Length-dependent thermal conductivity prediction of monolayer graphene using Molecular Dynamics

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(22M1626)

Motivation

Thermal Transport

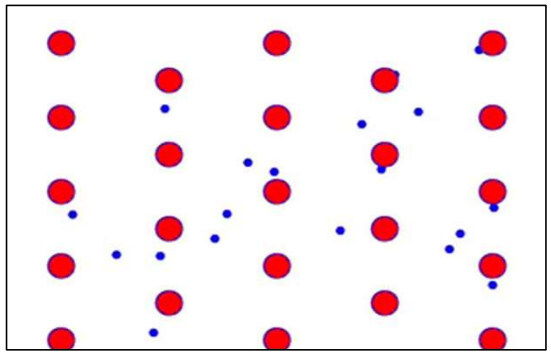

Fig1: Electrons transferring heat in metals.

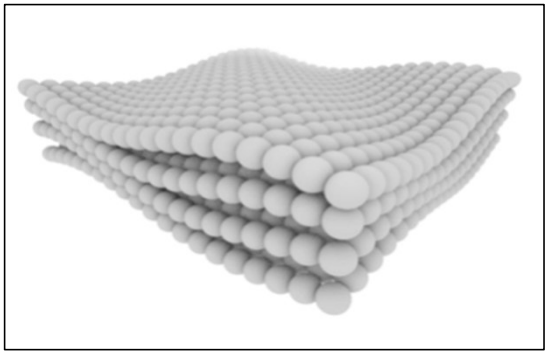

Fig2: Phonons transfer heat in semi-conductors and insulators.

The need for atomistic simulation techniques?

- Electronic devices are in the nanoscale regime.
- Phonon mean free path is of the same length scale as the size of the devices.
- The study of heat transport is no longer possible in the continuum scale.
- Experimental difficulties associated with such length scales.

Image source: *1. kaiserscience.wordpress.com* *2. Public Domain; Sean Kelley via NIST*

Introduction

Key points:

- Phonons as classical particles.
- Newton's laws of motion are used to predict trajectories with an interatomic potential or force field.
- Steady state thermal non-equilibrium condition maintained by thermostats.
- Heat flux is measured and temperature gradient calculated.
- Fourier's law of heat conduction is applied to estimate the thermal conductivity

$$J^{\alpha} = -\sum_{\beta} \kappa^{\alpha\beta} \frac{\partial T}{\partial x^{\beta}}$$

