

# Reproducing MD simulations in

Thermal transport in SiGe superlattice thin films and nanowires:  
Effects of specimen and periodic lengths

*Keng-hua Lin, and Alejandro Strachan*  
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## **Thermal transport in SiGe superlattice thin films and nanowires: Effects of specimen and periodic lengths**

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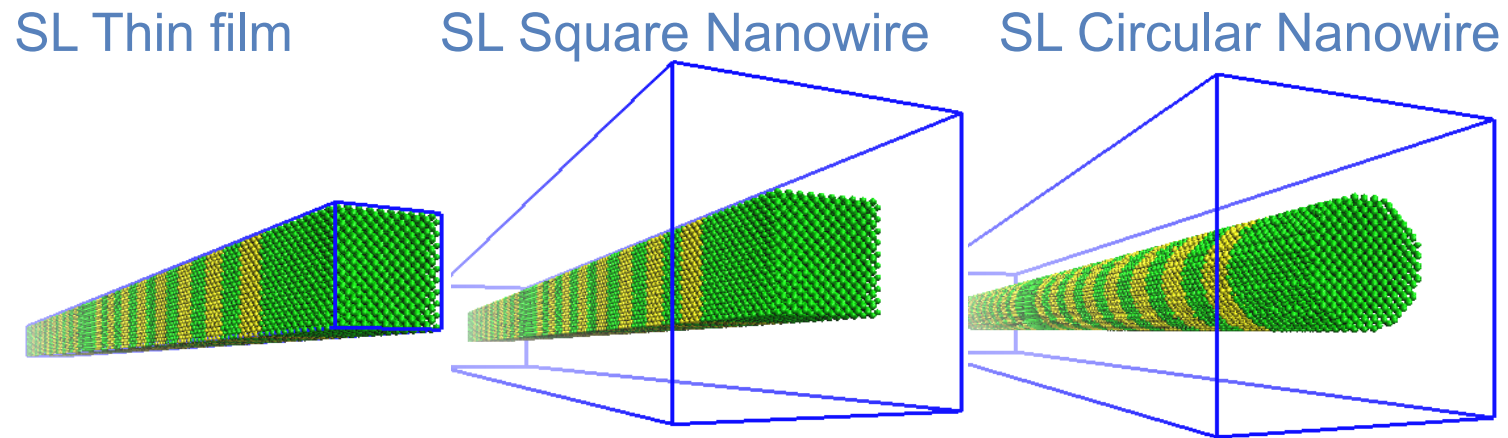
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We compute the thermal conductivity of superlattice (SL) thin films and nanowires for various SL periods and total specimen lengths using nonequilibrium molecular dynamics. Both types of materials exhibit similar behaviors with respect to SL period but the thermal conductivity of the thin films exhibits a significantly higher sensitivity to the specimen length. Notably, the thermal conductivity of SL thin films is smaller than those of the corresponding nanowires for specimen lengths below approximately 35 nm. These results arise from the complex dependence of the conductivities of the interfaces and the SL components on the specimen size and period. These trends and observations are explained using a simple phonon model that builds on the relationship between the cumulative thermal conductivity and the phonon wavelength.

DOI: [10.1103/PhysRevB.87.115302](https://doi.org/10.1103/PhysRevB.87.115302)

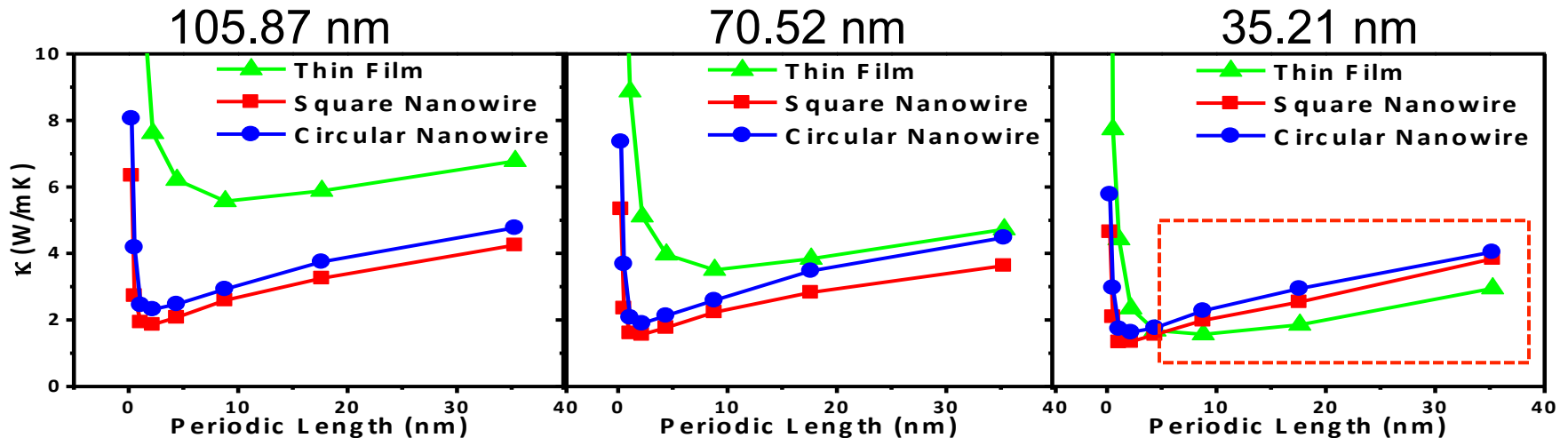
PACS number(s): 65.80.-g, 68.65.Cd, 63.22.-m, 63.22.Np

