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The nature of phase transition in GeTe - the parent compound of the phase-change materials

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Germanium telluride (GeTe) has attracted an intense renewed interest in the past few years for its relevance and high performance as a phase-change material as such and in combination of the form (GeTe)m(Sb2Te3)n which find useful applications in modern non-volatile data storage devices. Apart from this technological interest, there is a very fundamental issue regarding whether the ferroelectric-to-paraelectric phase transition in GeTe is order-disorder or displacive in its origin. Also, the underlying physics of the crystal volume contraction which assists the structural transformation in GeTe remains far from clear.

Our contribution presents results of the high-resolution neutron powder diffraction experiments performed on a spallation neutron source which allow for a better understanding of the structural changes across the rhombohedral-to-cubic phase transition in GeTe. We also report on the phonon dynamics in GeTe which we gain from the inelastic neutron scattering experiments along with the density functional theory calculations that show conclusively the displacive type of the phase transition rather than the order-disorder one suggested by some x-ray absorption fine structure experiments and the pair-distribution function analysis. The structural phase transition in GeTe is shown to be driven by the condensation of exactly three components of the triply degenerate optical transverse soft-phonon mode at the Brillouin zone center. Results of the current work indicate that the local atomic potentials are single-well which strongly supports the displacive nature of the phase change in crystalline GeTe. Our considerations are relevant not only for GeTe but can be applicable to other ferroelectric materials like barium titanate as well as manganites showing colossal magnetoresistance, e.g., lanthanum manganite which are known to exhibit similar phenomena.

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