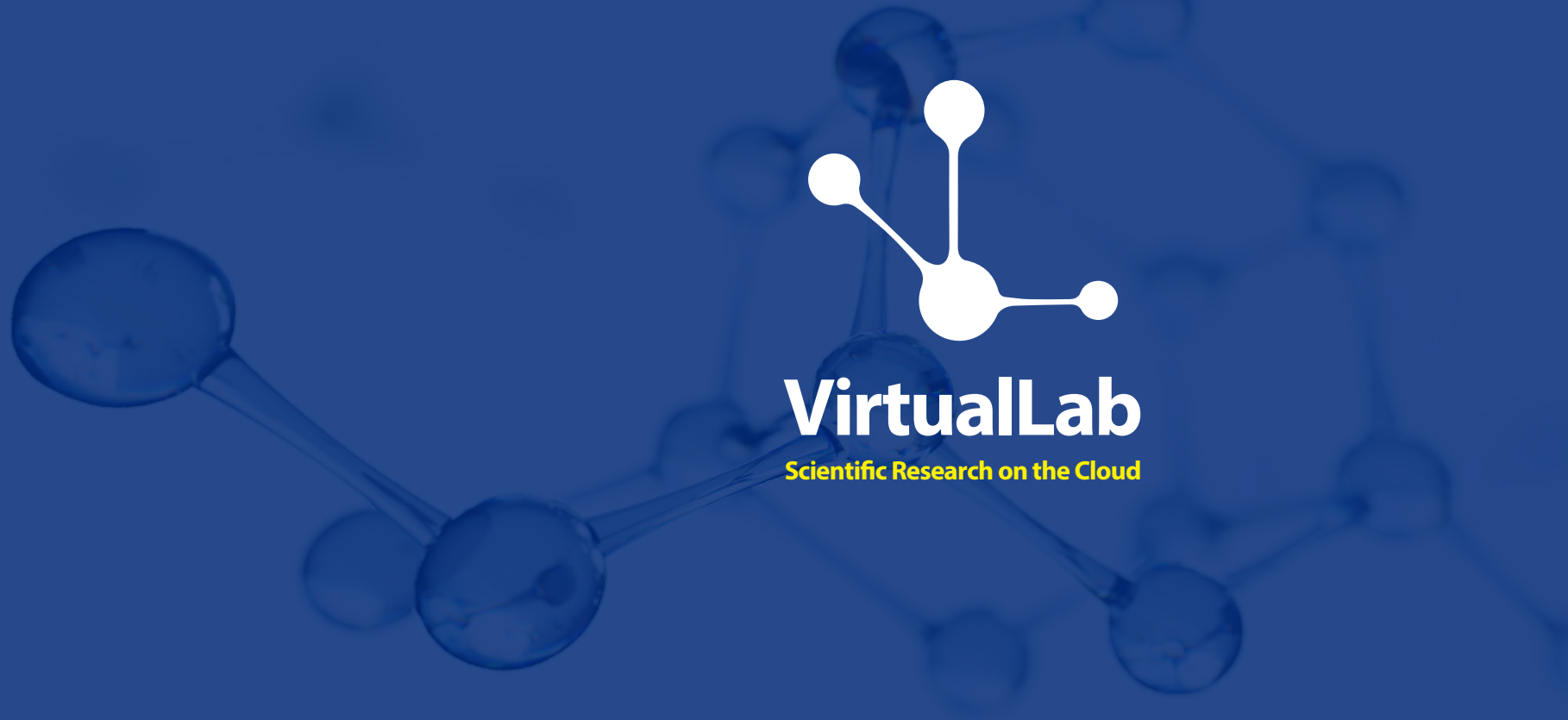
Materials Square : How to Reduce the Barriers to Entry for LAMMPS ?