Studied thermal transport on various semiconductor superlattices



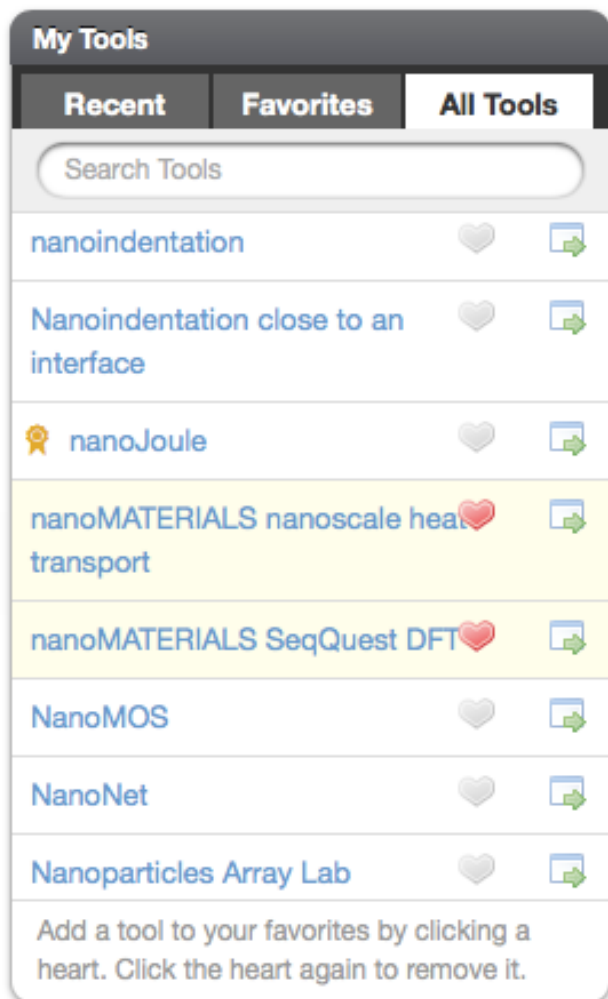
- Thin film and nanowire configurations
- Focused on how characteristic sizes affect thermal transport
  - Superlattice period
  - Total specimen length

## Thermal conductivity vs. superlattice period for three specimen lengths



- Thermal conductivity decreases with decreasing period until it reaches a minimum, further reduction leads to an increase in thermal conductivity – this is well known
- For long specimens thermal conductivity of wires is smaller than thin films – this is expected due to surface scattering
- Reducing specimen length reduces thermal conductivity – also well known – but the decrease in thin film is much more marked -> key result of the paper
- For short specimens thermal conductivity of thin films is predicted to be smaller than that of nanowires – surprising & interesting





From the tools menu launch  
“nanoMATERIALS nanoscale heat  
transport”

## About the tool:

Build nanoscale semiconductor samples and heterostructures and compute their thermal transport using MD

## Learn more about MD:

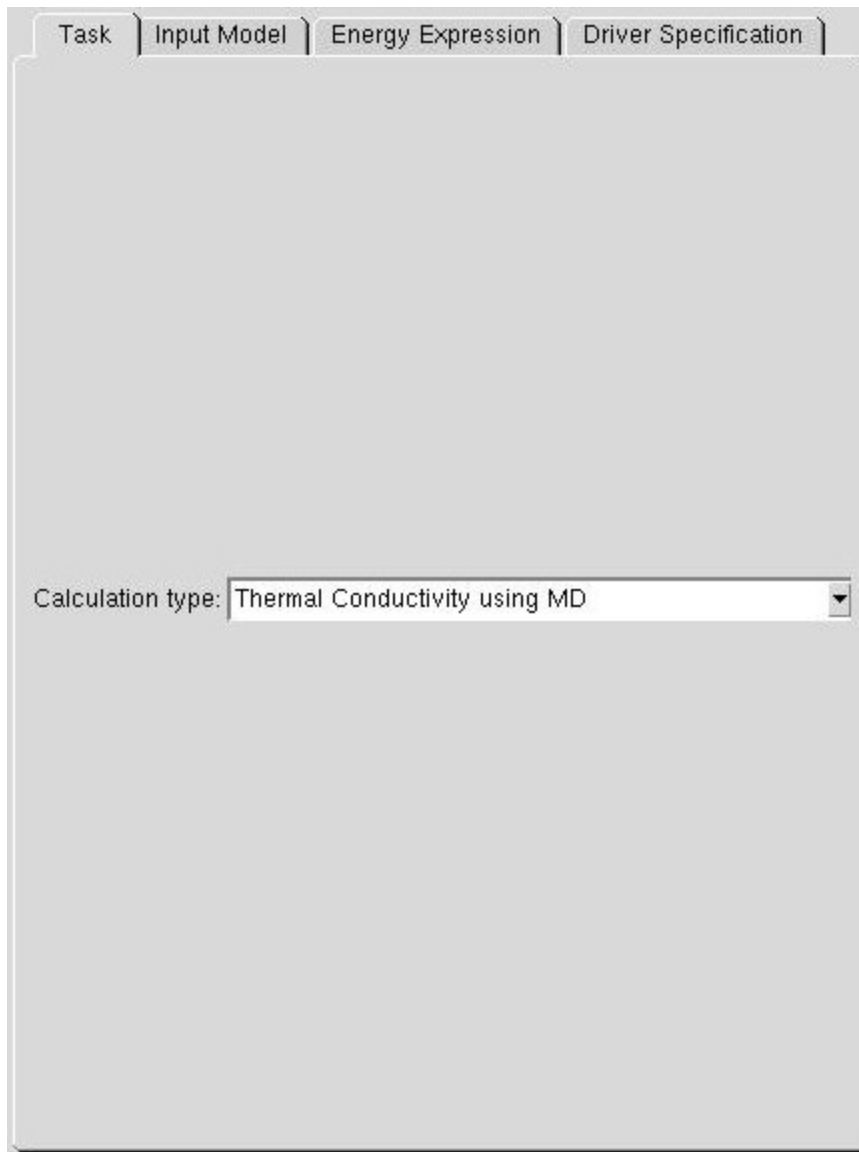
- nanoHUB-U course “Atoms to Materials”  
<https://nanohub.org/courses/FATM>
- <https://nanohub.org/topics/MD>  
**and thermal transport**
- nanoHUB-U course “Atoms to Materials”  
<https://nanohub.org/courses/FATM>