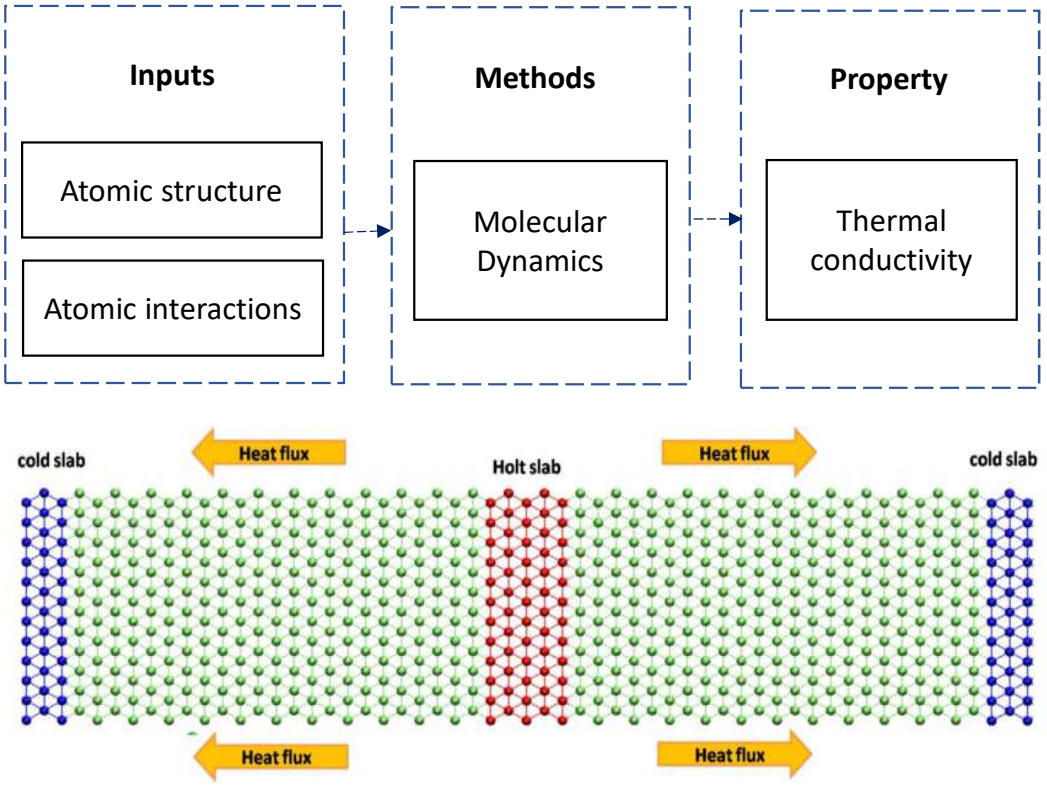

Fig3: Schematic of a simulation setup for NEMD

Image source: https://www.researchgate.net/figure/a-Schematic-of-NEMD-simulation-domain

A case study: Graphene

- Graphene's has high RT mobility and thermal conductivity.
- No dangling bonds.
- Used to transfer heat faster.

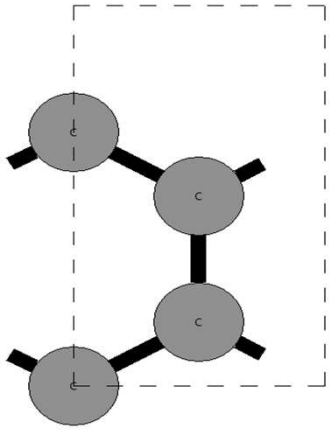

Fig4: Unit Cell of graphene

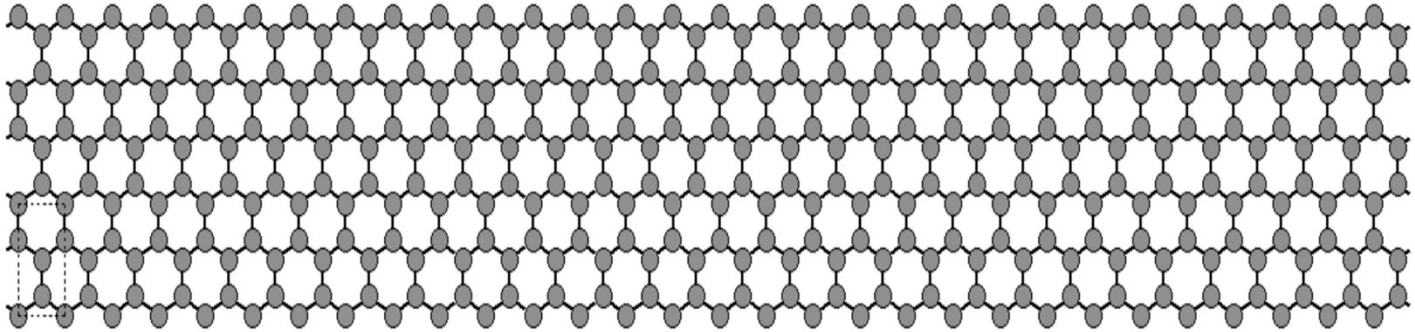

Fig5: 2 Honey Comb Lattice structure of graphene

Fig6: Adequate vacuum to avoid interactions between different layers

Structure Relaxation

Simulation parameters

Ensemble	:	NPT
Atom_style	:	atomic
Units	:	metal
Pair_style	:	tersoff
Pressure	:	0 bars
Temperature	:	300 K
Timestep	:	1 femtosecond
Run Time	:	1 nanosecond

