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Phonon Dispersions and Relaxation Times in AgSbTe₂ and PbTe¹

OLIVIER DELAIRE, JIE MA, ANDREW MAY, Oak Ridge National Laboratory, CHRIS CARLTON, MIT, MICHAEL MCGUIRE, Oak Ridge National Laboratory, LINDSAY VANBEBBER, University of Tennessee, DOUGLAS ABERNATHY, GEORG EHLERS, TAO HONG, ASHFIA HUQ, WEI TIAN, VEERLE KEPPENS, Oak Ridge National Laboratory, YANG SHAO-HORN, MIT, BRIAN SALES, Oak Ridge National Laboratory — The thermoelectric material AgSbTe₂ had attracted much interest due to its high thermoelectric figure-of-merit, and its anomalously low thermal conductivity for a nominally simple rock-salt structure, which is glass-like even in bulk single-crystals. We present results of systematic neutron scattering investigations of the phonon density-of-states, dispersions, and relaxation times in AgSbTe₂, and contrast these with PbTe. A detailed account of the thermal conductivity is obtained in terms of microscopic phonon mean-free-paths, providing good agreement with bulk transport measurements.

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