VirtualLab

Scientific Research on the Cloud

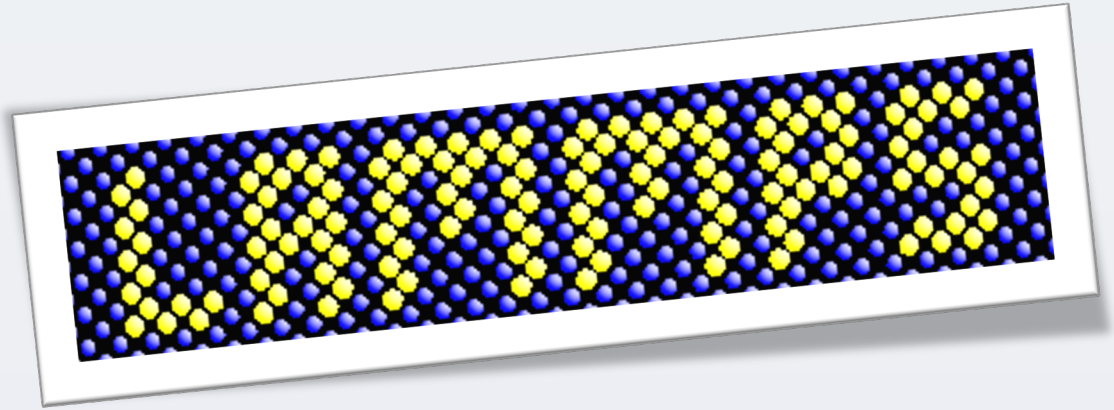
Virtual Lab, Inc
Minkyu Park (VP)

Classical molecular dynamics Code

Atomic-scale simulation

Huge Community

Open-**S**ource



Good Scalability

Transparent

Well-Documented/**W**ell-Communicated

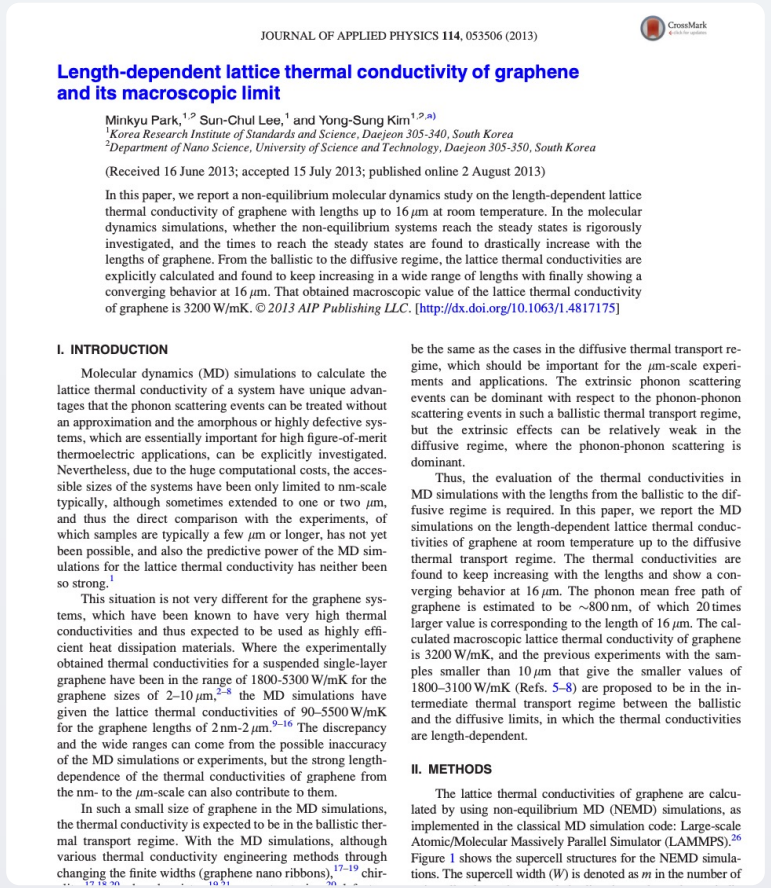
(Special Thanks to Steve)

Feasibility (User-package)

WHY LAMMPS ?

I ALSO HAVE USED LAMMPS IN MY STUDIES SINCE 2012

- Calculate diffusive lattice thermal conductivity of Graphene
- Non-Equilibrium molecular dynamics (Direct method)
- Length : ~ 16 μm (around 5M atoms)
- Tersoff potential with the parameter set*
- Results : 3,200 W/m-K at 16 μm



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Length-dependent lattice thermal conductivity of graphene and its macroscopic limit

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In this paper, we report a non-equilibrium molecular dynamics study on the length-dependent lattice thermal conductivity of graphene with lengths up to 16 μm at room temperature. In the molecular dynamics simulations, whether the non-equilibrium systems reach the steady states is rigorously investigated, and the times to reach the steady states are found to drastically increase with the lengths of graphene. From the ballistic to the diffusive regime, the lattice thermal conductivities are explicitly calculated and found to keep increasing in a wide range of lengths with finally showing a converging behavior at 16 μm. That obtained macroscopic value of the lattice thermal conductivity of graphene is 3200 W/mK. © *2013 AIP Publishing LLC*. [http://dx.doi.org/10.1063/1.4817175]

