Hopping timescales and the phonon-liquid electron-crystal picture in thermoelectric copper selenide

DAVID VONESHEN, HELEN WALKER, Science and Technology Facilities Council, KEITH REFSON, JON GOFF, Royal Holloway University of London — Suppression of heat transport is essential to improve the efficiency of thermoelectric devices to convert waste heat into useful power and state-of-the-art materials have achieved thermal conductivities comparable to glasses. Recently, it was suggested that sub-lattice melting in superionic Cu$_2$Se leads to a suppression of transverse phonons and dramatic further reduction in thermal conductivity to liquid-like values [H. Lui et al. Nat. Mater., 11, 422 (2012)]. The validity of this process depends critically upon relative timescales involved. Using neutron spectroscopy we have measured both the ion transport and lattice dynamics in Cu$_2$Se. We find that the hopping timescales are too slow to significantly affect lattice vibrations and that the transverse phonons persist at all temperatures. While we observe substantial changes to the phonon spectrum they occur well below the transition to the superionic phase. Instead we attribute the ultra-low thermal conductivity to anharmonicity arising from the crystal structure.

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