Evidence for phase transition in the incoherent lattice fluctuations, lattice distortion and local microstructure of pure and implanted SrTiO$_3$

KALYAN SASMAL, WEI-KAN CHU, Texas Center for Superconductivity Department of Physics, University of Houston, TX, USA — Low temp Rutherford Backscattering Spectrometry-Axial Ion Channeling used to probe displacive structural phase transition (PT) & Jahn-Teller (JT) lattice distortion in perovskite SrTiO$_3$. It provides direct evidence of incoherent lattice fluctuations as function of temp across non-ferroelectric (FE) 2$^\text{nd}$ order antiferrodistortive cubic to body-centered tetragonal structural PT at Curie-Weiss $T_0$ =105 K, caused by antiphase tilting of TiO$_6$ octahedra by minimizing Gibbs free energy, opens bandgap & weakens FE instability by reducing cross gap hybridization. Defects in semiconducting SrTiO$_3$ narrows large band gap & raises Fermi level into conduction band & ensures conductivity. JT effect occur for degenerate filled & empty molecular orbitals.

Critical channeling angle $\psi_c$ & ratio of minima of angular RBS-ICh spectral yield $\chi_{\text{min}}$ for Sr & Ti sublattices determine JT lattice distortion in transition element (Fe, Cr etc.) implanted SrTiO$_3$. Similar $\psi_{1/2}$ values for Sr sublattice indicates no displacement of Sr. Distortion of Ti sublattice infers implanted Fe & Cr is actually located in Ti positions but not in interstitial positions. Temp dependence of Thermal vibrational amplitudes of Sr & Ti also displacements of Ti$^{4+}$ are calculated based on Linhard’s continuum model. Implanted SrTiO$_3$ shows a minor tetragonal phase corresponds to lattice expansion along c-axis & it’s not randomly oriented. Local microstructure & atomic distortions studied with HR-TEM (FIB prepared), XPS, GID-XRD & Raman Scattering.

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