I. INTRODUCTION

Molecular dynamics (MD) simulations to calculate the lattice thermal conductivity of a system have unique advantages that the phonon scattering events can be treated without an approximation and the amorphous or highly defective systems, which are essentially important for high figure-of-merit thermoelectric applications, can be explicitly investigated. Nevertheless, due to the huge computational costs, the accessible sizes of the systems have been only limited to nm-scale typically, although sometimes extended to one or two μm, and thus the direct comparison with the experiments, of which samples are typically a few μm or longer, has not yet been possible, and also the predictive power of the MD simulations for the lattice thermal conductivity has neither been so strong.[1]

This situation is not very different for the graphene systems, which have been known to have very high thermal conductivities and thus expected to be used as highly efficient heat dissipation materials. Where the experimentally obtained thermal conductivities for a suspended single-layer graphene have been in the range of 1800-5300 W/mK for the graphene sizes of 2–10 μm,[2–8] the MD simulations have given the lattice thermal conductivities of 90–5500 W/mK for the graphene lengths of 2 nm-2 μm.[9–16] The discrepancy and the wide ranges can come from the possible inaccuracy of the MD simulations or experiments, but the strong length-dependence of the thermal conductivities of graphene from the nm- to the μm-scale can also contribute to them.

In such a small size of graphene in the MD simulations, the thermal conductivity is expected to be in the ballistic thermal transport regime. With the MD simulations, although various thermal conductivity engineering methods through changing the finite widths (graphene nano ribbons),[17–19] chir-

be the same as the cases in the diffusive thermal transport regime, which should be important for the μm-scale experiments and applications. The extrinsic phonon scattering events can be dominant with respect to the phonon-phonon scattering events in such a ballistic thermal transport regime, but the extrinsic effects can be relatively weak in the diffusive regime, where the phonon-phonon scattering is dominant.

Thus, the evaluation of the thermal conductivities in MD simulations with the lengths from the ballistic to the diffusive regime is required. In this paper, we report the MD simulations on the length-dependent lattice thermal conductivities of graphene at room temperature up to the diffusive thermal transport regime. The thermal conductivities are found to keep increasing with the lengths and show a converging behavior at 16 μm. The phonon mean free path of graphene is estimated to be ~800 nm, of which 20 times larger value is corresponding to the length of 16 μm. The calculated macroscopic lattice thermal conductivity of graphene is 3200 W/mK, and the previous experiments with the samples smaller than 10 μm that give the smaller values of 1800–3100 W/mK (Refs. 5–8) are proposed to be in the intermediate thermal transport regime between the ballistic and the diffusive limits, in which the thermal conductivities are length-dependent.

II. METHODS

The lattice thermal conductivities of graphene are calculated by using non-equilibrium MD (NEMD) simulations, as implemented in the classical MD simulation code: Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS).[26] Figure 1 shows the supercell structures for the NEMD simulations. The supercell width (W) is denoted as m in the number of

* Optimized by Lindsay and Broido

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Lattice Thermal Conductivity Calculation

I. Simulation Modeling

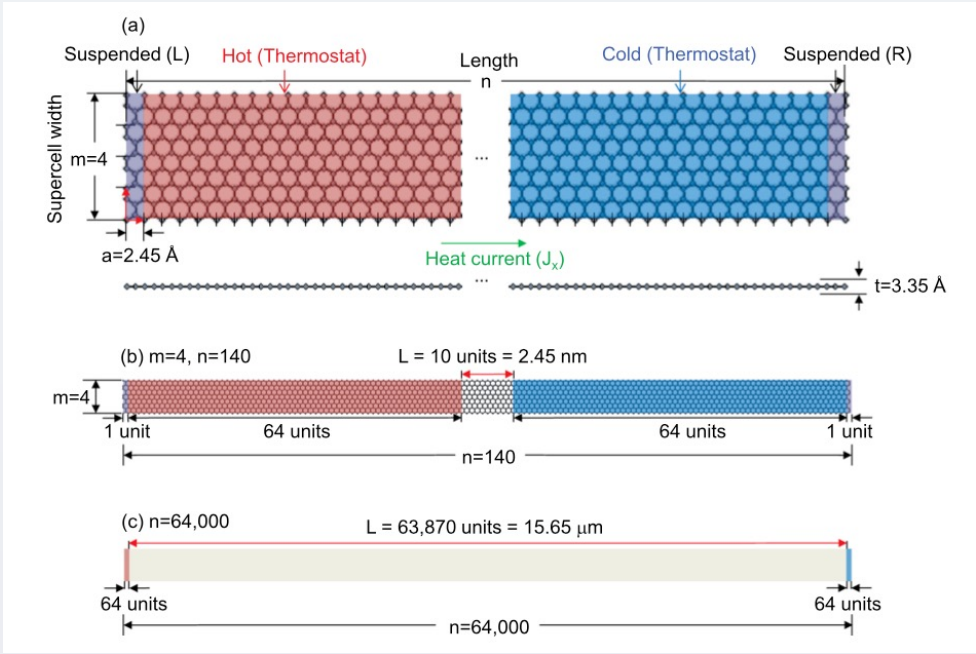
$m = 4$ (Supercell width)