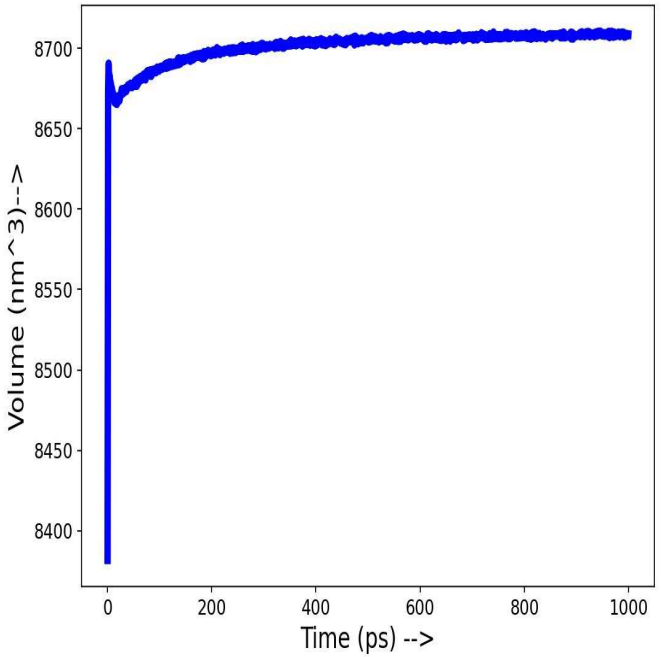

Fig7: Convergence of volume

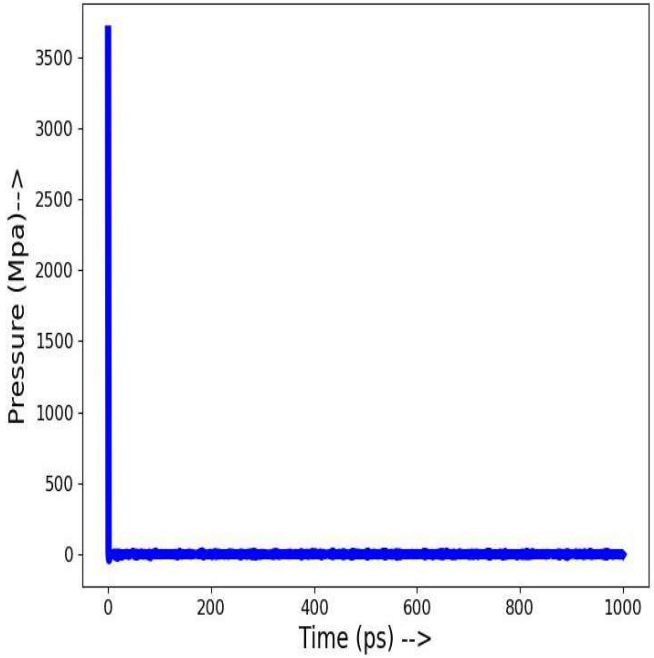

Fig8: Convergence of pressure

Thermal conductivity calculation

Simulation parameters

Ensemble	:	NVE
Thermostats	:	Langevin
Hot reservoir	:	320 K
Cold reservoir	:	280 K
Timestep	:	1 femtosecond
Equilibration	:	1 nanosecond
Production	:	3 nanoseconds

