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Supplementary information

Anharmonic lattice dynamics of Te and its counter-intuitive strain dependent lattice thermal conductivity

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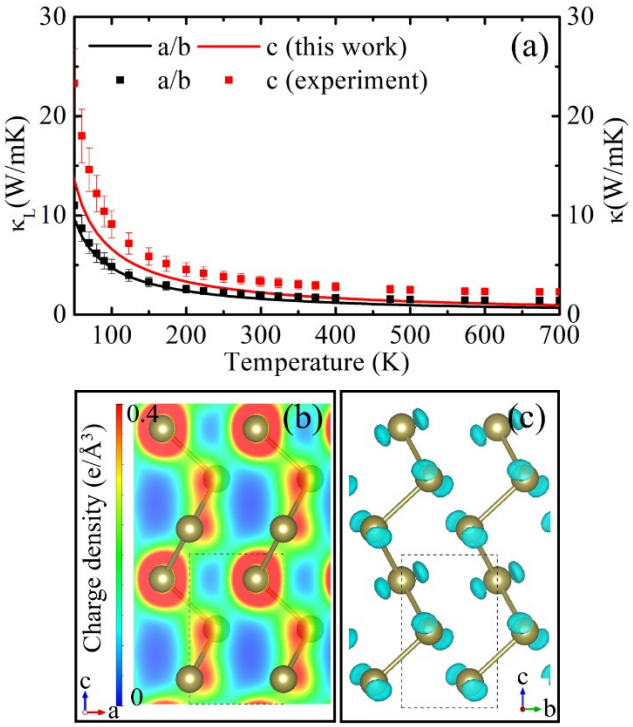

Fig. S1: (a) Lattice thermal conductivity of Te as a function of temperature from DFT calculation (solid curves). The discrete symbols with error bars are the total thermal conductivity from

previous experiment [1]. (b) Charge density distribution, and (c) electron localization function (ELF) of Te. The iso-surface of ELF is set to 0.9 to highlight the lone pair electrons.

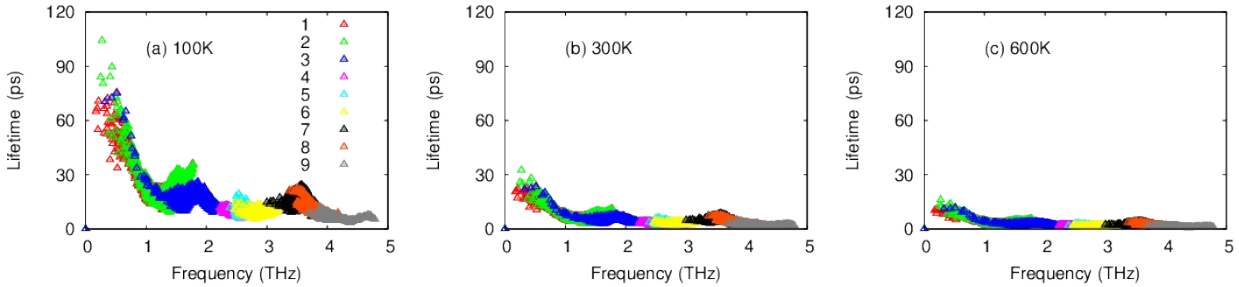

Fig. S2: Phonon lifetimes of Te at (a) 100 K, (b) 300 K, and (c) 600 K, as calculated using the third-order force constants. Phonon modes at a particular q-point are sorted by their frequencies from low to high.

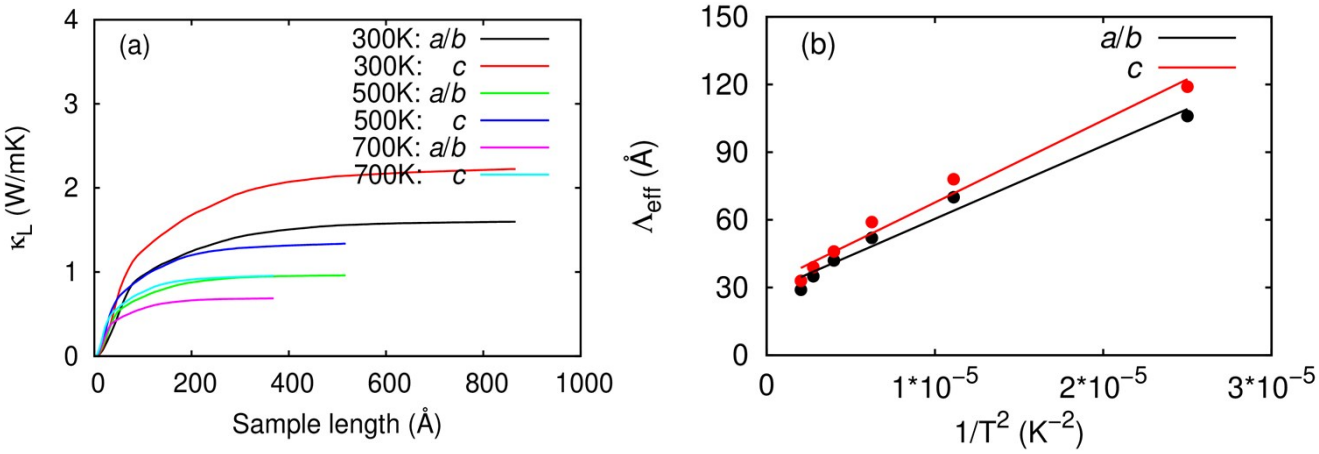

Fig. S3 (a) Lattice thermal conductivity of tellurium as a function of sample length calculated using the single-mode relaxation-time method. (b) Effective phonon mean free path plotted against $1/T^2$.

Reference

1. Ho, C.Y., R.W. Powell, and P.E. Liley, *Thermal conductivity of the elements.* Journal of Physical Chemical Reference Data, 1972. **1**(2): p. 279-421.