Supplementary Information for Phonon Scattering in the Complex Strain Field of a Dislocation in PbTe

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Supplementary note 1

The temperature distributions of the model with dislocation density 6.68×10^{15} m^{-2} in addition to the pristine structure P Model in the NEMD simulations, from which we determined the length of the LSR region. It starts from the position where temperature distribution begins to deviate from the linear distribution and ends in the position where temperature distribution comes back to the linear distribution, and the length is the distance in the horizontal direction between the two purple solid circles, see the Fig. S1b.

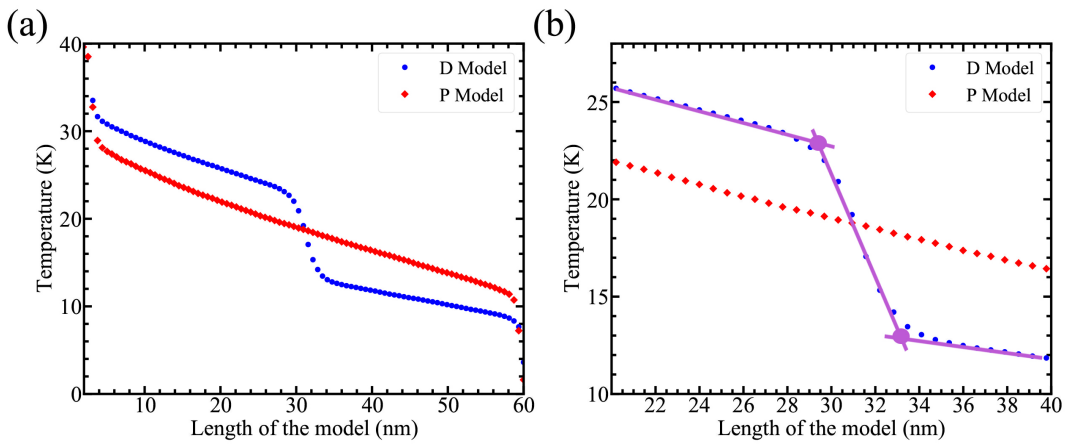

Fig. S1: (a) The temperature distributions of the model with dislocation density 6.68×10^{15} m^{-2} in addition to the pristine structure P Model in the NEMD simulations. (b) Magnified view showing of the sharp reduction in temperature near the dislocation.

Supplementary note 2

The phonon density of states (DOS) of the dislocation D Model and pristine structure P Model were calculated using the Fourier transform of the velocity autocorrelation function of the atoms in the selected volume containing the dislocation. The position corresponding to this selected volume was used in the P Model. Equilibrium molecular dynamic simulations under 20 K were conducted using the same models in the NEMD simulations.

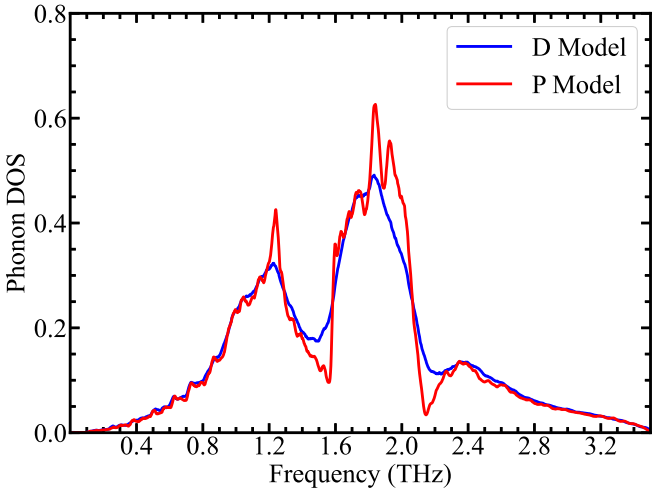

Fig. S2: Phonon density of states of the model with dislocation density 3.34×10^{15} m^{-2} D Model and pristine structure P Model.

Supplementary note 3

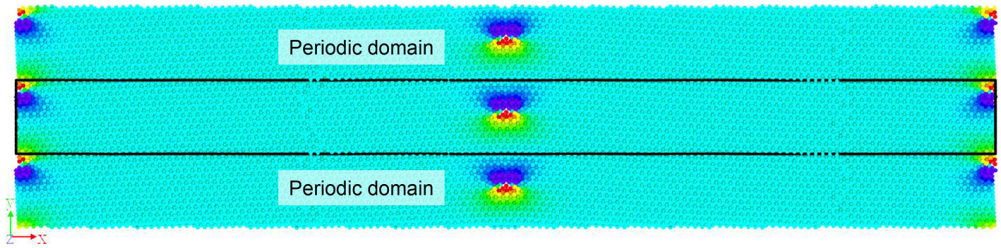

Fig. S3: The normal strain ϵ_{xx} in the the model with dislocation density 6.68×10^{15} m^{-2}. The negative strain region was close enough to the positive strain region of the nearest periodic domain to allow dislocation interactions.