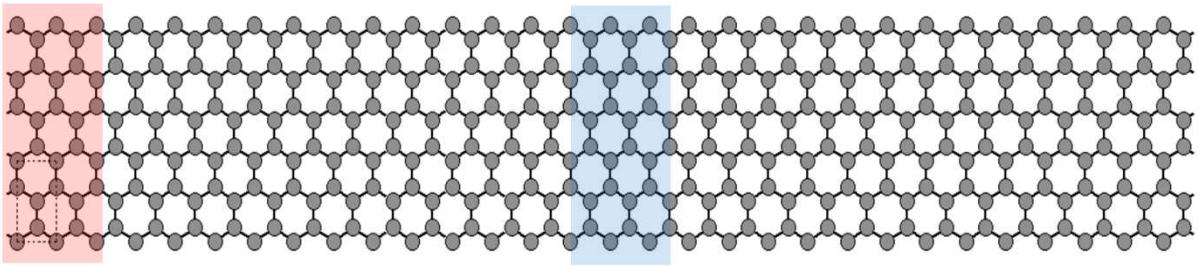

Fig9: Schematic of the simulation setup

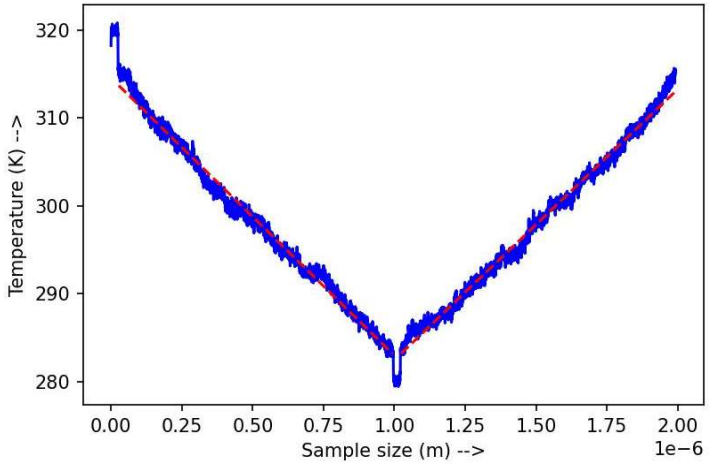

Fig10: Temperature gradient developed in the graphene sheet

Thermal conductivity calculation

```
#----------------------------------------------------------------------Production run final----------------------------------------------------------------

fix             E_in      HOT       langevin  ${thi}  ${thi}    0.05  590804    tally     yes
fix             E_out     COLD      langevin  ${tlo}  ${tlo}    0.05  28859     tally     yes

thermo_style    custom    step  temp      c_Thot    c_Tcold   f_E_in    f_E_out   v_tdiff   f_AVE

variable        x_bin     equal     (1/(${x_grid}))
variable        value     format    x_bin %.10g
compute         x bins    all       chunk/atom          bin/1d    x         lower     ${value}  units     reduced
fix             4 all     ave/chunk $p      $s     $d   x_bins    temp ave running file profile.${u}.${v}.${r}.langevin overwrite
variable        start_time equal time
run             ${r4}

#-----------------------------------------------------------------------Post Processing-------------------------------------------------------------

variable                  Q_hot          equal     f_E_in
variable                  Q_cold         equal     f_E_out
variable                  len_y          equal     ly
variable                  prod_time      equal     ${r4}*${dt}
variable                  len_x          equal     lx

print                     ${Q_hot}       append    heat_in_val.dat   screen no
print                     ${Q_cold}      append    heat_out_val.dat  screen no
print                     ${len_y}       append    length_y.dat      screen no
print                     ${prod_time}   append    time_val.dat      screen no
print                     ${len_x}       append    length_x.dat      screen no
print                     $r             append    res_thick_val.dat screen no
```

