In-situ Exploration of the Correlation between Domain Evolution and First-order Phase Transition in (K, Na)NbO_3 Based Single Crystal

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Domains and domain walls of ferroic materials have attracted dramatically interest due to the crucial influences on piezoelectric and dielectric properties as well as the performances of related nano-applications. It is worthy to consider the relationship of temperature dependent domain evolution and interior structural transformation. Raman spectroscopy, as a necessary tool to analyze the internal structure in nano/micro-scale, is employed to *in-situ* combine with piezoresponse force microscopy (PFM) in order to clarify the correlation between ferroelectric domains and structure information. In (K, Na)NbO_3 (KNN) based ferroelectrics, clear hysteresis nature in adjacent phases (R-O, O-T) has been found, namely thermal hysteresis effect.[1] It indicates that the orthorhombic (O) to tetragonal (T) conversion belongs to ferroelectric first-order phase transition. Here, the unambiguously reversible evolutions of 90°/180° domain walls companied with O-T phase transition have been investigated in $LiNbO_3$ modified $(K_{0.5}Na_{0.5})NbO_3$ single crystal during heating and cooling processes, as shown in Figure 1. The surface corrugations, 90° domain walls and reciprocal 180° *c*-domains as well as their evolution have been presented by temperature dependent PFM. The results confirm that ferroelectric domain formation keeps the closed relationship with interior structural change. Differences of internal stress among various phases can be obtained by analyzing the vibrational modes of NbO_6 octahedron. It promotes further to discuss the formation of 60° domain walls and the density of 90° domain boundaries in KNN based single crystal. The 180° domain with polarization reversal can also be seen during the phase transition. The present study affords an effective opportunity to explore the stable performance in a broad temperature range for domain-wall dependent ferroelectric devices.

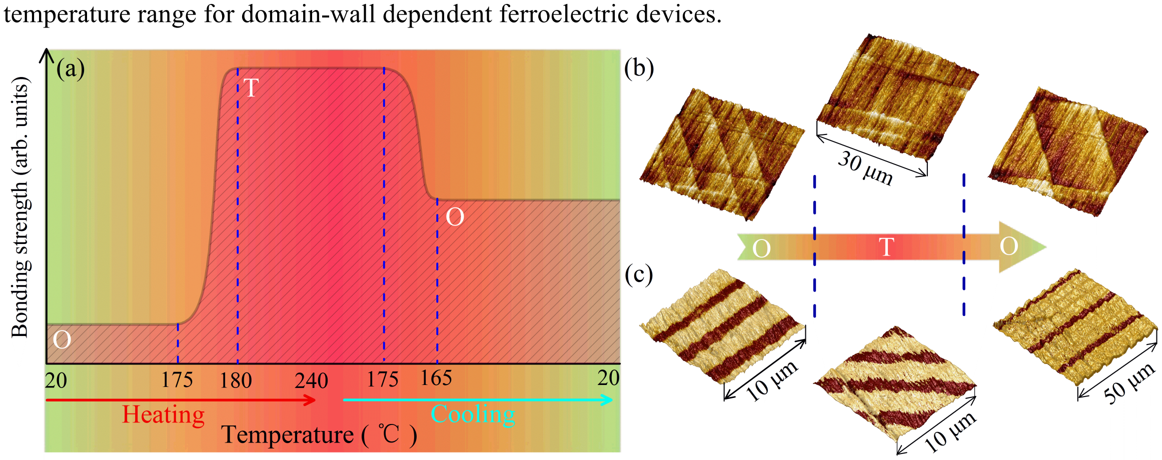

Figure 1. (a) General trend in temperature dependent bonding strength in various phases. (b)-(c) Three-dimensional topography images and in-plane domain evolution are illustrated during heating and cooling processes, respectively. All scales are 30 μm in (b).

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