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TUNING OXYGEN VACANCY CONCENTRATION AT STRONTIUM TITANATE GRAIN BOUNDARIES

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Tuning Oxygen Vacancy Concentration at Strontium Titanate Grain Boundaries

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A great number of electronic devices derive their scientifically interesting and technologically important properties from electrically active interfaces, which include: grain boundaries, ferroelectric domains, electrode-film interfaces etc. The electrical activity of such interfaces originates from a convoluted yet tractable interplay among numerous interfacial variables, including local atomic structure, defect chemistry and resultant localized changes in electronic structure. This is the basis for formation of interfacial trapped charge, and space-charge potential, which modify substantially under applied bias.

Our study utilizes oriented bicrystals of $SrTiO_3$ as model systems to understand the nonlinear transport, capacitance and space-charge phenomena. Bulk donor (Nb) doped $SrTiO_3$ bicrystal exhibits a non-linear I-V behavior with resistivity almost 4 orders of magnitude higher than its single crystal counterpart. This behavior is attributed to the presence of electrostatic potential barrier at the grain boundary. The grain boundary potential barrier can be tailored by oxidation/reduction excursions as well as by grain boundary specific doping with transition metal elements, such as manganese (Mn). The tuning occurs as a result of change in the defect chemistry specifically at interfaces. By tuning processing parameters one can manipulate oxygen vacancy concentration as well as variable valence states exhibited by Mn (as Mn^{2+} and Mn^{3+}) in order to tailor grain boundary barrier characteristics, particularly $__B$ (barrier height). Diverse analytical techniques such as EELS and Z-contrast imaging are employed in conjunction with macroscopic electrical measurements (four probe I-V) to obtain predictive structure-property relations for interfaces in $SrTiO_3$.