Supporting Information for

The energy level of the $Fe^{2+/3+}$-transition in $BaTiO_3$ and $SrTiO_3$ single crystals

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The Reproducibility of the stepwise re-oxidation experiment

In addition to the sample in the main text which was prepared by reducing in the vacuum (sample 1), second sample (sample 2) was prepared by reducing in H_2/Ar atmosphere. In the preparation of sample 2, the $BaTiO_3$ was annealed in the glass tube with a H_2 5%—Ar gas flow at 60 sccm for 12h at 800°C and subsequently quenched to the room temperature without being exposed to the air. Pt electrodes were deposited on both surfaces without surface cleaning unlike the sample 1.

Figure S1 (a) shows Arrhenius plots of the samples 1 and 2. The conductivity of two samples went down in a quite similar way except for some points; in particular, the temperature at which the conductivity starts deviating from linear line was slightly different between sample 1 (~250°C) and Sample 2 (~270°C) and the decrement of the conductivity observed in each loop was wider in sample 2 than sample 1. Nevertheless, Figure S1(b) shows that the evolutions of the activation energy of two samples, which were almost identical to each other confirming the reproducibility of a relationship between the evolution of the conductivity and that of activation energy.

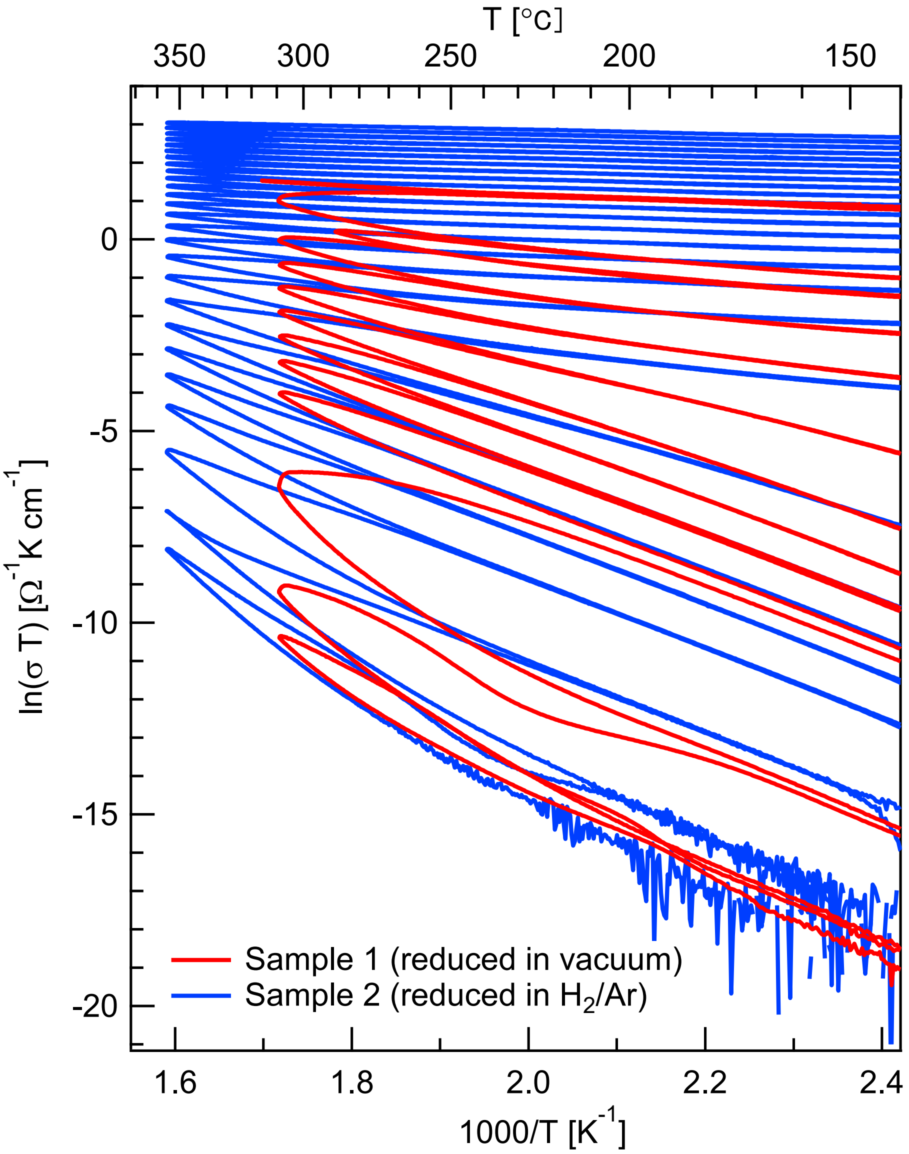

Figure S1. Conductivity of $BaTiO_3$ samples during stepwise re-oxidation.

