Boosting thermoelectric performance by defect chemistry engineering

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Thermoelectric (TE) harvesting is expected to play an important role in future sustainable energy technologies, provided by simplicity, excellent scalability and reliability, and self-sufficiency to enable mobile or remote applications. Donor-substituted strontium titanates are amongst the most promising oxide thermoelectrics, mainly for conversion of high temperature heat sources with enhanced Carnot efficiency, overcoming critical shortcoming of intermetallic-based thermoelectrics (toxicity and limited thermal and redox stability). Recent work in our group boosted the high-temperature thermoelectric performance in tantalum - (Fig. 1, top left graph), niobium and tungsten-substituted strontium titanates, by shifting prevailing structural defects from Ruddlesden-Popper-type (SrO^{RP}) and other oxygen-rich defects (O''_{shear}), confirmed by TEM (Fig. 1), to oxygen (Vö) and cation nonstoichiometry (V''_{Sr}). This unique approach of defect chemistry engineering can be combined with complementary microstructural design to further promote electrical transport and suppress thermal leakage, thus opening new possibilities to upgrade $SrTiO_3$-based thermoelectrics.

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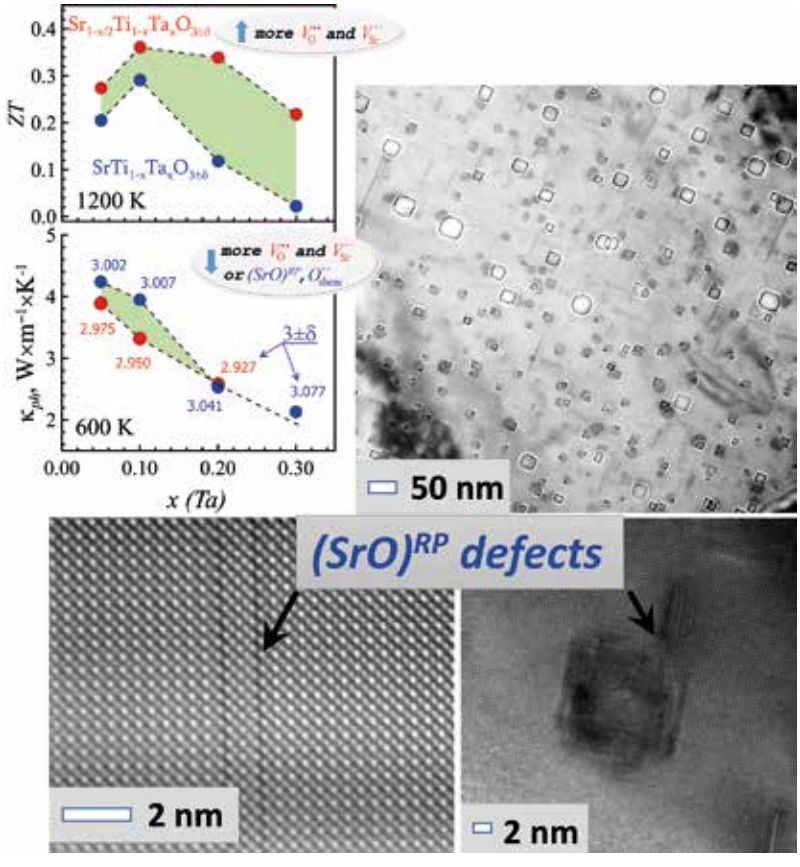

FIGURE 1
The top left graph shows dimensionless figure of merit (ZT) and lattice thermal conductivity (κ_{ph}) of $SrTi_{1-x}Ta_xO_{3\pm\delta}$ (blue circles) and $Sr_{1-0.5x}Ti_{1-x}TaxO_{3\pm\delta}$ (red circles) ceramics. The numbers indicate total oxygen content, obtained from thermogravimetry data. The green area illustrates *ZT* enhancement and κ_{ph} reduction due to defects engineering. High-resolution TEM images of $Sr_{1.05}Ti_{0.9}Nbo_{.1O3\pm\delta}$ lamellar sample, confirming the formation of Ruddlesden-Popper-type defects, are also shown.