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# To determine the thermal conductivity of a silicon nanowire using MD simulation

ES 631 Advanced Heat Transfer

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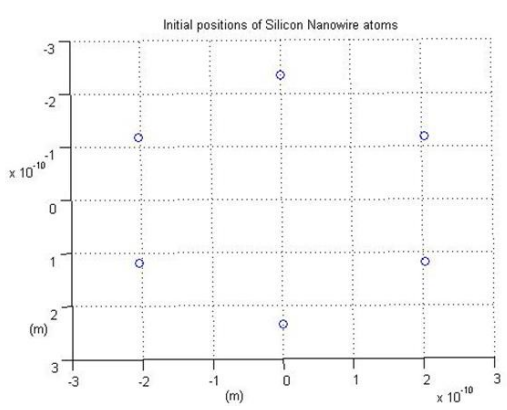
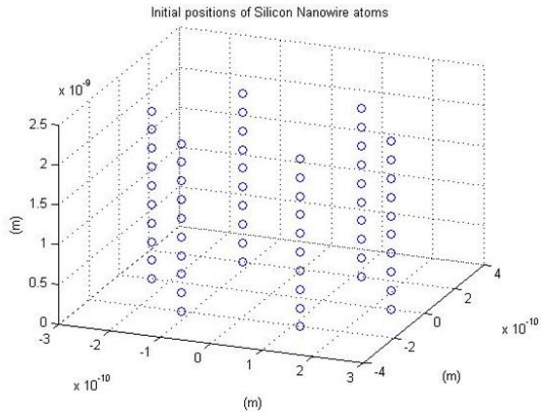
**Objective:** The goal of the present work is to estimate the thermal conductivity of a infinitely long silicon nanotube from molecular dynamic simulation using the Green–Kubo formula. We begin with estimation of the initial position and velocity of each Si atoms in the nanotube followed by integration of equation of motion using velocity verlet algorithm subjected to appropriate initial and boundary conditions.

### Methodology and Matlab code sequence:

## Initial positions [*siliconstructure.m*]

A Matlab routine has been written to fix the initial position of all atoms. Assuming hexagonal structure for Si we take into consideration ten cross sections of Si layers as our computational domain with six atoms in each layer. The center of the first layer are fixed at (0,0,0). Periodic boundary condition is implemented for distances.




The coordinates are calculated as

$$x = r_o \cos\theta$$
$$y = r_o \sin\theta$$
$$z = z$$

Initial velocity: The initial velocities were assigned using normal distribution with mean zero and standard deviation $\sqrt{\frac{k_B T}{m}}$ where m is the mass of the system i.e. $m_{si}$*number of particles.

Center of mass velocity is maintained at zero by

$$V_{CMx} = V_x - V_{mean(x)}$$

$$V_{CMy} = V_y - V_{mean(x)}$$

$$V_{CMz} = V_z - V_{mean(z)}$$

## Distances [*distances.m*]:

Distances and relative positions were computed between every bonded pair.

## Inter atomic potential and forces [*weber.m*]:

The inter-atomic potential dictates how the atoms or the molecules interact with each other in a system. The force acting on the system is determined by taking the gradient of the potential of the system. An empirical potential for Si is the Stillinger-Weber potential which has a pair potential and three body potential. For the sake of simplicity we take into account the distance based potential as,

$$u_2(r_{ij}) = \begin{cases} \varepsilon A_{sw}\left[B_{sw}\left(\frac{\sigma}{r_{ij}}\right)^4 - 1\right]\exp\left[\left(\frac{r_{ij}-a}{\sigma}\right)^{-1}\right] & r_{ij} < a \\ 0 & r_{ij} \geq a \end{cases}$$

**Table 1 Recommended parameters in the Stillinger Weber potential for Si []**

| | | | |
|---|---|---|---|
| $\varepsilon$=3.4723*10$^{19}$ J | $\sigma$= 0.20951 nm | $A_{sw}$=7.049556277 | $B_{sw}$=0.6022245584 |
| a=1.80$\sigma$ | $\lambda$= 21 | $\gamma$=1.2 | |

The forces are defined as,

$$F_{ij} = \frac{du_2}{dr_{ij}}$$

$$F_{ij} = \varepsilon A_{sw}\left[-4B_{sw}\sigma^4(r_{ij})^{-5}\right]\exp\left(\frac{r_{ij}-1}{\sigma}\right)^{-1} - \left(B_{sw}\left(\frac{\sigma}{r_{ij}}\right)^4 - 1\right)\exp\left(\frac{r_{ij-1}}{\sigma}\right)^{-1}$$

## *forceComponents.m:*

It converts all the interatomic forces acting on each atoms into a combined vector force for each atom.