## Objective

Build heterostructures and compute their thermal conductivity

## Approach

- Thermal conduction using MD simulations in LAMMPS
  - <http://lammmps.sandia.gov>
- Use a method by Müller-Plathe to compute thermal conductivity
  - F. Müller-Plathe, J. Chem. Phys. 106, 6082 (1997).

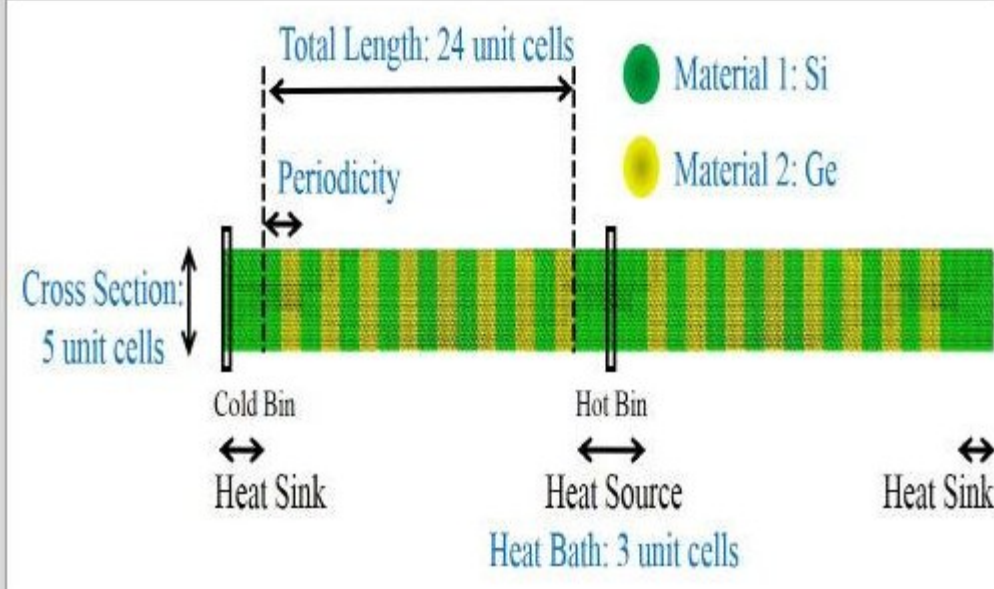
A screenshot of a software interface for setting up a simulation. At the top, there are four tabs: "Task", "Input Model", "Energy Expression", and "Driver Specification". The "Input Model" tab is currently selected. Below the tabs is a large, empty grey rectangular area. At the bottom of this area, there is a label "Calculation type:" followed by a dropdown menu. The dropdown menu is open, showing the text "Thermal Conductivity using MD" and a small downward-pointing arrow on the right side.

The default calculation type is set to thermal conductivity, so move on to the “Input Model” tab

Task | Input Model | Energy Expression | Driver Specification

Create your own structure?:  no

Use pre-built structure



Total Length: 24 unit cells

Material 1: Si

Material 2: Ge

Periodicity

Cross Section: 5 unit cells

Cold Bin

Hot Bin

Heat Sink

Heat Source

Heat Bath: 3 unit cells

Prebuilt structure:

- Si/Ge nanolaminate (Periodicity: 4 unit cells)
- Si/Ge square nanowire (Periodicity: 0.5 unit cell)
- Si/Ge square nanowire (Periodicity: 1 unit cell)
- Si/Ge square nanowire (Periodicity: 2 unit cells)
- Si/Ge square nanowire (Periodicity: 4 unit cells)
- Si/Ge square nanowire (Periodicity: 8 unit cells)
- Si/Ge nanolaminate (Periodicity: 0.5 unit cell)
- Si/Ge nanolaminate (Periodicity: 1 unit cell)
- Si/Ge nanolaminate (Periodicity: 2 unit cells)
- Si/Ge nanolaminate (Periodicity: 4 unit cells)
- Si/Ge nanolaminate (Periodicity: 8 unit cells)

The tool supplies prebuilt structures for square nanowire and nanolaminate simulations