$l = 140 – 64{,}000$ unitcell (Transport length)

Lattice constant = 2.45 Å, Thickness = 3.35 Å

Thermostats = 64 unitcell (each ends)

Last each ends are suspended



Lattice Thermal Conductivity Calculation

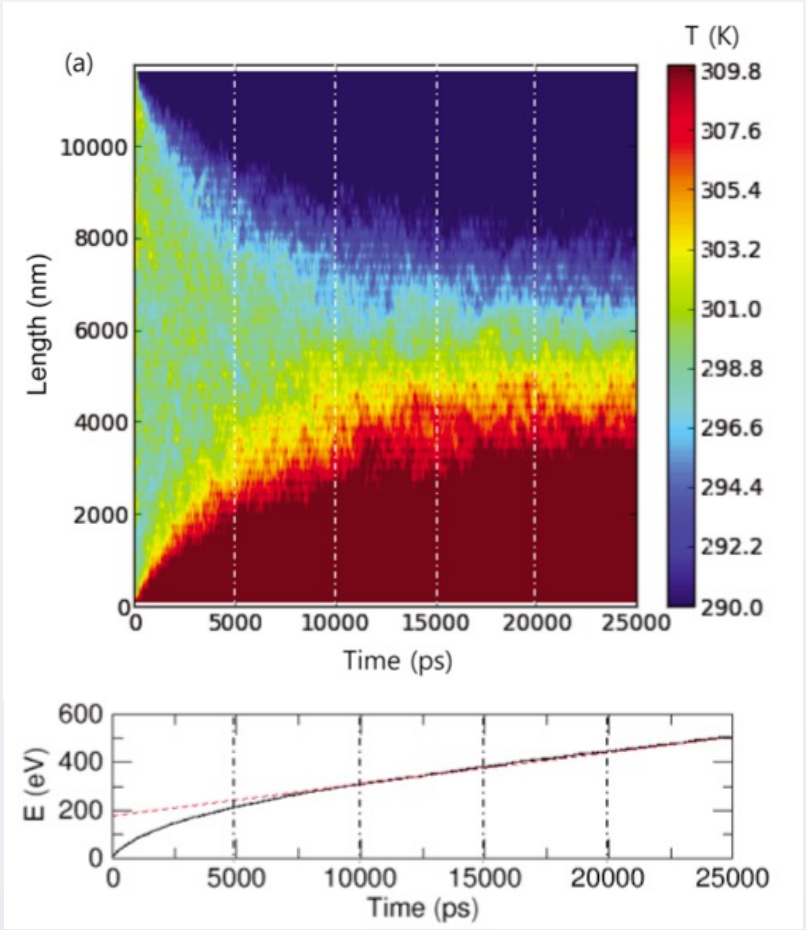
II. Calculation Details & Issues

Fourier's law : $J = \mathrm{K}\left(\frac{\Delta T}{L}\right)$

Heat flux (J) can be calculated by cumulative E (E_{cum})

