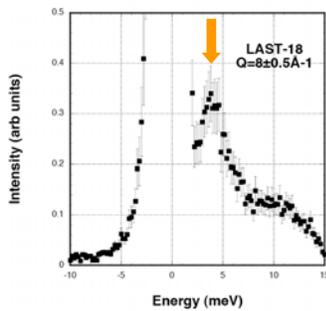
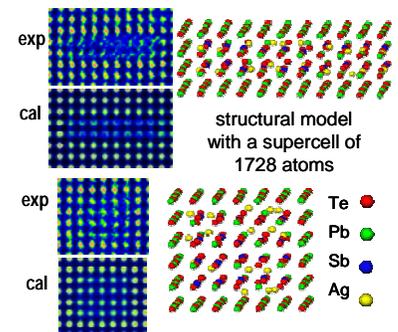
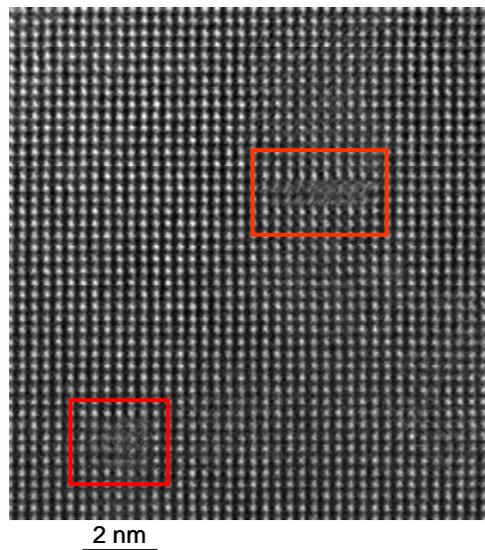


STRUCTURE ORIGIN OF THE ENHANCED THERMOELECTRIC POWER

Today approximately 60% of the energy consumption in the US is lost, mostly through waste heat. Development on thermoelectric technology that converts waste heat, for example the heat from radiator in automobiles, to electricity can lead to significant energy savings. Many recent advances in thermoelectric materials are attributed to nanoscale phenomena, where nanoprecipitates are used to modify thermal and electronic transport for improved thermoelectric performance. A prerequisite for understanding properties of these complex materials is an accurate description of the atomistic structure of their nanoscale constituents. In collaboration with researchers at General Motors recently we have studied one of the best performing thermoelectric compounds they developed, PbTe-AgSbTe₂, to understand the structural origin of the enhanced thermoelectric properties using aberration corrected electron microscopy. By directly observe unprecedented small precipitates, especially their size (below 2nm), shape (cube and plate) and spatial distribution we were able to identify their roles for the superior thermoelectric behavior. Density functional theory (DFT) calculations with supercomputers allow us to compare experiment with theoretical models and to determine the structure of the nanoprecipitates. Extensive calculations demonstrate the nucleation and atomic arrangement of the nanoprecipitates is driven by the interplay of electric dipolar interactions and strain fields. These findings provide crucial insights for the development of advanced nanocomposite thermoelectric materials.



Inelastic neutron scattering showing a phonon resonant peak at 4meV ($\lambda r \sim 1.8$ nm) in PbTe-AgSbTe₂. Corresponding defects (right) with the same length scale were identified using advanced electron microscopy.



Two typical defects present in the sample that are responsible to the enhanced thermoelectric properties. Their structures have been determined by comparison of experiments and DFT calculations.

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