Each prebuilt structure has the same specimen length (29.32 nm) but varies in periodicity

Running one simulation for each prebuilt structures will generate the data needed to plot thermal conductivity vs. periodic length



Task | Input Model | Energy Expression | Driver Specification

Thermalization run before thermal conductivity calculation?  no

Temperature equilibration run before thermal conductivity calculation?  no

**Thermal Conductivity Calculation**

Ensemble: NVT

Temperature:

Pressure:

MD Time Step:

Number of MD Steps:  + -

Swapping Frequency (Steps):  + -

**Periodic Tasks**

Write to Trajectory (Steps):  + -

Write to Temperature File (Steps):  + -

**Data Analysis**

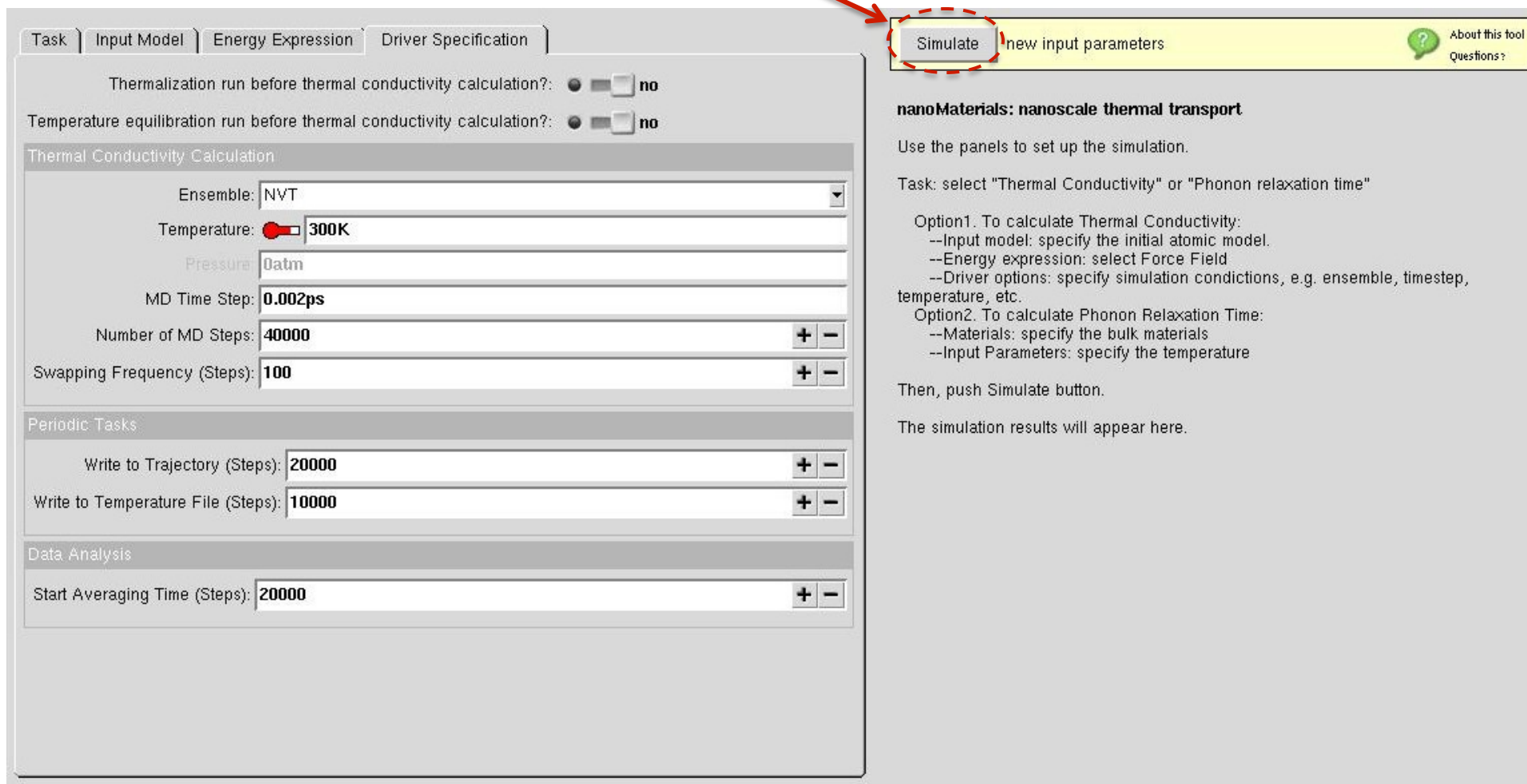
Start Averaging Time (Steps):  + -

The “Energy Expression” tab can be skipped as it only shows the use of the Stillinger-Weber interatomic potential

The “Driver Specification” tab lists MD simulation parameters that can be adjusted if desired, but can be left as is

For improved results, increase the “Number of MD Steps” to 100,000 and set the “Start Averaging Time” to 50,000. This will give the specimen more time to reach steady-state and increase the amount of averaging points, but at the cost of a longer simulation

Click "Simulate" to begin the simulation



Task | Input Model | Energy Expression | Driver Specification

Thermalization run before thermal conductivity calculation?:  no

Temperature equilibration run before thermal conductivity calculation?:  no

Thermal Conductivity Calculation

Ensemble: NVT

Temperature: 300K

Pressure: 0atm

MD Time Step: 0.002ps

Number of MD Steps: 40000 + -

Swapping Frequency (Steps): 100 + -

Periodic Tasks

Write to Trajectory (Steps): 20000 + -

Write to Temperature File (Steps): 10000 + -

Data Analysis

Start Averaging Time (Steps): 20000 + -

**Simulate** new input parameters

About this tool Questions?