$$\kappa = \frac{Q}{A * t} \frac{1}{\left(\frac{dT}{dx}\right)}$$

Convergence study

Length : 250 nanometres

Reservoir : 20 nanometres

Width : 2.5 nanometres

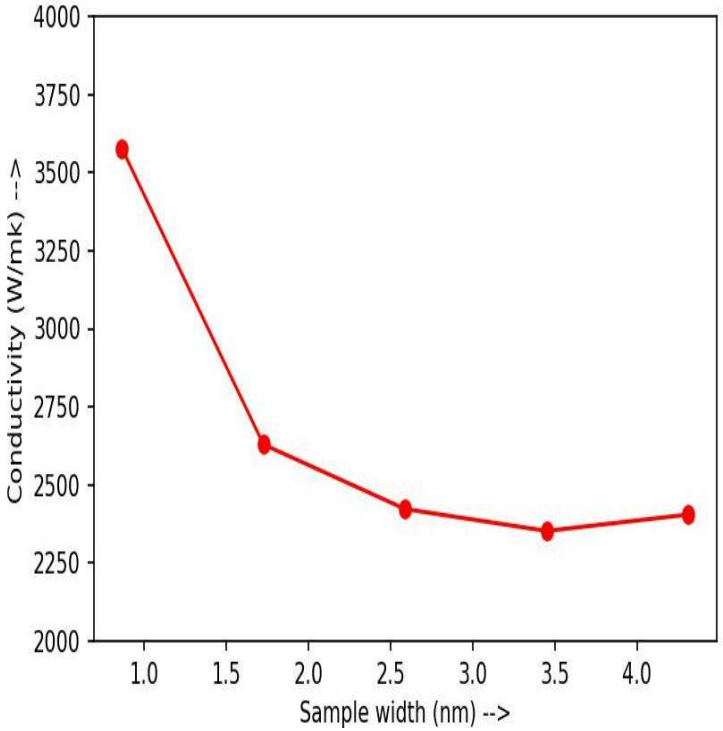

Fig11: Thermal conductivity convergence with width of sheet

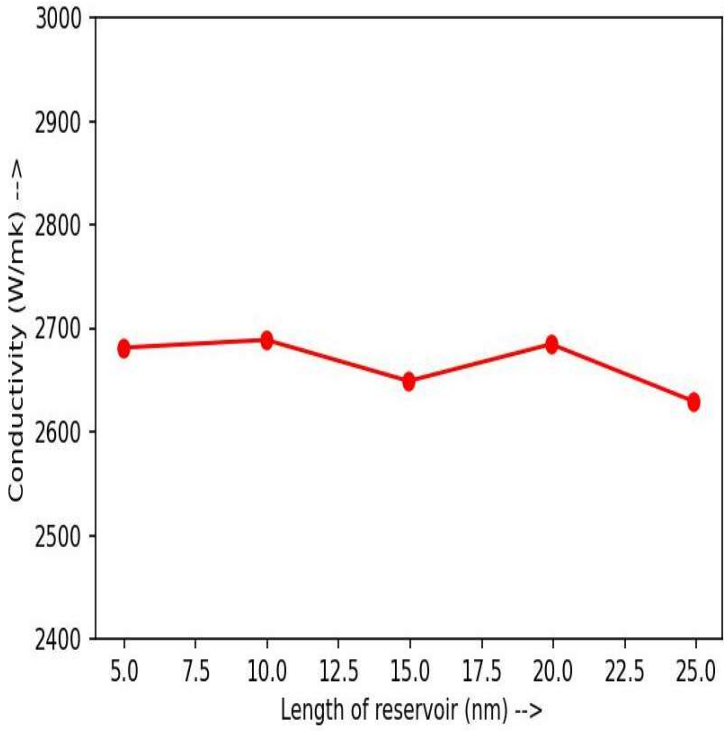

Fig12: Thermal conductivity convergence with length of reservoirs

Comparison with literature

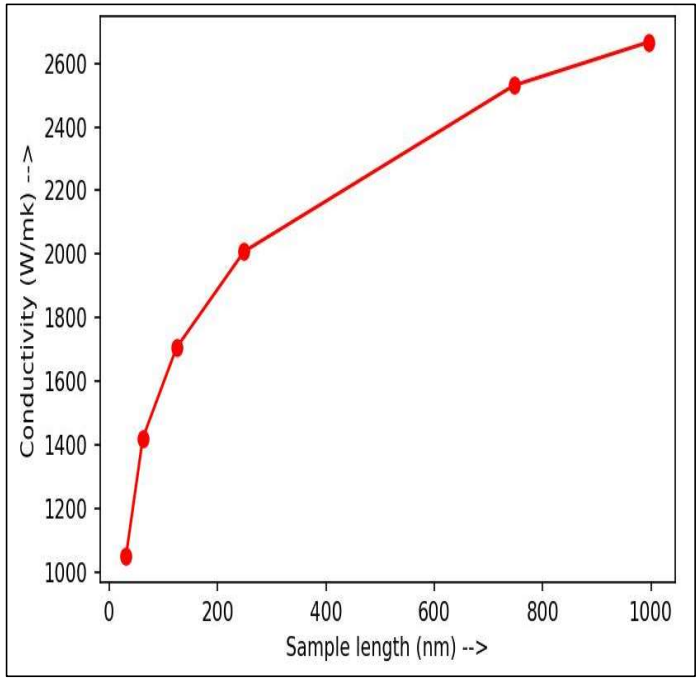

Fig13: Thermal conductivity vs length of the sample

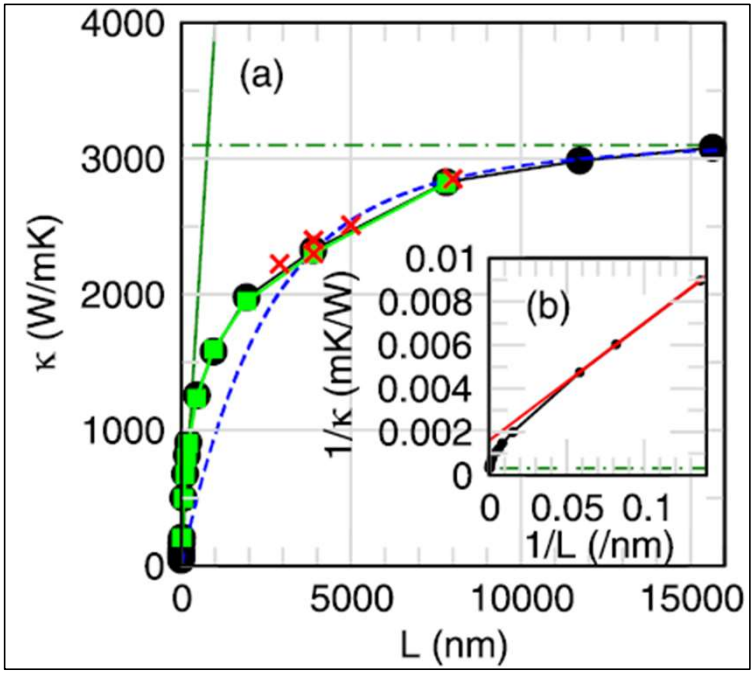

Fig14: Thermal conductivity vs length of the sample (Literature)

Discussion

Strong Length Dependence:

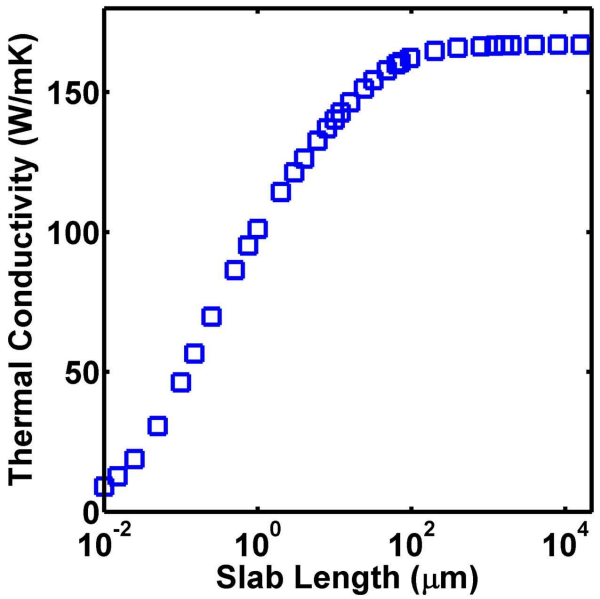

Fig15: Length dependence thermal conductivity of Si slab

Deviations from the paper:

κ at 1 μm ($Wm^{-1}K^{-1}$)	~2700	~1800
Thermostat	Langevin	NVT
Boundary	Periodic	Fixed
Simulation time	3 ns	20 ns
Temperature difference	40 K	60 K