Table S1. The impurity concentrations measured by GDMS technique

Elements	Concentration (ppm)	Concentration (cm^{-3})	Elements	Concentration (ppm)	Concentration (cm^{-3})
Li	< 0.05	$< 2.6\times10^{16}$	Pd	< 0.5	$< 1.7\times10^{16}$
Be	< 0.01	$< 4.0\times10^{15}$	Ag	< 100	$< 3.4\times10^{18}$
B	0.05	1.7×10^{16}	Cd	< 1	$< 3.2\times10^{16}$
F	1	1.9×10^{17}	In	0.5	1.6×10^{16}
Na	< 5.4	$< 8.5\times10^{17}$	Sn	4.6	1.4×10^{17}
Mg	0.66	9.8×10^{16}	Sb	< 0.79	$< 2.4\times10^{16}$
Al	0.26	3.5×10^{16}	Te	10	2.8×10^{17}
Si	0.55	7.1×10^{16}	I	0.1	2.9×10^{15}
P	< 0.1	$< 1.2\times10^{16}$	Cs	0.1	2.7×10^{15}
S	< 0.1	$< 1.1\times10^{16}$	La	< 0.5	$< 1.3\times10^{16}$
Cl	< 0.1	$< 1.0\times10^{16}$	Ce	< 0.05	$< 1.3\times10^{15}$
K	< 0.1	$< 9.3\times10^{15}$	Pr	< 0.05	$< 1.3\times10^{15}$
Ca	95	8.6×10^{18}	Nd	0.05	1.3×10^{15}
Sc	< 0.5	$< 4.0\times10^{16}$	Sm	< 0.1	$< 2.4\times10^{15}$
V	< 0.05	$< 3.6\times10^{15}$	Eu	< 0.05	$< 1.2\times10^{15}$
Cr	0.36	2.5×10^{16}	Gd	0.05	1.2×10^{15}
Mn	0.11	7.3×10^{15}	Tb	5	1.1×10^{17}
Fe	4.7	3.0×10^{17}	Dy	0.05	1.1×10^{15}
Co	< 0.05	$< 3.1\times10^{15}$	Ho	< 0.05	$< 1.1\times10^{15}$
Ni	0.36	2.2×10^{16}	Er	0.05	1.1×10^{15}
Cu	< 0.5	$< 2.9\times10^{16}$	Tm	< 0.05	$< 1.1\times10^{15}$
Zn	< 1	$< 5.5\times10^{16}$	Yb	< 0.05	$< 1.0\times10^{15}$
Ga	< 0.05	$< 2.6\times10^{15}$	Lu	< 0.05	$< 1.0\times10^{15}$
Ge	< 0.5	$< 2.5\times10^{16}$	Hf	< 0.5	$< 1.0\times10^{16}$
As	< 0.1	$< 4.8\times10^{15}$	W	< 5	$< 9.9\times10^{16}$
Se	< 0.1	$< 4.6\times10^{15}$	Re	< 0.05	$< 9.7\times10^{14}$
Br	< 0.1	$< 4.5\times10^{15}$	Os	< 0.05	$< 9.5\times10^{14}$
Rb	< 5	$< 2.1\times10^{17}$	Ir	< 0.05	$< 9.4\times10^{14}$
Sr	≤ 1100	$\leq 4.5\times10^{19}$	Pt	< 0.5	$< 9.3\times10^{15}$
Y	< 100	$< 4.1\times10^{18}$	Hg	< 0.1	$< 1.8\times10^{15}$
Zr	780	3.1×10^{19}	Tl	< 0.05	$< 8.9\times10^{14}$
Nb	< 50	$< 2.0\times10^{18}$	Pb	< 0.05	$< 8.7\times10^{14}$
Mo	< 5	$< 1.9\times10^{17}$	Bi	< 0.01	$< 1.7\times10^{14}$
Ru	< 0.1	$< 3.6\times10^{15}$	Th	< 0.01	$< 1.6\times10^{14}$
Rh	< 0.2	$< 7.0\times10^{15}$	U	< 0.01	$< 1.5\times10^{14}$