Invited Paper

Nanostructure and Interfacial Structures of Ferroelectric Epitaxial Thin Films

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Ferroelectric thin films are considered to have a great potential for tunable microwave device applications, such as microwave tunable phase shifters, filters, oscillators, and antennas due to their relatively high dielectric constant, low dielectric loss and large electric field tunability. Special attention has been paid to the ferroelectric (Ba,Sr)TiO_3 and Ba(Zr,Ti)O_3 thin films due to their promise in microelectronic applications. Ferroelectric (Ba,Sr)TiO_3 films exhibit high dielectric constant but with relatively high loss tangent, especially at microwave frequencies which limits their practical applications, while $Ba(Zr_xTi_{1-x})O_3$ films exhibit field-controlled nonlinear dielectric constant and even more chemically stable properties than $(Ba_{1-x}Sr_x)TiO_3$ and good combination of high tunability and relatively low loss. In an attempt to achieve optimum properties of ferroelectric thin films, enormous efforts have been made to improve the film quality in terms of epitaxy, microstructure, composition, and interface control. In this invited talk, we will present an overview of the recent development of lead-free ferroelectric $(Ba_{1-x}Sr_x)TiO_3$ and $Ba(Zr_xTi_{1-x})O_3$ thin films. Specifically, we will present:

(1) Microstructure of epitaxial $(Ba_{1-x}Sr_x)TiO_3$ films and their atomic interface structure with respect to the MgO substrate. The identification of the initial grown TiO_2 monolayer of the $(Ba_{1-x}Sr_x)TiO_3$ film and the effect of the substrate surface structure (steps, terraces and kinks) on the film microstructure. (Figure 1)

(2) Twin-coupled multi-oriented nano-finger structures formed in the epitaxial $Ba(Zr_xTi_{1-x})O_3$ films and the evolution of such novel structures: Four types of the twin domains formed by coherently joining their {111} or {110} with the epilayer. The transition from the epilayer to nanofingers accomplished by alternatively introducing {111} and {110} plane twin boundaries, which results in gradual reduction of the lateral size of the epitaxial grains and eventually drives the epitaxial structure into twin-coupled nanofingers. $Ba(Zr_xTi_{1-x})O_3$ thin films with such novel structures are highly desirable for the design of microwave components operating at very low voltages. (Figure 2)

(3) Recent development of the interface structure studies of the ferroelectric epitaxial thin films in a two-dimensional (2-D) space using plan-view transmission electron microscopy (TEM). Interfacial structures have been a very important issue because their characteristics determine the epitaxial behavior, microstructure and physical properties of the films. Traditionally, interfacial structures have been studied using cross-sectional TEM and the structural information is limited in 1-D space. The 2-D interface studying provides critical structural (such as local strain) information that is lacking from the cross-section TEM. (Figure 3)

(4) Development of interface regulated [Ba(Zr,Ti)O_3)//(Ba,Sr)TiO_3)] multilayered films for new properties that are not available in the individual component materials. (Figure 4)

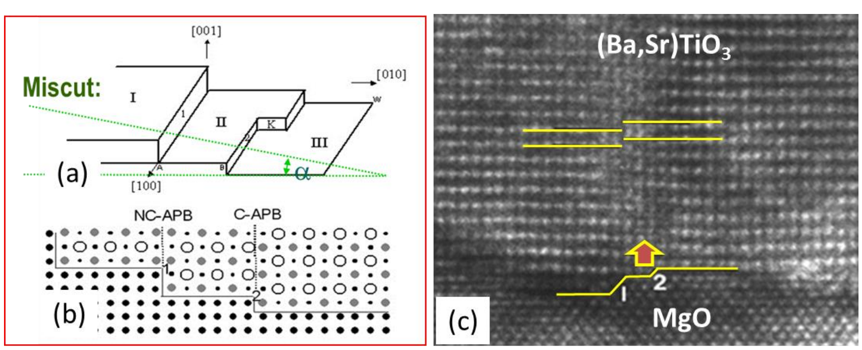

Figure 1 Illustration of the substrate surface (a) showing steps, terraces and kinks and (b) (Ba,Sr)TiO_3/MgO interface along the $[100]_{MgO.}$ (c) HRTEM image of (Ba,Sr)TiO_3/MgO interface.