$$E_{cum}(t) = [E_{hot}(t) - E_{Cold}(t)]/2$$

Calculate slope, ***E*** as a function of ***t*** at the steady state



Lattice Thermal Conductivity Calculation

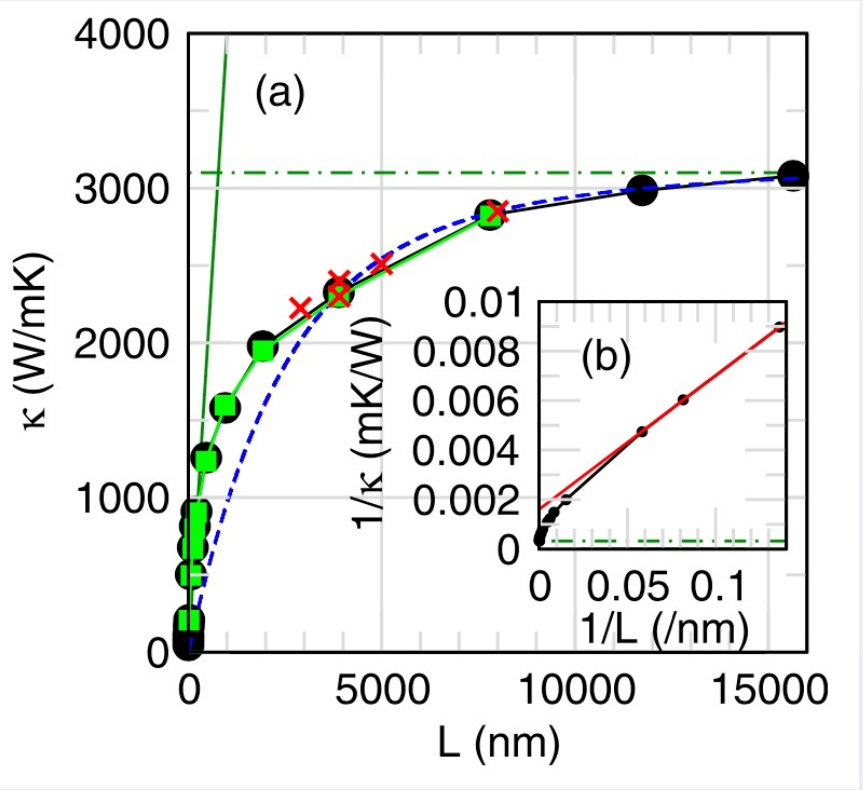
III. Results

$K_{diffusive}$ of Graphene is 3,200 W/m-K at 16 μm

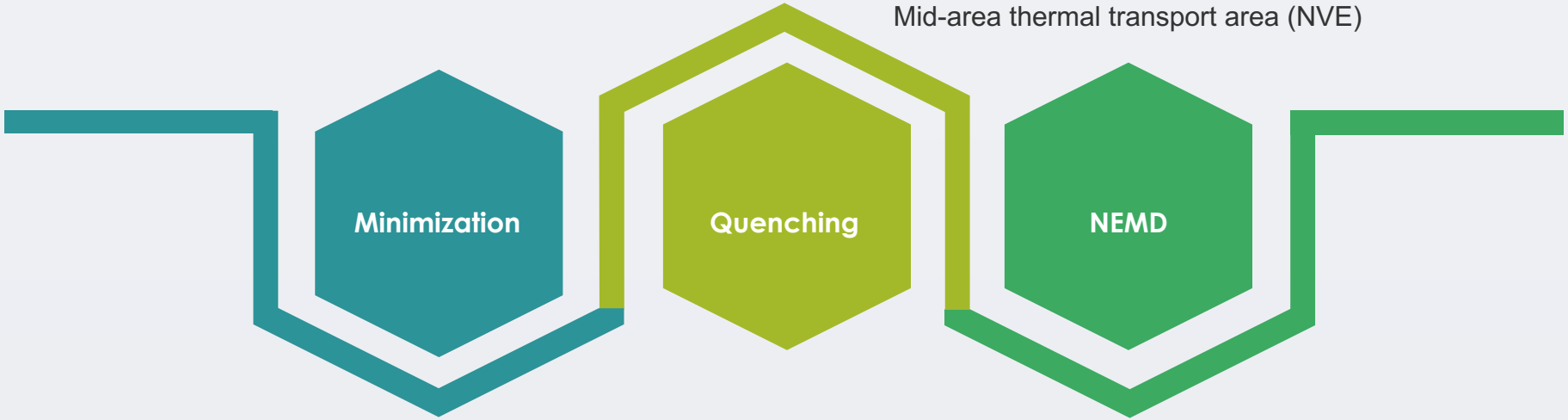
This is also well-match with previous reports

Mode-independent phonon MFP = 865 nm (ref. 775 nm)

(Phenomenological high-order heat transport eq.)



