of the BaTiO₃(111) film on Pt(111)/MgO(111), (b) boundary of the BaTiO₃(111) film and Pt(111) film, and (c) SAED of boundary of the BaTiO₃(111) film and Pt(110) film.

Table S1. Elastic constants and tensile stress in the plane of the growth direction of (100)-, (110)-, and (111)-oriented film.

Orientation of the film	Elastic constants	Calculated elastic constants (GPa)	Lattice expansion (%)	Estimated tensile stress (GPa)
(100)	C_{11}	173	1.50	2.60
(110)	$(C_{11} + C_{12})/2 + C_{44}$	237.5	4.25	10.09
(111)	$(C_{11} + 2C_{12} + 4C_{44})/3$	256.33	6.22	15.94

Table S2. Properties of thin films prepared from a variety of film orientations measured at 1 kHz and 0.1 V and DC resistivity at 300 kV/cm.

Orientation of the film	Thickness (nm)	Measured capacitance (nF)	Dielectric constant	tan (delta)
BaTiO ₃ (100)/Pt(100)/MgO(100)	165	11.68	1107	0.043
BaTiO ₃ (110)/Pt(110)/MgO(110)	160	22.10	2030	0.058
BaTiO ₃ (111)/Pt(111)/MgO(111)	165	22.54	2072	0.061

Table S3. DC resistivity of thin films prepared from a variety of film orientations measured at 300 kV/cm.

Orientation of the film	Resistivity ($\Omega \cdot \text{cm}$)
BaTiO ₃ (100)/Pt(100)/MgO(100)	5.91×10^8
BaTiO ₃ (110)/Pt(110)/MgO(110)	4.48×10^8
BaTiO ₃ (111)/Pt(111)/MgO(111)	8.70×10^7