$SrTiO_3$ thin films: A Ferroelectric

Beamline: X23A2

Category of Researcher: PRT member

Technique: NEXAFS

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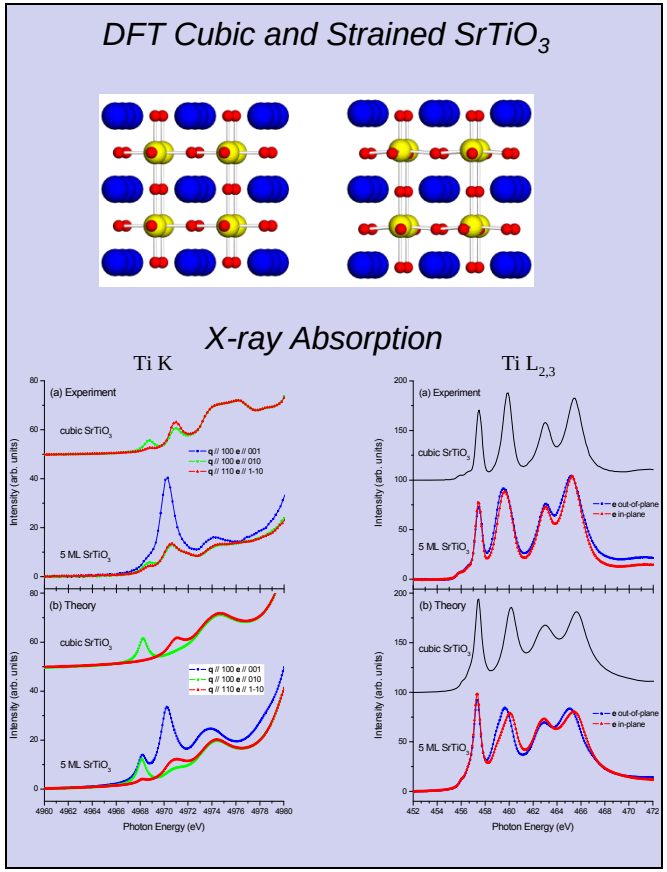
Publication: Ferroelectric distortion in $SrTiO_3$ thin films on Si(001) by x-ray absorption fine structure spectroscopy, *Phys. Rev. B, Rapid Communications*, 75, 140103(R) (2007).

Motivation: To study the local atomic and chemical environment of the strain-induced ferroelectric phase transition in $SrTiO_3$ thin films grown coherently on Si using first principles theoretical modeling of both the local atomic structure and the x-ray absorption near-edge fine-structure spectra.

Results: Ti-*K* and Ti-$L_{2,3}$ x-ray absorption fine-structure near-edge spectra of $SrTiO_3$ thin films grown coherently on Si(001) reveal the presence of a ferroelectric (FE) distortion at room temperature. The ferroelectric distortion manifests itself as an enhancement of the Ti *1s – 3d* transition which becomes dipole allowed (due to *3d-4p* hybridization) in the ferroelectric state. This unique phase ($SrTiO_3$ is normally not ferroelectric at any temperature) is a direct consequence of the compressive biaxial strain achieved by coherent epitaxial growth and has now been used to make ferroelectric-RAM.



Top: (Left) Structure of cubic $SrTiO_3$. (Right) Structure of tetragonally distorted $SrTiO_3$ on Si(001) as calculated by DFT. The distorted structure reveals both the AFD and FE distortions.
Bottom: Bethe-Salpeter calculations of the Ti-K (Left) and Ti-$L_{2,3}$ (Right) near edge structures using the atomic coordinates of the theoretical structures (Top).