Effect of Heterointerface on Transport Properties of In-situ Formed MgO/titanate Core-shell Nanowires

Kazuki Nagashima, Takeshi Yanagida, Hidekazu Tanaka, Syu Seki, Akinori Saeki, Seiichi Tagawa and Tomoji Kawai.*

Institute of Scientific and Industrial Research, Osaka University, 8-1 Mihogaoka, Ibaraki, Osaka 567-0047 (Japan)

E-mail: yanagi32@sanken.osaka-u.ac.jp.

Supporting Information

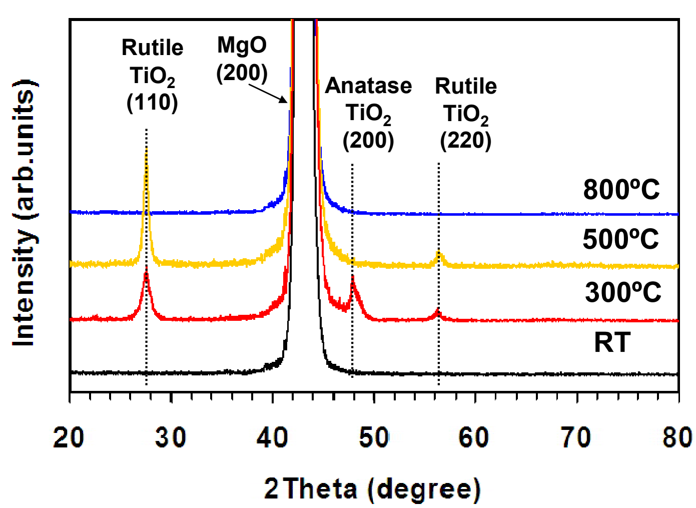

Figure S1. XRD pattern of the titanate thin films on MgO (100) single crystal substrate. These films were fabricated at 10^{-3} Pa of the oxygen pressure and the film thickness was controlled to be 100 nm.

Figure S1 shows the XRD data of the titanate thin films grown on MgO (100) single crystal substrate when varying the substrate temperature. The thin films grown at 300 ºC showed the epitaxial growth of mixed (110) oriented rutile structure and (100) oriented anatase structure. (110) oriented rutile structure was seen in the thin film grown at the substrate temperature of 500 ºC. On the other hand, such titanate peaks were no longer observable for the thin film grown at 800 ºC.