**nanoMaterials: nanoscale thermal transport**

Use the panels to set up the simulation.

Task: select "Thermal Conductivity" or "Phonon relaxation time"

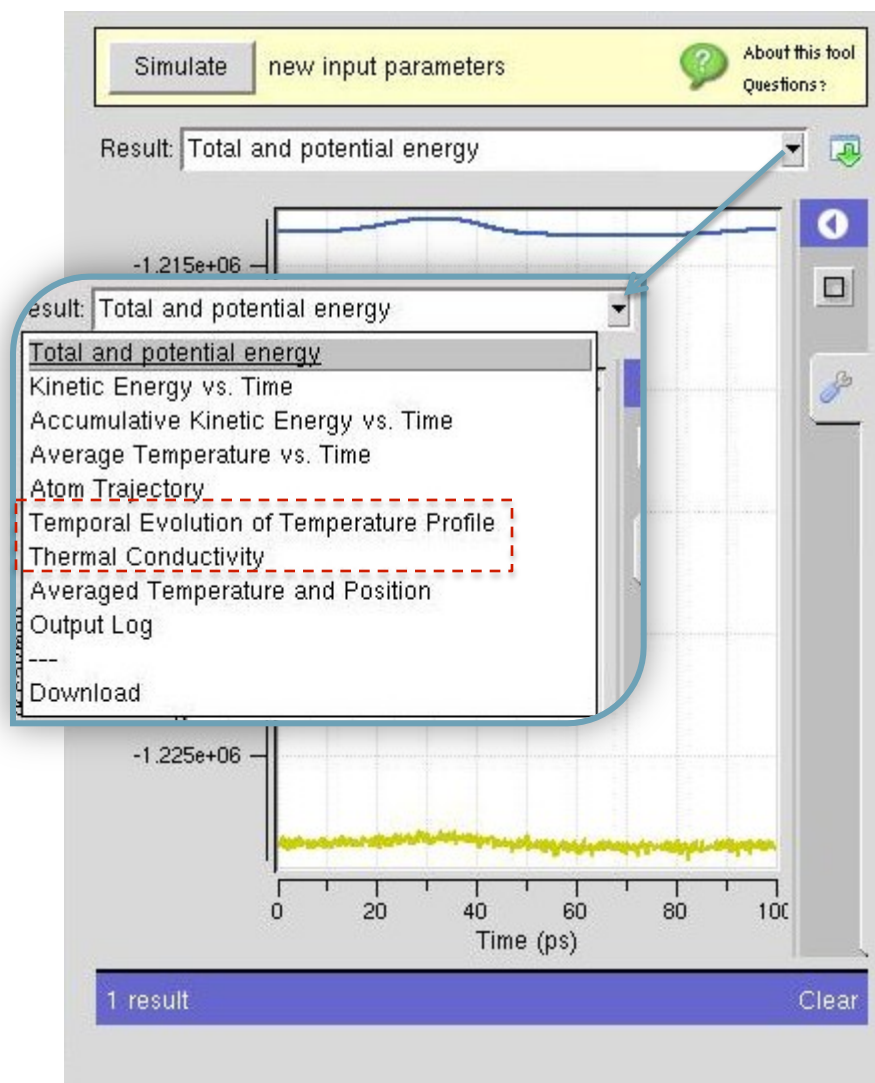
Option1. To calculate Thermal Conductivity:  
 --Input model: specify the initial atomic model.  
 --Energy expression: select Force Field  
 --Driver options: specify simulation conditions, e.g. ensemble, timestep, temperature, etc.

Option2. To calculate Phonon Relaxation Time:  
 --Materials: specify the bulk materials  
 --Input Parameters: specify the temperature

Then, push Simulate button.

The simulation results will appear here.

Allow for 1-4 hours for the simulation to run



Once the simulation finishes, the simulation results panel will appear

The “Thermal Conductivity” page contains the results of interest, and the “Temporal Evolution of Temperature Profile” page is useful to view