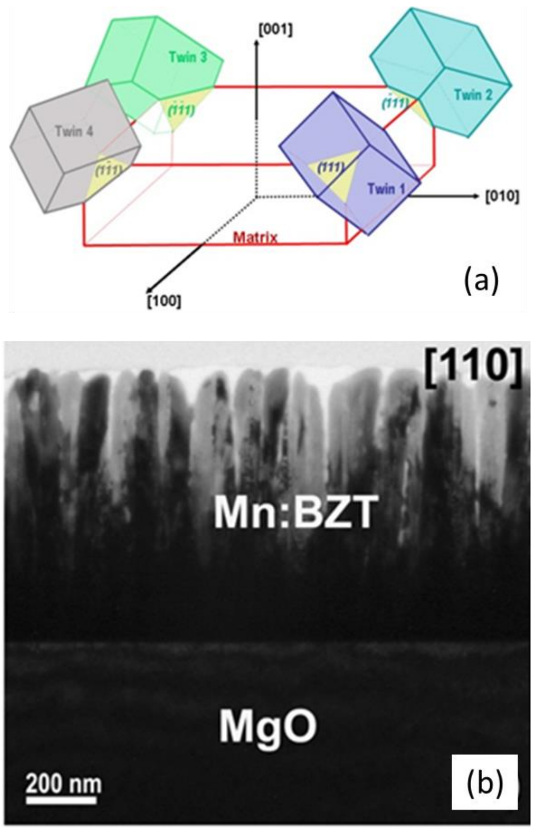

Figure 2 (a) Illustration of four types of twins formed by joining {111}. (b) XTEM of Ba(Zr,Ti)TiO_3/MgO showing nanofinger structures.

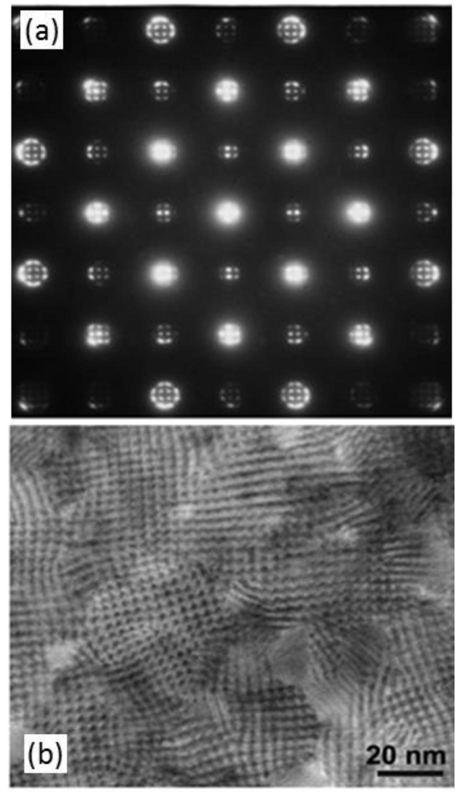

Figure 3 (a) Electron diffraction pattern and (b) HRTEM image of a 2-D (Ba,Sr)TiO_3/MgO interface.

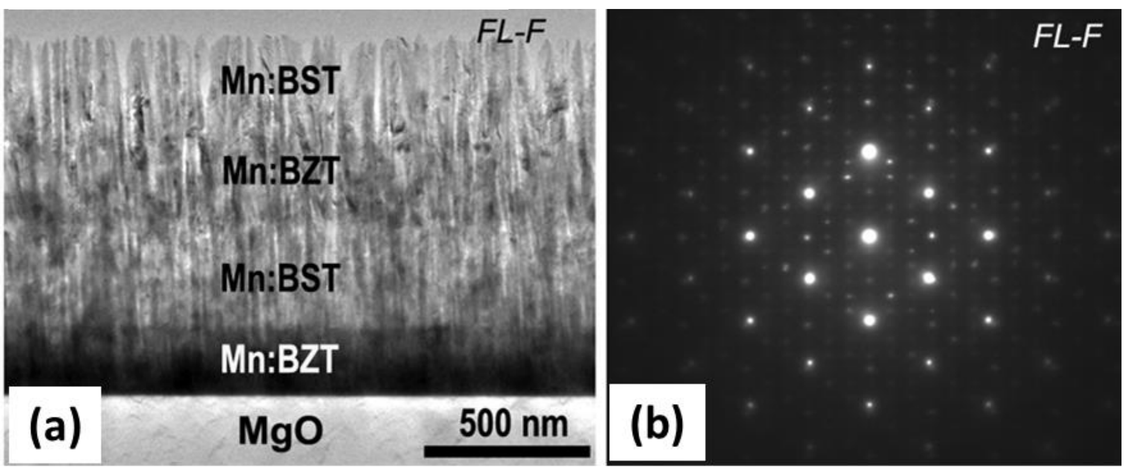

Figure 4 (a) Cross-section TEM and (b) electron diffraction pattern of a Mn:(Ba,Sr)TiO_3// Mn:Ba(Zr,Ti)O_3 multilayered structure.