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Dynamics of the phase-change material GeTe across the structural phase transition

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Despite successful application of the phase-change materials from the ternary Ge–Sb–Te system in a variety of optical data storage devices (CDs, DVDs and blue-ray disks) as well as in non-volatile random access memories (non-volatile RAM) [1–2], a comprehensive understanding of the mechanism underlying the phase transitions in the GST compounds is still lacking. A typical example is the temperature induced structural phase transition in GeTe, which is the parent compound of the GST phase-change materials. In particular, the nature of phase transition (displacive or order-disorder) and the driving force of the rhombohedral-to-cubic phase transformation at $T_c \approx 600$˚K along with accompanying effects (volume contraction and disappearance/persistence of the Peierls distorted Ge–Te bonds above T_c) still remain a source of controversy in spite of numerous experimental and theoretical studies carried out over last 30 years [3–10].
This presentation addresses results of the inelastic neutron scattering (INS) experiments on powder GeTe samples and ab initio molecular dynamics (AIMD) simulations which have been undertaken to revisit lattice dynamics of GeTe as a function of temperature and examine behaviour of the local versus average structure of this compound across the structural phase transition. Generally, results of our experimental and theoretical research support observations provided by the so-called local probes (EXAFS and PDF analysis of the high-energy x-ray scattering).

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