Result: Thermal Conductivity

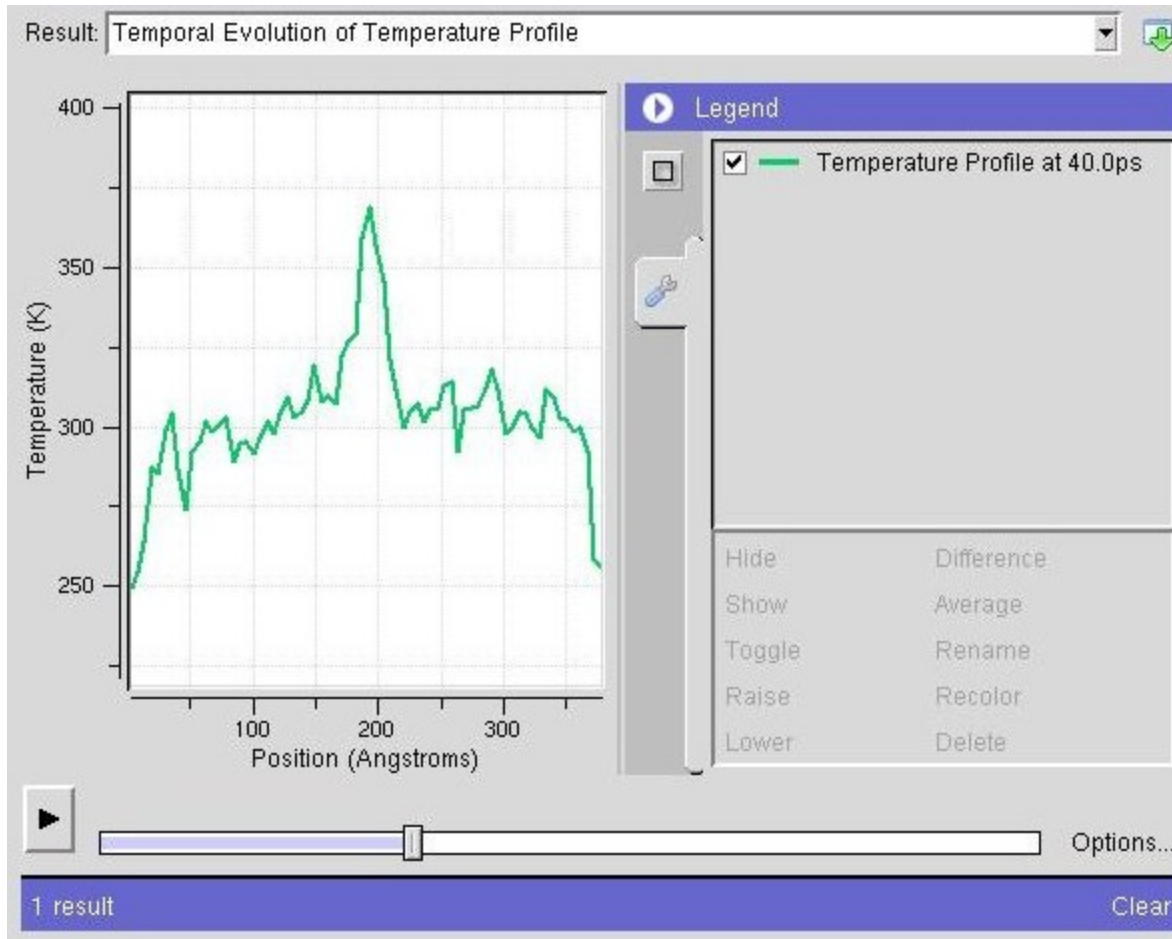
```
Thermal Conductivity including Material and Contacts: 0.27445 (W/mK)
Material Thermal Conductivity: 0.35832 (W/mK) from layer 3 ~ 26
KE: 6074.73920 Kcal/mol
Lx: 39.85034 Angstroms
Ly: 39.63897 Angstroms
Time: 400.00000 ps
Total Bin Number: 54
Number of Heatbath: 3
```

Find:

1 result

The “Thermal Conductivity” page gives the  $\kappa$  values for the material with contacts and for just the material

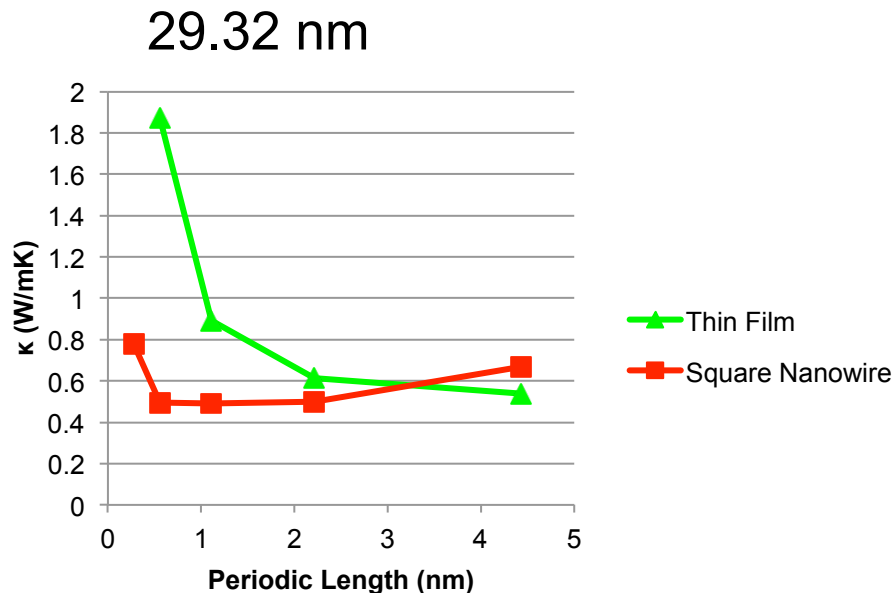




The “Temporal Evolution of Temperature Profile” page depicts the temperature profile of the specimen at periodic timesteps, which can be set as one of the simulation parameters. The slider at the bottom is used to cycle through the profiles

