Heterostructural Alloying – A Design Tool to Improve Functionality

Scientific Achievement

Metastable (SnCa)Se with improved thermoelectric functionality was realized by combining theory-guided alloying with non-equilibrium growth.

Significance and Impact

Alloying to target desired structures is emerging as a powerful materials design tool for applications requiring multi-property optimization. In this case, a factor of 100 increase in the power factor, which depends on Seebeck coefficient and electrical resistivity, is achieved in going from orthorhombic SnSe to cubic $Sn_{0.84}Ca_{0.16}Se$ (Fig. 2).

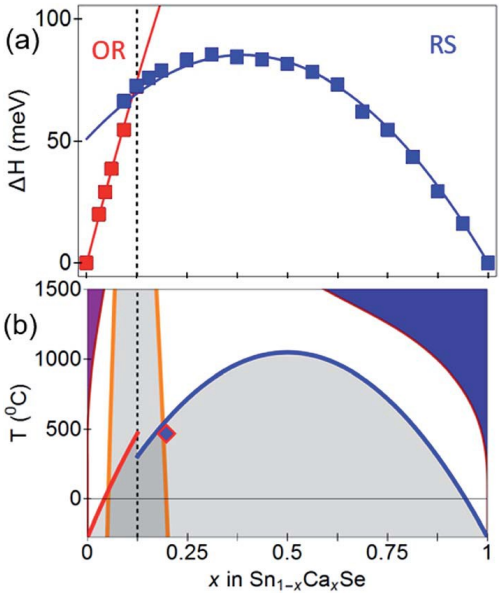

Fig. 1: Predicted phase diagram. Isotropic rock-salt (RS) structure desired.

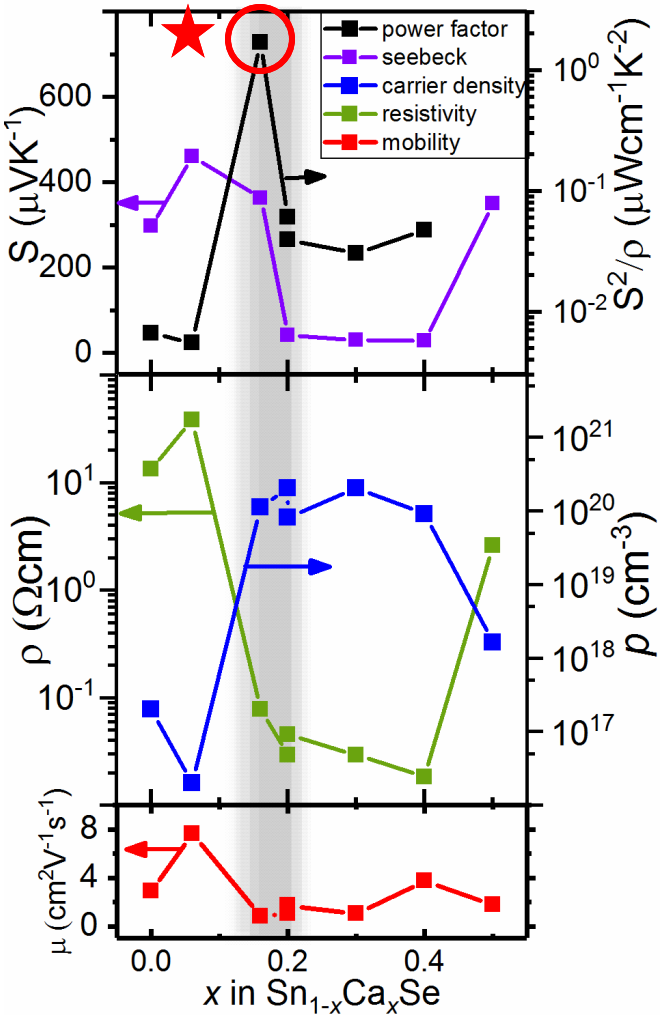

Fig. 2: Measured transport properties of PLD-grown (SnCa)Se thin films.

Research Details

Theory: DFT/RPA accurately calculates alloy phase diagrams (Fig. 1).

Synthesis: $Sn_{1-x}Ca_xSe$ films by pulsed laser deposition (PLD).

Characterization: Crystal structure by X-ray diffraction, decomposition microstructures by scanning transmission electron microscopy / energy-dispersive X-ray spectroscopy, transport measurements by Hall effect, Seebeck effect, electrical resistivity. Optical absorption determines bandgap and thickness.

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