# Thermopower in highly reduced n-type ferroelectric and related perovskite oxides and the role of heterogeneous nonstoichiometry

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Abstract: Nonstoichiometric perovskite-structured alkaline-earth titanates with ferroelectric, paraelectric, and paraelastic phases were investigated for thermoelectric properties. Depending on the degree of reduction, different trends are noted. In ferroelectric $BaTiO_3$, thermopower anomalies are observed in and around the paraelectric (Pm3m)-ferroelectric (P4mm) and ferroelectric (P4mm)-ferroelectric (Cmm2) phase transition temperatures, and the nature of these trends was found to depend on the degree of reduction. This indicates a coupling between the thermoelectric effect and the ferroelectric phase transition, a phenomena also noted in the recent work of Kolodiazhnyi [T. Kolodiazhnyi, Phys. Rev. B 78, 045107 (2008)]. Heavily reduced $SrTiO_{3-\delta}$ showed a strong metallic behavior in the thermopower and conductivity data without anomalies as the phase is paraelastic in the temperature range studied. The nature of the reduction from the low oxygen partial pressure anneals is heterogeneous; clusters of defects similar to 3 nm wide meander through the crystallites. The defective regions have high oxygen vacancy concentrations, and the chemical nature of the Ti changes from $Ti4^+$ to $Ti3^+$. The complex nature of the thermochemical reduction near the metal-insulator transition will challenge simple physical models for oxide thermoelectrics. Traditional thermopower models are discussed in relation to the reported thermopower and the conductivity in the paraelectric and ferroelectric phases.