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Title: Local ferroelectric polarization switching driven by nanoscale distortions in thermoelectric

Sn0.7Ge0.3Te

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Abstract:

A remarkable decrease in the lattice thermal conductivity and enhancement of thermoelectric figure of merit were recently observed in rock-salt cubic SnTe, when doped with germanium (Ge). Primarily, based on theoretical analysis, the decrease in lattice thermal conductivity was attributed to local ferroelectric fluctuations induced softening of the optical phonons which may strongly scatter the heat carrying acoustic phonons. Although the previous structural analysis indicated that the local ferroelectric transition temperature would be near room temperature in Sn0.7Ge0.3Te, a direct evidence of local ferroelectricity remained elusive. Here we report a direct evidence of local nanoscale ferroelectric domains and their switching in Sn0.7Ge0.3Te using piezoeresponse force microscopy(PFM) and switching spectroscopy over a range of temperatures near the room temperature. From temperature dependent (250-300 K) synchrotron X-ray pair distribution function (PDF) analysis, we show the presence of local off-centering distortion of Ge along the rhombohedral direction in global cubic Sn0.7Ge0.3Te. The length scale of the Ge2+ offcentering is 0.25-0.10 Å near the room temperatures (250-300 K). This local emphatic behaviour of cation is the cause for the observed local ferroelectric instability, thereby low lattice thermal conductivity in Sn0.7Ge0.3Te.

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