Lattice Thermal Conductivity Calculation



Relaxation

conjugate-gradient method

Main Calculation

Fix each 64 unitcells set cold sink and hot source (thermostats, NVT)
Mid-area thermal transport area (NVE)

Quenching

NVE – NPT – NVE – NPT -NVE

Lattice Thermal Conductivity Calculation

- Set up units, atom style
- Load atomic coordinate
- Define interatomic forcefield
- Set up variables

```
#-------------------------------------------------------------------------
# Minimization --> Quenching Processs --> NEMD for thermal conductivity
#-------------------------------------------------------------------------
#            min -->> nve1 -->> npt1(600-600)
#                     nve2 -->> npt2(600-300)
#                     nve3 -->> npt3(300-300)   -->> nve4
#             After equilibration, perform NEMD
#-------------------------------------------------------------------------
units                  metal
atom_style             atomic
dimension              3
boundary               p p p
#-------------------------------------------------------------------------
read_data              data.pos
mass                   1 12.0107

pair_style             airebo 3 1 0
pair_coeff             * * CH.airebo C
#-------------------------------------------------------------------------
#          Variables for quenching process
variable               N           equal     count(all)
variable               P           equal     1.0125
variable               T1          equal     600.0
variable               T2          equal     300.0
variable               Tdamp       equal     v_dt*100
variable               Pdamp       equal     v_dt*1000
variable               dt          equal     0.0005          # INPUT
variable               run_nve1    equal     100000
variable               run_nve2    equal     200000
variable               run_nve3    equal     100000
variable               run_nve4    equal     200000
variable               run_npt1    equal     2000000
variable               run_npt2    equal     200000
variable               run_npt3    equal     2000000
variable               rndn        equal     135753
#-------------------------------------------------------------------------
```

Lattice Thermal Conductivity Calculation

- Run Relaxation and NVE calculation
- After that repeat twice NPT and NVE

  (To remove artificial defect on the system)
- Next step, thermal transport calculation

```
# Relaxation
neighbor            2.0 bin
neigh_modify        every 10  delay 0 check yes
fix                 br all box/relax iso 0.0 vmax 0.001
min_style           cg
minimize            1.00e-30 1.00e-30 100000 1000000
unfix               br
reset_timestep      0

# NVE 1
timestep            ${dt}
thermo_style        custom step temp etotal pe ke enthalpy press lx ly lz vol density
thermo              1000
fix                 nve1 all nve
variable            Temp   equal  temp
variable            ETOT   equal  etotal/v_N
variable            KE     equal  ke/v_N
variable            PE     equal  pe/v_N
variable            Pr     equal  press
fix                 ave_nve1 all ave/time 100 10 1000 v_Temp v_ETOT v_PE v_KE v_Pr ave window 2 file temp_nve1.out
dump                pos_xyz  all custom 50000 nve1_*.xyz id type x y z
dump_modify         pos_xyz sort id
run                 ${run_nve1}
unfix               nve1
unfix               ave_nve1
undump              pos_xyz
write_restart       restart.nve1
reset_timestep      0
```

Lattice Thermal Conductivity Calculation

- Run main calculation

  (At that time, there was not another choice)

```
# Thermal conductivity calculation, NVT (Thot)- NVE (transport) - NVT (Tcold)
fix                     fixth   grth nvt temp ${Th} ${Th} ${Tdamp}
fix                     fixtc   grtc nvt temp ${Tc} ${Tc} ${Tdamp}
fix                     fixtm   grtm nve

variable                encum   equal (f_fixtc-f_fixth)/2.
variable                endel   equal (-f_fixtc-f_fixth)/2.

thermo_style            custom  step c_th c_tm c_tc f_fixth f_fixtc v_encum v_endel v_heat_x v_heat_y v_heat_z

dump                    dmp_them all custom 1000 md_rescaling.traj id element xu yu zu vx vy vz
dump_modify             dmp_them sort id
```

- Today, there are several thermal

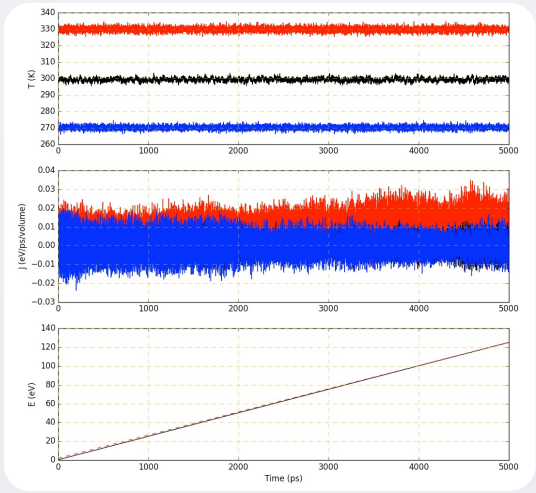
  conductivity calculation packages available.

