Investigation of Grain Boundary Features of Nano-grained $BaTiO_3$ Oxides Using By HVEM

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1. Introduction

$BaTiO_3$ ceramics with their crystallites critically reduced into nano-size and with at tetragonal phase at room temperature have been widely used in various electronic devices because of their unique and useful electrical characteristics [1,2], while the application of the nano-crystalline $BaTiO_3$ ceramics with a cubic structure to electronic devices is not available. It has been reported that the physical properties of nano-sized particles are affected by their size [3-5]. It is necessary to develop the novel fabrication of nano-crstalline $BaTiO_3$ with tetragonal phase for reasonable electronic devices containing nano-crystallites. The crystallites, which are surrounded by neighboring crystallites in polycrystalline $BaTiO_3$, are considered to be in a significantly different situation from the individual powders with the same size. The understanding of the structural variation of the nano-grained $BaTiO_3$ synthesized from nano-powders is very indispensable for the improvement of the nano-electronic technology.

In this study, the nano-sized $BaTiO_3$ with tetragonal phase were synthesized by hot-press sintering of nano-powders coated with Mn. The transition of the crystal structure of the nano-sized $BaTiO_3$ were tried to be observed.

2. Experimental

To prepare fine nano-sized $BaTiO_3$ powders, mixture solutions of Ba (Barium acetate (99.9%)), and Ti (titanium isopropoxide (99.9%)) precursors were added into a KOH solution (500mL) with vigorous agitation. The starting nano-powders, which were homogeneously coated with Mn, were used to produce the nano-sized $BaTiO_3$ powders with chemically-modified surfaces; uniaxial hot-press sintering of the surface-coated powders was carried out at low temperature. The crystalline structure of the nano-powders and the nano-meter-size barium titanate was analyzed by X-ray diffractometry (XRD; Philips, PW3719). To cross-check the phase of the ceramics, we used a Raman spectroscopy and a transmittance microscopy (TEM, CM200, Philips) facilities. The

chemical features of the ceramics were investigated by a X-ray photoelectron spectroscopy (XPS, 2803-S, SSI) and a secondary ion mass spectroscopy (SIMS, PHI-7200, Perkin-Elmer). To understand the relation of the grain boundary features and the transition of the crystal structural of nano-grained $BaTiO_3$ oxides, the high resolution transmission electron microscopy (HRTEM) images near the grain boundary of the samples were obtained by a high voltage electron microscopy (HVEM, JEOL); the resolution of HVEM is 0.12 nm at 1.25 MV.

3. Results and discussion

The crystal phase of the nano-grained $BaTiO_3$ ceramics, which were synthesized by hot-press sintering of the $BaTiO_3$ nano-powders coated with Mn, were discussed in terms of the effect of the grain boundary features. The nano-grained $BaTiO_3$ ceramics prepared from the non-coated $BaTiO_3$ nano-powders show a mixed state of the cubic and the tetragonal phase; on the other hand, the nano-grained $BaTiO_3$ ceramics prepared from the $BaTiO_3$ nano-powders coated with Mn exhibit only the tetragonal phase. The effect of the grain boundary features resulted in the phase transition from the cubic to the tetragonal phase, even though the grain size of the nano-grained $BaTiO_3$ ceramics is about 40 nm.

References

[1] H. Ihrig and W. Puschert, J. Appl. Phys., 48 (1997) 3081.

[2] M.-B. Park and N.-H. Cho, J. Am. Ceram. Soc., 84 (2001) 1937.

[3] F. Zhang, S.-W. Chan, J. E. Spanier, E. Apak, Q. Jin, R. D. Robinson, and I. P. Herman, Appl. Phys. Lett., 80 (2002) 17.

[4] S. Tsunekawa, R. Sivamohan, S. Ito, A. Kawazoe, and A. Kasuya, Phys. Rev. Lett., 85 (2000) 3440.

[5] X. Li and W.-H. Shih, J. Am. Ceram. Soc., 80 (1997) 2844.

[6] M. Anliker, H. R. Brugger and W. Kanzig, Helv. Phys. Acta, 27 (1954) 99.

[7] B. D. Begg, E. R. Vance and J. Nowontny, J. Am. Ceram. Soc., 77 (1994) 3186.

[8] K. Unchino, E. Sadanaga and T. Hirose, J. Am. Ceram. Soc., 72 (1989) 1555.

[9] M.-B. Park and N.-H. Cho, Solid State Ionics, 154-155 (2002) 407.