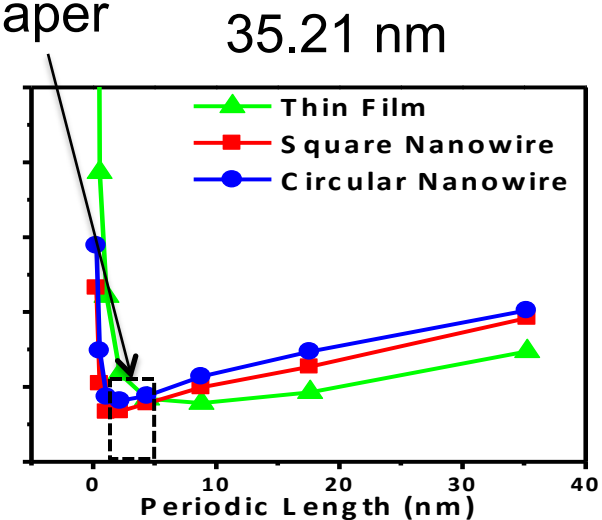
Looking at the temperature profiles reveals when the specimen reaches steady-state within the simulation

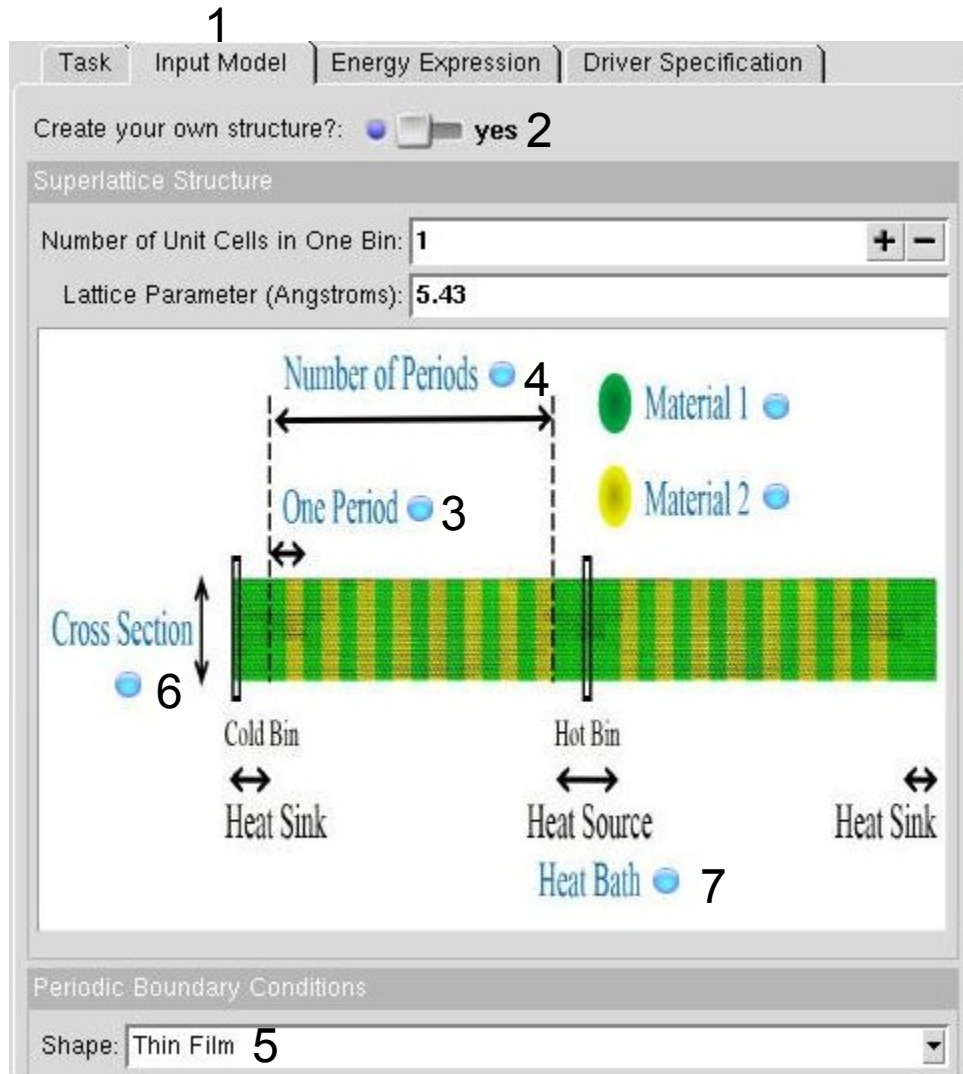
By collecting and mapping the thermal conductivities for each of the prebuilt structures, the following curves are generated:



Similar behavior of the two curves is clearly seen, as the thin film thermal conductivity becomes greater than the square nanowire thermal conductivity at lower periodic lengths

These results correspond to this portion of the graph provided in the paper





To simulate longer SiGe structures, as used in the paper, go back to the “Input Model” tab (1) and click “Create your own structure” (2)