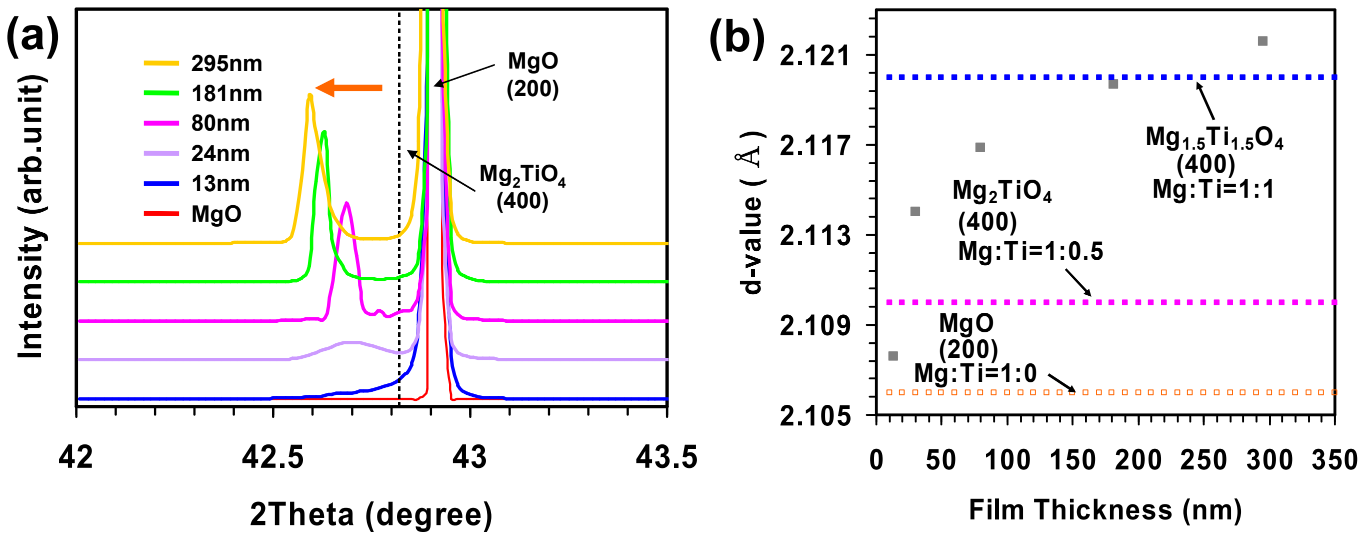

Figure S2. Structural analysis of the $(Mg,Ti)_3O_4$ thin films. (a) XRD pattern of the $(Mg, Ti)_3O_4$ spinel thin films on MgO (100) single crystal substrate. (b) Thickness dependence of the lattice constant of $(Mg,Ti)_3O_4$ thin films. All thin films were fabricated at 800 ºC and 10^{-3} Pa.

To clarify the nature of titanate thin films grown MgO (100) under the substrate temperature of 800 ºC, the crystallinity of titanate thin films was investigated, and the XRD data is shown in Figure S2a. The film thickness was varied from 13 to 295 nm to investigate the mixing nature between MgO and titanate. The presence of peaks around 42.6-42.7 degree can be seen, and the peak angle decreases with increasing the thickness. Comparison between the d-values estimated from the peaks and the lattice constants of possible $(Mg,Ti)_3O_4$ spinel structures is shown in Figure S2b. It can be seen that these peaks can be fairly identified as mixed spinel structures. In addition, increasing the thickness resulted in the increase of the d-value, approaching to $Mg_{1.5}Ti_{1.5}O_4$ structure. This trend can be readily understood in terms of increasing Ti component with increasing the thickness due to the distribution of Mg diffusion from the substrate. Thus the mixing nature between MgO and titanate dominates the crystal structures formed at 800 ºC, resulting in the $Mg_{2-x}Ti_{1+x}O_4$ spinel structures.

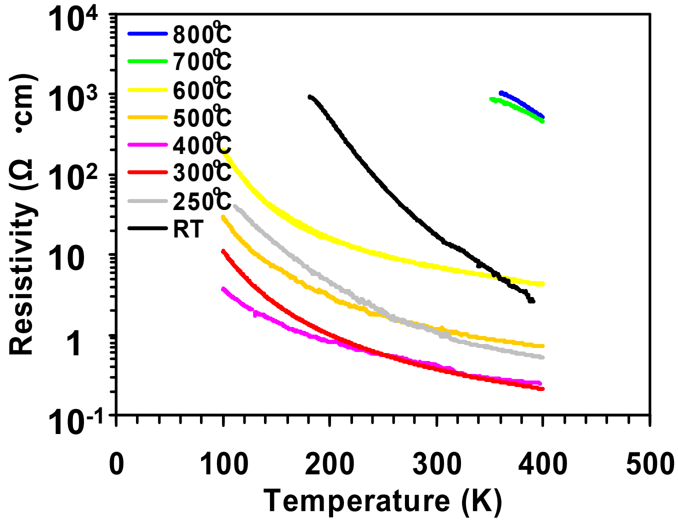

Figure S3. Transport properties of the titanate thin films grown on MgO (100) single crystal substrate. The films were fabricated at 10^{-3} Pa of oxygen pressure and the film thickness was 100 nm. The measurement was performed by using four probe method.

Figure S3 shows the effect of growth temperature on the transport properties of titanate thin films grown on MgO substrate. Firstly the resistivity decreases when increasing the temperature from RT to 300 ºC, through the minimum around 300-400 ºC and then increases drastically with increasing the temperature. This trend can be interpreted in terms of (1) the enhancement of the film crystallinity the temperature range between RT and 400 ºC and (2) the formation of insulative $Mg_{2-x}Ti_{1+x}O_4$ spinel structures for higher temperature range.