Nano-Structure of PLD-Grown Epitaxial $PbTiO_3/BaTiO_3$ Superlattices by Synchrotron X-ray Diffraction

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By combining different ferroelectric layers, such as $PbTiO_3$ (PTO), $BaTiO_3$,(BTO) into artificially modulated structures, it is possible to investigate the role that size and interface play in the ferroelectric phase transition, the ferroelectric coupling across dielectric layers, the effects of strain on the ferroelectric properties. The physical behaviour of such compounds is primarily by their epitaxial crystalline quality, their composition and their structural perfection. We have extended a diffraction model[(1)], previously applied on metallic and semiconductor multilayers, to the more complex case of $(PTO/BTO)_n$ perovskite superlattices. The entire (001) diffraction profiles of the $(BaTiO_3/PbTiO_3)_n$ superlattices are fitted over 8 orders of diffraction (L=1 to 8). We evaluate the coherence length, the interface roughness, the discrete thickness fluctuations, and the intra-layer gradients of strain and atomic diffusion in the <001> growth direction.

Probing the reciprocal space along <100> and <010> shows the distribution and orientations of coherent domains and their respective unit cell dimensions parallel to the growth plane. Our diffraction measurements support the presence of {a} domains, i.e. the polar axis of $PbTiO_3$ is parallel to the surface, as a result of large lattice relaxation.

[1] Fullerton et al., *Phys. Rev.*, 1992, **B45**, 9292.

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