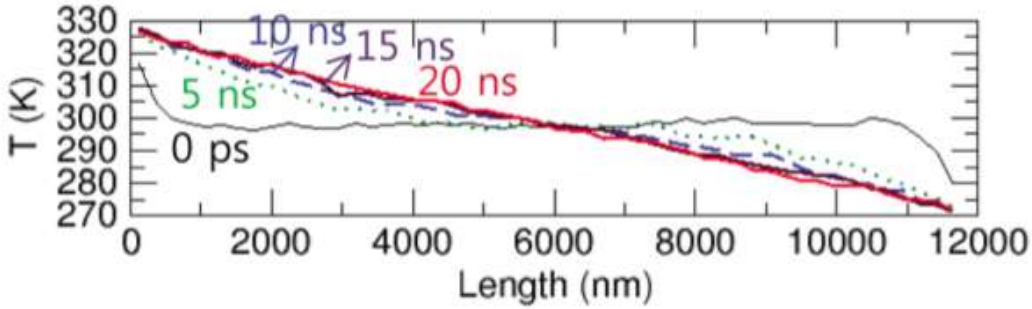

Fig16: Temperature gradient at different simulation times

Image source: *Zhang, Hang, et al. "Length dependent thermal conductivity measurements yield phonon mean free path spectra in nanostructures." Scientific Reports 5.1 (2015): 9121.*

References

1. Park, Minkyu, Sun-Chul Lee, and Yong-Sung Kim. "Length-dependent lattice thermal conductivity of graphene and its macroscopic limit." *Journal of Applied Physics* 114.5 (2013): 053506.

2. Zhang, Hang, et al. "Length dependent thermal conductivity measurements yield phonon mean free path spectra in nanostructures." *Scientific Reports* 5.1 (2015): 9121.

3. Gu, Xiaokun, Zheyong Fan, and Hua Bao. "Thermal conductivity prediction by atomistic simulation methods: Recent advances and detailed comparison." *Journal of Applied Physics* 130.21 (2021): 210902.

4. LAMMPS: Examples > Kappa > in.langevin

Thank You