Thermal Conductivity Simulator

First-time User Guide

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Introduction

- This tool is designed to calculate the thermal conductivity of one of the most important semiconductor material, that is, silicon. The reverse non-equilibrium molecular dynamics (RNEMD) technique is used.
- The tool uses LAMMPS software package for the RNEMD simulation.
- With this tool you can calculate the thermal conductivity of Silicon for any rectangular dimensions and at any temperature.
The RNEMD Method

- This method uses the `fix thermal/conductivity` command in LAMMPS, which implements the rNEMD algorithm of Muller-Platthe.
- Kinetic energy is swapped between atoms in two different layers of the simulation box.
- This induces a temperature gradient between the two layers. The fix tallies the cumulative energy transfer ($Q$) that it performs.
- Dividing the energy transferred by time ($t$) and the cross-sectional area ($A$) of the simulation box yields a heat flux.
- Heat flux, $\dot{q} = \frac{Q}{At}$
- The ratio of heat flux to the slope of the temperature profile gives the thermal conductivity.
Lines of best-fit are plotted and their slopes averaged to get the temperature gradient.

\[ k = \frac{\dot{q}}{dT/dz} = \frac{\dot{q}}{\text{average slope}} \]
1. Thermal Conductivity Simulator

- Go to https://nanohub.org/
- Log in to nanoHUB. If you do not have a nanoHUB account then create one.
- From My Tools on nanoHUB dashboard, search for “Thermal Conductivity Simulator” and then launch the tool.
- You can also go directly to https://nanohub.org/tools/thermalcond and launch the tool.
2. Inputs

This is the tool interface. You will input your specifications here.
2. Inputs

Currently the only material choice is Silicon. However, more materials can be added upon request.

Set your desired temperature here.

Set your desired dimensions.

Note that:

- The minimum x and y dimensions are 3nm, to ensure a minimum number of atoms in each layer for appropriate temperature measurements.
- Previous research works shows that the z-dimension should be at least 33nm long (about 60 unit cells) to get results with close accuracy to experiments.
- The x, y and z dimensions will be automatically slightly adjusted as shown below:

For proper diamond lattice, resetting length values to:

\[ x = 3.258612 \text{ nm} \]
\[ y = 3.258612 \text{ nm} \]
\[ z = 33.129225 \text{ nm} \]
2. Inputs

Once you have entered all the desired specifications, click the ‘simulate’ button to generate your structure.
3. Wait for simulation results
4. Explore Simulation Results

- Average Heat flux (W/m²)
- Thermal Conductivity (W/m.K)
- Average Heat flux (W/m²)
4. Explore Simulation Results
If you have any queries or feature requests, feel free to contact us at our email addresses given on first page.

Researchers should cite this work as: