Supporting information for

Structural Property-Induced Different Phonon--Twin-Boundary Scattering in Diamond

Huicong Dong [a, b, c], Shuaichao Yu [b], Zhihao Feng[a, b, c, d*], Bin Wen[b]**

[a] School of Materials Science and Engineering, Hebei University of Science and Technology, Shijiazhuang 050018, China

[b] State Key Laboratory of Metastable Materials Science and Technology, Yanshan University, Qinhuangdao 066004, China

[c] Hebei Key Laboratory of Material Near-net Forming Technology, Hebei University of Science and Technology, Shijiazhuang 050018, China

[d] Steel Ball Technology Innovation Center of Hebei Province, Handan 056038, China

This file includes:

Discussion 1: Sample length dependence of TB thermal resistance

Discussion 2: Time Domain Normal Mode Analysis (TDNMA)

Discussion 3: Phonon wave packet method

Figure S1 The temperature difference as a function of the sample length in the case of the (111)/[110] TB fitted to a shifted exponential.

Figure S2 The kinetic of the atoms as a function of the running steps in the (310)/[001] sample with a wave packet of 16.0168THz frequency. The left and right mean the kinetic energy of the phonon wave-packet at each side of the grain boundary interface.

*Corresponding author. E-mail: fengzhihao_edu@163.com (Zhihao Feng)
**Corresponding author. E-mail: wenbin@ysu.edu.cn (Bin Wen)

Discussion 1: Sample length dependence of TB thermal resistance

According to the previous work by Watanabe et al[1], it can be obtained that the interface thermal resistance shows a strong dependence on the system size along the heat transport direction, which is also considered in our work. To reduce the efforts, here, the (111)/[110] TB has been chosen as a typical case for study, and the length of the simulation cell ranges from 20 to 300 nm.

As shown in Figure S1, the temperature jump ΔT shows a strong system size L_Z dependence for (111)/[110], and ΔT reaches an asymptotic value at about 180 nm. Besides, our results also show great consistency with the following equation

$$\Delta T = T_{\infty} + A\exp(-L_Z / L_0) \quad (1)$$

The values of parameters A and L_0 obtained from the fit are 40.1 K and 217.4 nm, respectively. Thus, to eliminate this effect, all sample lengths of the four have all been set around 300nm.

Discussion 2: Time Domain Normal Mode Analysis (TDNMA)

In TDNMA[2], the atomic velocities v and atomic displacements μ are conducted onto normal mode coordinates of systems. The normal mode coordinates $q(\boldsymbol{k},v,t)$ and its time derivative $\dot{q}(\boldsymbol{k},v,t)$ can be obtained by following

$$q(\boldsymbol{k},v,t)=\sum_{j,l}(\frac{m_j}{N})^{\frac{1}{2}}\exp(-i\boldsymbol{k}\cdot r_{j,l}^{0})e_j^{*}(\boldsymbol{k},v)\cdot\mu(j,l,t) \tag{2}$$

$$\dot{q}(\boldsymbol{k},v,t)=\sum_{j,l}(\frac{m_j}{N})^{\frac{1}{2}}\exp(-i\boldsymbol{k}\cdot r_{j,l}^{0})e_j^{*}(\boldsymbol{k},v)\cdot v(j,l,t) \tag{3}$$

where $r_{j,l}^{0}$ is the equilibrium position of atom with index j at lattice site l, $\mu(j,l,t)$ and $v(j,l,t)$ are the corresponding displacement and velocity at time t. N is the number of unit cell, $e(k,v)$ is the phonon eigenvector, m_j is the atom mass, k is the wave vector, and v is the index of polarization.

The potential and kinetic energies of normal modes can be calculated by

$$U(\boldsymbol{k},v,t)=\frac{1}{2}\omega(\boldsymbol{k},v)^2q^{*}(\boldsymbol{k},v,t)q(\boldsymbol{k},v,t) \tag{4}$$

$$T(\boldsymbol{k},v,t)=\frac{1}{2}\dot{q}^{*}(\boldsymbol{k},v,t)\dot{q}(\boldsymbol{k},v,t) \tag{5}$$

Thus, the total energy of normal modes can be obtained by

$$E(\boldsymbol{k},v,t)=U(\boldsymbol{k},v,t)+T(\boldsymbol{k},v,t) \tag{6}$$

The phonon lifetime $\tau(\boldsymbol{k},v)$ is relevant to the temporal decay of the total energy[3] as

$$\frac{\langle E(\boldsymbol{k},v,t)E(\boldsymbol{k},v,0)\rangle}{\langle E(\boldsymbol{k},v,0)E(\boldsymbol{k},v,0)\rangle}=\exp(-t/\tau(\boldsymbol{k},v)) \tag{7}$$

The phonon mean and thermal conductivity along x direction can be expressed under the relaxation time approximation[4,5] by

$$\lambda_x(\boldsymbol{k},v)=\left|v_{g,x}(\boldsymbol{k},v)\right|\tau(\boldsymbol{k},v) \tag{8}$$

$$k_x(\boldsymbol{k},v)=c(\boldsymbol{k},v)v_{g,x}^{2}(\boldsymbol{k},v)\tau(\boldsymbol{k},v) \tag{9}$$

where $v_{gx}(\boldsymbol{k},v)$ is the phonon group velocity along the x direction and $c(\boldsymbol{k},v)$ is the mode specific heat capacity.

Discussion 3: Phonon wave packet method

To obtain energy transmission coefficients of wave packet across twin boundaries, the phonon wave packet (PWP) method is used, whose basic idea is to build a Gaussian PWP from a single branch of the phonon dispersion curve with narrow frequency range and a well-defined polarization[6]. To create a wave packet centered at a wave vector k_0 in branch λ, atoms are displaced according to[7]

$$u_{il\mu}(k_0,\lambda) = A\varepsilon_{i\mu\lambda}(k_0,\lambda)\exp[ik_0(z_1-z_0)]\exp[-(z_1-z_0)^2/\eta^2] \tag{10}$$

where $u_{il\mu}$ is the μth component of displacement for atom i in the lth unit cell. The wave packet is initially located at $z=z_0$ with amplitude A. The parameter η controls the width of the wave packet, and $\varepsilon_{i\mu\lambda}$ is the polarization vector for band λ at k_0. In all simulations, A = 0.0001 Å, $\varepsilon_{i\mu\lambda}$ = 1, z_0 = 1000 a, and η = 100 a, where a is the lattice constant of the material in which the wave packet is generated. To set the initial velocities of atoms, time dependence is added to the displacement. By differentiating the displacement concerning time, we can obtain

$$v_{il\mu}(k_0,\lambda) = -i\omega(k_0,\lambda)u_{il\mu}(k_0,\lambda) \tag{11}$$

References

[1] Watanabe T, Ni B, Phillpot S, et al. Thermal conductance across grain boundaries in diamond from molecular dynamics simulation. J. Appl. Phys., 2007, 102(6): 063503.

[2] Zhang C, Sun Q. Gaussian approximation potential for studying the thermal conductivity of silicene. J. Appl. Phys., 2019, 126(10): 105103.

[3] Ladd A, Moran B, Hoover W. Lattice thermal conductivity: A comparison of molecular dynamics and anharmonic lattice dynamics. Phys. Rev. B, 1986, 34(8): 5058.

[4] McGaughey A, Kaviany M. Quantitative validation of the Boltzmann transport equation phonon thermal conductivity model under the single-mode relaxation time approximation. Phys. Rev. B, 2004, 69(9): 094303.

[5] Turney J, Landry E, McGaughey A, et al. Predicting phonon properties and thermal conductivity from anharmonic lattice dynamics calculations and molecular dynamics simulations. Phys. Rev. B, 2009, 79(6): 064301.

[6] Ju S, Liang X. Investigation on Interfacial Thermal Resistance and Phonon Scattering at Twist Boundary of Silicon. J. Appl. Phys. 2013, 113, 053513.

[7] Schelling P; Phillpot S, Keblinski P. Phonon Wave-Packet Dynamics at Semiconductor Interfaces by Molecular-Dynamics Simulation. Appl. Phys. Lett. 2002, 80, 2484-2486.

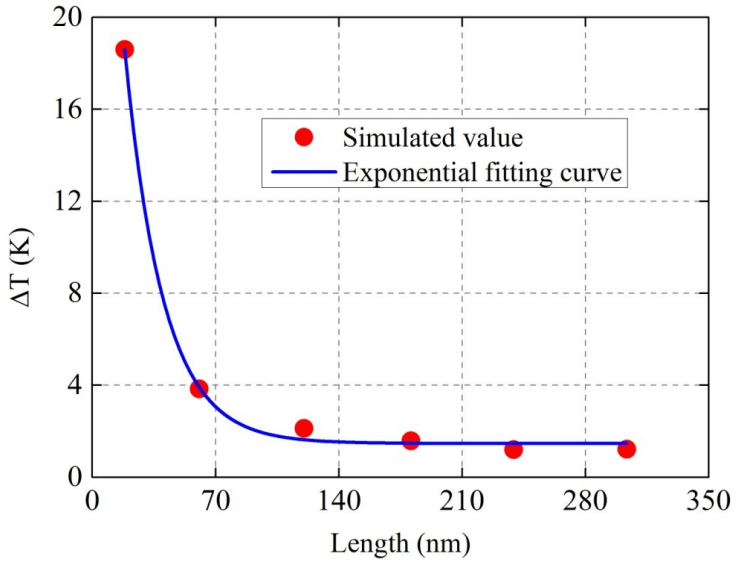

Figure S1. The temperature difference as a function of the sample length in the case of the (111)/[110] TB fitted to a shifted exponential.

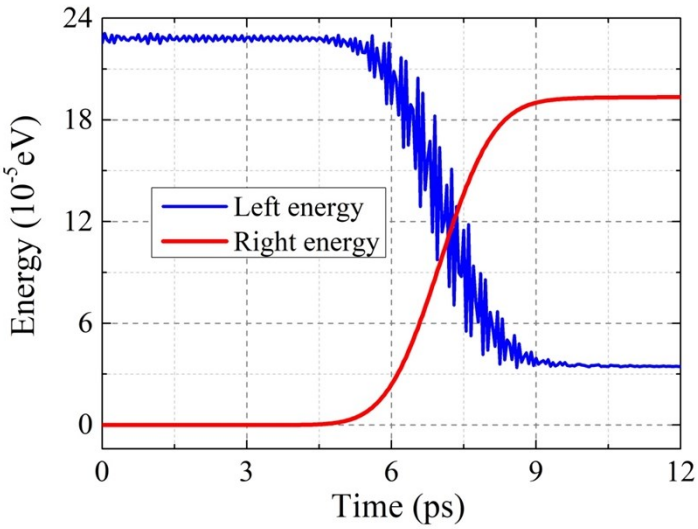

Figure S2. The kinetic of the atoms as a function of the running steps in the (310)/[001] sample with a wave packet of 16.0168THz frequency. The left and right mean the kinetic energy of the phonon wave-packet at each side of the grain boundary interface.