

Abstract Submitted  
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**Evidence for phase transition in the incoherent lattice fluctuations, lattice distortion and local microstructure of pure and implanted SrTiO<sub>3</sub>** 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<sub>3</sub>. It provides direct evidence of incoherent lattice fluctuations as function of temp across non-ferroelectric (FE) 2<sup>nd</sup> order antiferrodistortive cubic to body-centered tetragonal structural PT at Curie-Weiss T<sub>0</sub> =105 K, caused by antiphase tilting of TiO<sub>6</sub> octahedra by minimizing Gibbs free energy, opens bandgap & weakens FE instability by reducing cross gap hybridization. Defects in semiconducting SrTiO<sub>3</sub> 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  $\chi_{\min}$  for Sr & Ti sublattices determine JT lattice distortion in transition element (Fe, Cr etc.) implanted SrTiO<sub>3</sub>. 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<sup>4+</sup> are calculated based on Linhard's continuum model. Implanted SrTiO<sub>3</sub> 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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