Lattice Thermal Conductivity Calculation

- After finish calculation, do post-process

  (python code, house-code)

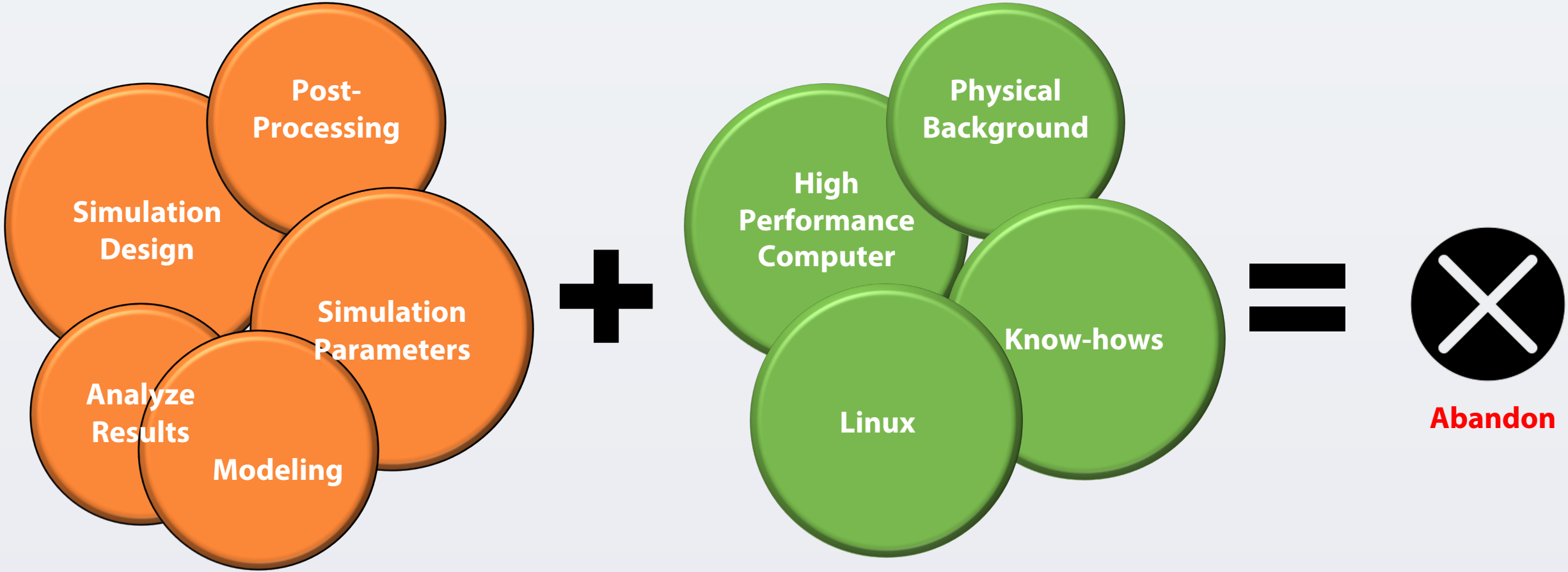
- Finally, I get nice figures !




```
# Post-process tool for Lattice Thermal Conductivity
# Written by MK (Virtual Lab)
# 2020. 05. 04.
# Update log.
# 2020. 05. 05.
# Parcing stdout_main -> temperature.dat

skip_raw = open('stdout_main').readlines()
ii = 0
for xx in skip_raw:
    if xx != '\n':
        if xx.split()[0] == 'Step':
            skip_raw_init = ii
        elif xx.split()[0] == 'Loop':
            skip_raw_final = ii
    ii += 1

new_temp = open("temperature.dat", 'w')
for xx in skip_raw[skip_raw_init+1:skip_raw_final]:
    new_temp.write(xx)

new_temp.close()

# step c_th c_tm c_tc f_fixth f_fixtc v_encum v_endel v_heat_x v_heat_y v_heat_z
#  0    1    2    3    4       5       6       7       8       9       10

import numpy as np

# Set-up variables
timestep = 0.0005              # ps
temperature_delta = 30*2       #
ll = 100; mm = 6; nn = 1       #
scalex = 9.4787998199; scaley = 16.4177627563; scalez = 3.2146000000 # lattice parameter
length = ll*scalex; width  = mm*scaley; height = nn*scalez
temp  = np.loadtxt("temperature.dat")
istep = temp[:,0] * timestep   # MD Time
temperature = temp[:,1:4]      # Temperature (Thot, Tmid, Tcold)
encum =  temp[:,6]/mm/nn       # Cumulative energy
flux  = temp[:,8:]             # Heatflux (Jx, Jy, Jz)

# To find the best fit
from scipy import stats
xx_best, yy_best = istep, encum
n_sampling = 10
sampling_list = range(0, len(encum), n_sampling)

p_list = []; ii = 0
while ii < len(sampling_list):
    slope, intercept, r_value, p_value, std_err = stats.linregress(xx_best[sampling_list[ii]:], yy_best[sampling_list[ii]:])
    p_list.append(r_value)
    if ii != 0 and p_list[ii] >= p_list[ii-1]:
        func = slope, intercept, r_value, p_value, std_err
    ii += 1
```