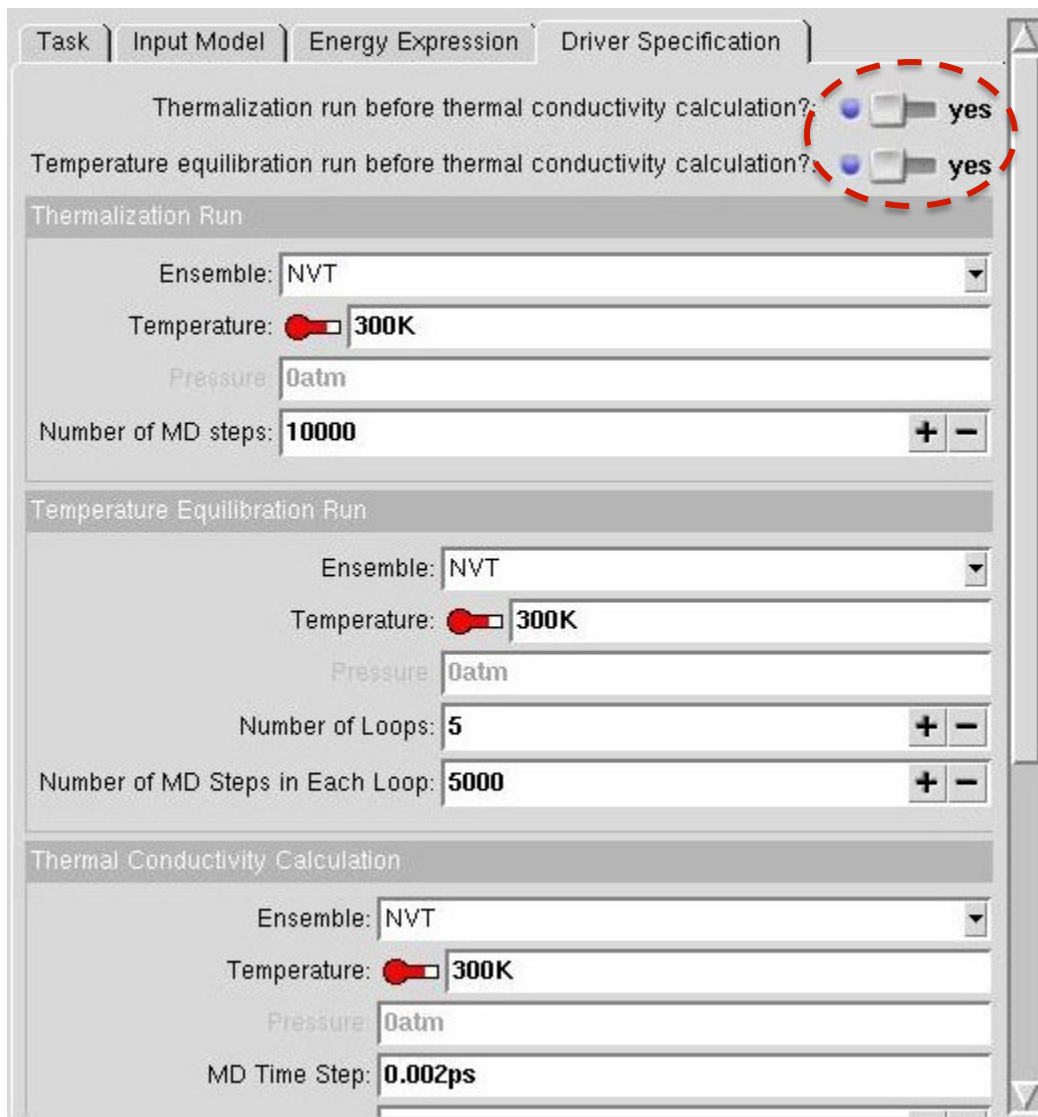
Use the “One Period” hotspot (3) to define the number of bins of each material per period

Use the “Number of Periods” hotspot (4) to adjust the total length of the structure

Use the “Shape” option (5) at the bottom is the option to choose between thin film (nanolaminate) and square nanowire structures

The “Cross Section” (6) and “Heat Bath” hotspots can also be adjusted if desired (7)

$$\text{Specimen length} = 2 \times (\text{number of periods} \times \text{periodic length} + \text{length of heat bath})$$



Task | Input Model | Energy Expression | **Driver Specification**

Thermalization run before thermal conductivity calculation?  yes

Temperature equilibration run before thermal conductivity calculation?  yes

**Thermalization Run**

Ensemble: NVT

Temperature: 300K

Pressure: 0atm

Number of MD steps: 10000

**Temperature Equilibration Run**

Ensemble: NVT

Temperature: 300K

Pressure: 0atm

Number of Loops: 5

Number of MD Steps in Each Loop: 5000

**Thermal Conductivity Calculation**

Ensemble: NVT

Temperature: 300K

Pressure: 0atm

MD Time Step: 0.002ps

Unlike the prebuilt structures, every newly generated structure needs to undergo thermalization and temperature equilibration as part of the simulation, so these options should be switched to 'yes' under the "Driver Specification" Tab

The default parameters for thermalization and temperature equilibration need only be adjusted if desired



Temperature Equilibration Run	
Ensemble:	NVT
Temperature:	300K
Pressure:	0atm
Number of Loops:	5
Number of MD Steps in Each Loop:	5000
Thermal Conductivity Calculation	
Ensemble:	NVT
Temperature:	300K
Pressure:	0atm
MD Time Step:	0.002ps
Number of MD Steps:	50000
Swapping Frequency (Steps):	100
Periodic Tasks	
Write to Trajectory (Steps):	10000
Write to Temperature File (Steps):	5000
Data Analysis	
Start Averaging Time (Steps):	30000

The remaining simulation parameters can be left at their default value, or can be adjusted for improved, but longer, simulations

The “Start Averaging Time” needs to be sufficiently large for the specimen to reach steady-state before averaging begins (> 40ps)

The “Number of MD Steps” needs to be sufficiently larger than the “Start Averaging Time” to generate a large number of data points (usually at least 40ps greater)

Once the parameters are set, begin the simulation.