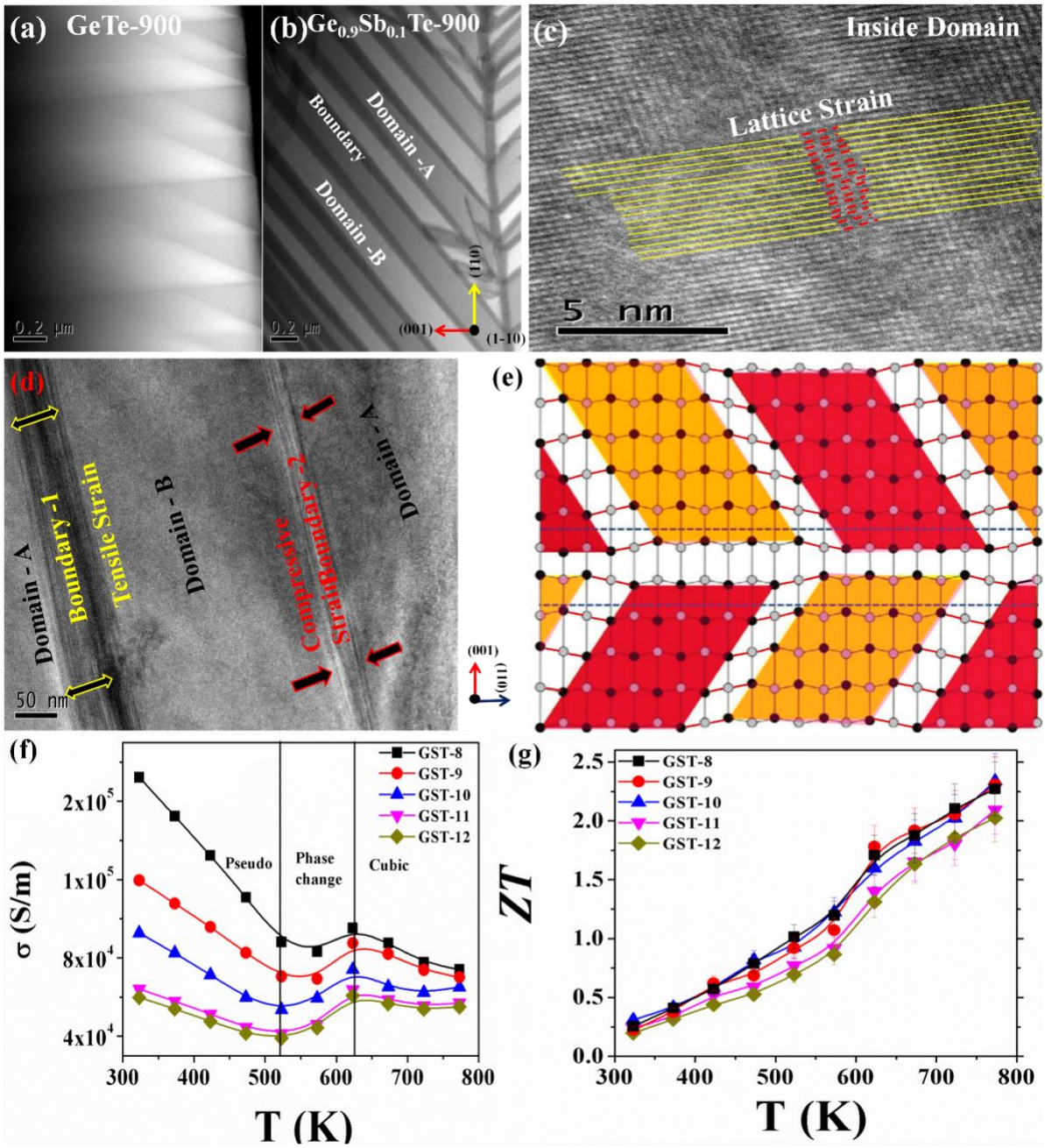
Synergistic optimization of thermoelectric performance of Sb doped GeTe with strained domain and domain boundaries

For the first time ***Dr Raman Sankar*** group have reported the systematic vacancy control of Ge in GeTe system by doping Sb in to the system. The concomitant carrier concentration (n) and the aliovalent Sb ion substitution led to an optimal doping level of x=0.10 to show ***ZT ~2.35 near 800 K***, which is ***significantly higher than*** those single- and multi-elementals substitution studies of GeTe system reported in literature. The prominent results were published in **Journal of Material Chemistry –A**, published by **Royal Society of Chemistry** on 13 Feb 2020.

Microdomain structural changes of undoped (a) GeTe-900, and (b) herringbone domain structure of $Ge_{0.9}Sb_{0.1}Te$-900 with thickened domain boundaries are shown in figure. (c) The amplified view of Sb doping-centre introduced local strain within the herringbone domain of $Ge_{0.9}Sb_{0.1}Te$, as revealed by the gradual displacement that is used to relieve the local strain. (d) Herringbone domain structures for $Ge_{0.9}Sb_{0.1}Te$-900 with alternating tensile/compressive domain boundaries. The inset shows a magnified view near the boundary with tensile strain. (e) Schematic representation of the herringbone domain with alternating tensile/compressive strains, replotted following the atomistic model proposed by Lee *et al.* with copyright permission. Figure (f) shows the electrical conductivity (σ) for $Ge_{1-x}Sb_xTe$-900 (x=0.08-0.12) as a function of temperature. It is found that σ(x) at 300 K decreases with increasing Sb substitution, which must be attributed to the reduction of carrier concentrations (*n*). Due to the synergetic effects of carrier optimization, band structure modulation, and enriched phonon scattering mechanisms to reduce thermal conductivity, the overall thermoelectric performance *ZT* for the Sb substituted GeTe system has reached a record high value of **~ 2.35 at ~800 K** through the single specie doping of Sb for $Ge_{0.9}Sb_{0.1}Te$, as summarized in figure (g).

Journal Link: **https://doi.org/10.1039/D0TA00628A**


(a) GeTe-900
(b) $Ge_{0.9}Sb_{0.1}Te$-900
Domain -A
Boundary
Domain -B
(110)
(001)
(1-10)
0.2 μm
0.2 μm
(c) Inside Domain
Lattice Strain
5 nm
(d)
Domain - A
Boundary -1
Tensile Strain
Domain - B
Compressive Strain
Boundary -2
Domain - A
50 nm
(e)
(001)
(011)
(f)
GST-8
GST-9
GST-10
GST-11
GST-12
Pseudo
Phase change
Cubic
σ (S/m)
T (K)
(g)
GST-8
GST-9
GST-10
GST-11
GST-12
ZT
T (K)