HOWEVER, “ANYONE” COULD DO THIS?

THERE ARE MANY BARRIERS TO ENTRY SIMULATION



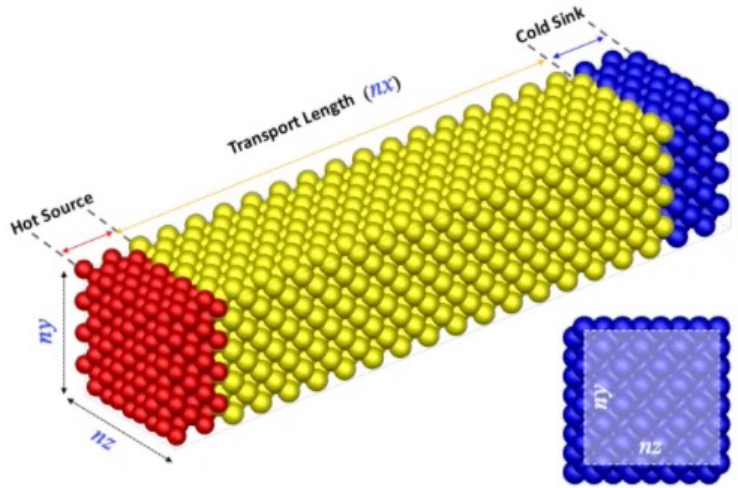
LAMMPS (Thermal Conductivity)

This job has been finished normally (id : 34053)

Simulation | Analysis

Potential table

ID	Type	Elements	Author	DOI
152	MEAM	W	Byeong-Joo Lee, M.I. Baskes, Hanchul Kim, and Yang Koo Cho	



Transport direction : x y z

Supercell : 150 2 2

1536 atoms

Temperature (K) : 300

Time (ps) : 500

Timestep (fs) : 0.5

Job Submit

Resource : On-Demand 48

Job Name : web_W_TC

Finish Notice : E-mail

Submitted

materials square

https://www.matsq.com

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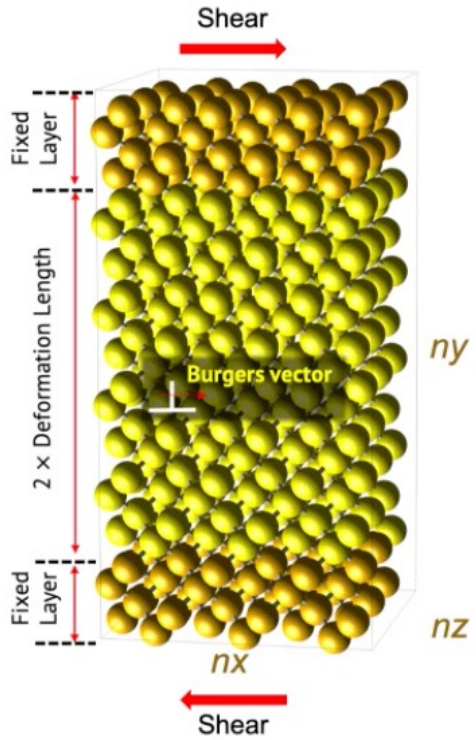
Ni edge dislocation

This job has been finished normally (id : 33505)

Simulation | Analysis

Potential table

ID	Type	Elements	Author	DOI
156	MEAM	Ni, Ti	W.-S. Ko et al.	



Crystal system : FCC BCC

Supercell : 30 40 4

28800 atoms

Dislocation type : Edge Screw

Poisson's ratio : 0.3

Displacement (Å) : 0.025

Total shear strain (%): 15

Total steps : 1158

Job Submit

Resource : On-Demand 36

Job Name : Ni edge dislocation test

Finish Notice : E-mail

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