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The Role of Strain on Grain Boundary Structure/Property Relations

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THE ROLE OF STRAIN ON GRAIN BOUNDARY STRUCTURE/PROPERTY RELATIONS

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Grain boundaries comprise arrays of dislocations that induce significant local strains even if the long-range strain fields are negligible. These short-range strains may be sufficient to lead to the spontaneous generation of point defects at high concentrations, changing the local stoichiometry and causing a valence imbalance. This is the origin of the electrical barriers at grain boundaries in $SrTiO_3$, where a combination of atomic-resolution Z-contrast microscopy, electron energy loss spectroscopy and first-principles theory shows the grain boundaries to be intrinsically non-stoichiometric[1]. The Ti:O ratio is increased at grain boundaries compared to the bulk, leading to excess electrons in the conduction band. In p-type bulk this leads to a p-n-p type of band structure. The same effect occurs in the structurally related high temperature superconductor, YBCO. As the charge carriers in this material are holes, the excess electrons at the boundary lead to a depletion zone which is non-superconducting. A structural unit model of the grain boundary structure is able to quantitatively explain the exponential decrease in superconducting critical current with grain boundary misorientation.

[1] M. Kim et al., "*Nonstoichiometry and the electrical activity of grain boundaries in $SrTiO_3$*", Physical Review Letters, **86**,4056 (2001).