Structural phase transitions in AgTa_{0.5}Nb_{0.5}O₃ thin films

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(Received 4 January 2010; accepted 9 May 2010; published online 22 June 2010)

Octahedral tilt transitions in epitaxial AgTa_{0.5}Nb_{0.5}O₃ (ATN) films grown on (001)_p (where p = pseudocubic) oriented SrRuO₃/LaAlO₃ and LaAlO₃ substrates were characterized by electron diffraction and high resolution x-ray diffraction. It was found that the ATN films exhibited octahedral rotations characteristic of the *Pbcm* space group, similar to those seen in bulk materials; however, the temperature of the M₃ \leftrightarrow M₂ phase transition has been suppressed by ~ 250 K due to the fact that the correlation length for rotations about c_p was significantly reduced. The average off-center B-cation displacements, which signify the degree of long-range order for these local cation positions, were negligibly small compared to bulk materials, as inferred from the near-zero intensity of the 1/4(00l)_p-type reflections. On cooling, pronounced ordering of B-cation displacements occurred at ≈ 60 K which is significantly lower compared to bulk (≈ 310 K). The onset of this ordering coincides with a broad maximum in relative permittivity as a function of temperature. It is believed that point and planar defects in thin ATN films disrupt the complex sequence of in-phase and antiphase rotations around c_p thereby reducing the effective strength of interactions between the tilting and cation displacements.

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