Supplementary note 4

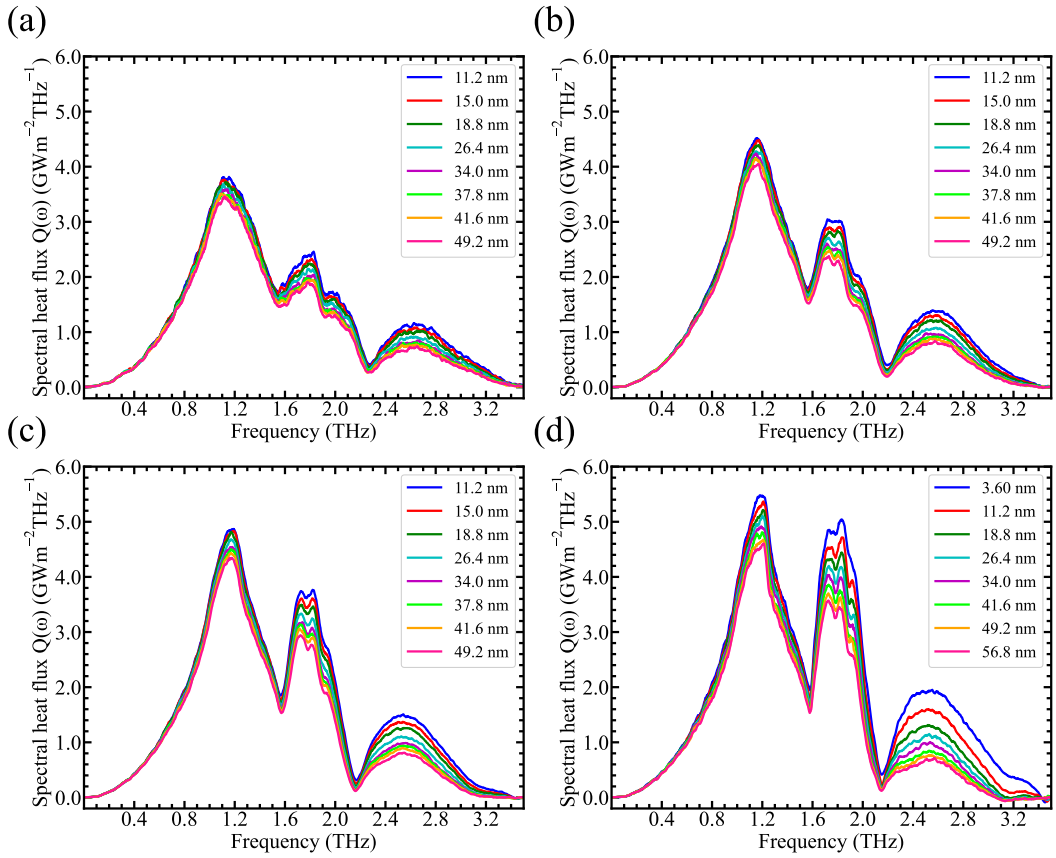

Fig. S4: Spectral heat fluxes of the different length models. (a), (b), and (c) are the highest (6.68×10^{15} m^{-2}), medium (3.34×10^{15} m^{-2}), and lowest (1.67×10^{15} m^{-2}) dislocation density models D Model, respectively. (d) Pristine structure P Model.

Supplementary note 5

A shear strain model was built for first-principles calculations. The Vienna Ab *initio* Simulation Package (VASP) was used to conduct DFT calculations.[2] The projector augmented wave (PAW)[3] method was used in conjunction with the revised Perdew-Burke-Ernzerhof for solids (PBEsol)[4] generalized gradient approximation (GGA)[5] for the exchange-correlation (xc) functional.[6] For structural relaxation, $16\times16\times16$ Monkhorst-Pack k-point meshes and

a plane wave basis with a kinetic energy cut-off of 330 eV were used. The force and energy convergence thresholds were 10^{-8}eV/Å. The configurations for calculating the second- and third-order force constants were generated by Phonopy and thirdorder.py in the ShengBTE package, respectively. A $2\times2\times2$ unit cell was used. The forces on the atoms were calculated using VASP, and the second- and third-order force constants were obtained by Phonopy and thirdorder.py in the ShengBTE package, respectively. The phonon dispersion was obtained from the second- and third-order force constants. By combining the second- and third-order force constants, the BTE was solved using the ShengBTE package to obtain the thermal conductivity, phonon group velocity, phonon scattering rate, and Grüneisen constant.

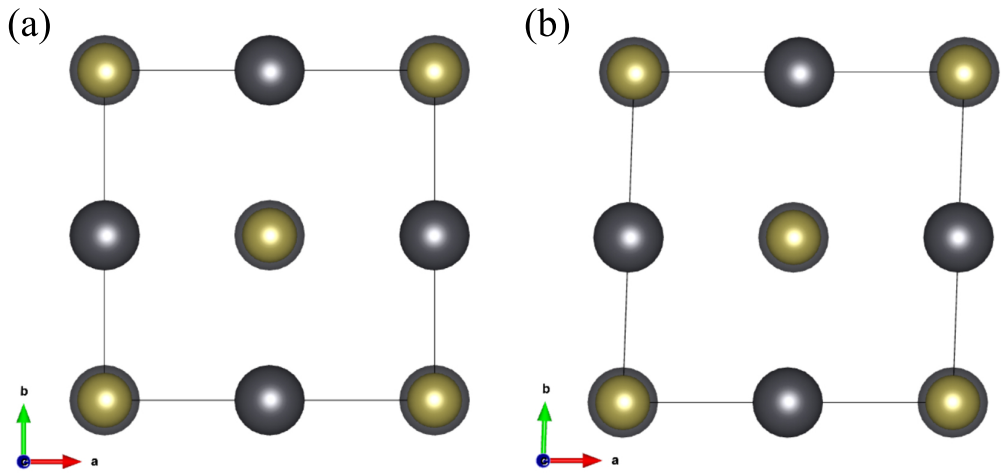

Fig. S5: Shear strain model built using first-principles calculations: (a) pristine model and (b) shear strain model. The angle between the **a** and **b** axis was 88°. The figure was produced using VESTA software.[1]

References

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