## Velocity verlet algorithm [*velocityVerlet.m*]:

After establishing the initial position, velocity and inter atomic potential, the next step is to integrate the equation of motion. We have used velocity verlet algorithm for the same. It gives us velocity, position and acceleration for the next time step.

Velocity Verlet Algorithm:
A related, and more commonly used, algorithm is the Velocity Verlet algorithm

1. Calculate $\vec{x}(t+\Delta t) = \vec{x}(t) + \vec{v}(t)\Delta t + \frac{1}{2}\vec{a}(t)\Delta t^2$
2. Derive $\vec{a}(t+\Delta t)$ from the interaction potential using $\vec{x}(t+\Delta t)$
3. Calculate $\vec{v}(t+\Delta t) = \vec{v}(t) + \frac{1}{2}(\vec{a}(t) + \vec{a}(t+\Delta t))\Delta t$

## Estimation of heat flux for one time step [*JQ.m*]

$$J_Q(t) = \frac{1}{V}\left[\sum_{i=1}^{N}\left(\vec{v}_i h_i + \frac{1}{2}\sum_{i=1, j\neq 1}^{N}(\vec{F}_{ij} \bullet \vec{v}_i)\right)\right]$$

Where,

$$h_i = \frac{p_i^2}{2m} + u_i$$

$u_i$ is the interatomic potential.

## Thermostat: [*thermostat.m*]

The purpose of thermostat is to enforce the temperature at desired value. It gives us scaling factor for velocity.

Berendsen Thermostat:

$$X^2 = 1 + \frac{\delta t}{\tau}\left(\frac{KE_0}{KE} - 1\right)$$

## Estimation of conductivity [*conductivity3.m*]

This code calculates the thermal conductivity using all the previous functions. It requires input of τ (thermostat parameter) and δt (time step) values. The values assumed are:

| | |
|---|---|
| τ | $1*10^{-31}$ |
| δt | $5*10^{-33}$ |

Green Kubo Method for thermal conductivity of an isotropic solid:

$$k(T) = \frac{V}{3k_B T^2}\int_0^\infty (J_Q(t) \bullet .J_Q(0)dt$$

$$= \frac{V}{3k_B T^2}\int_0^\infty \int \overline{J_Q(t) \bullet J_Q(0)}dt$$

After a simulation of ($M_t$ -l)Δt, the axial heat current is known for t = 0, Δt, 2Δt, ..., ($M_t$ -l)Δt. Thus, there are $M_t$ data points available for the calculation of the thermal conductivity. The auto-correlation function at a given time t = jΔt (with j = 0, 1, 2, ..., M, -1 ) can be calculated using:

$$\overline{J_Q(t) \bullet J_Q(0)} = \frac{1}{M}\sum_{k=1}^{M} J_Q(t_k) \bullet J_Q(t_k + t)$$

$$M = M_t - \frac{t}{\Delta t_s} = M_t - j$$

where M = M, - j and ti corresponds to t = 0. Consider a simulation of 100Δt . The third term (j = 2) of the auto-correlation function can be expressed as:

$$HCACF(2\Delta t) = \frac{1}{9}\left[J_Q(0)J_Q(2\Delta t) + J_Q(\Delta t)J_Q(3\Delta t) + ...\right]$$

The integration of the HCACF in is thus limited by the precision of the auto-correlation function, which is influenced by the length of the simulation and by the number of time steps.

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## Results and conclusion:

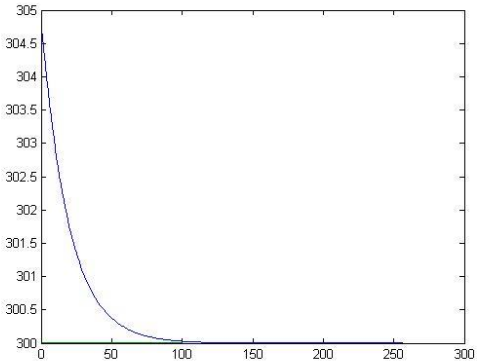
Thermal conductivity calculated by each run of random number generation varies as the assigned initial velocities are varying.

The table below shows mean and standard deviation of initial velocities and corresponding thermal conductivity.

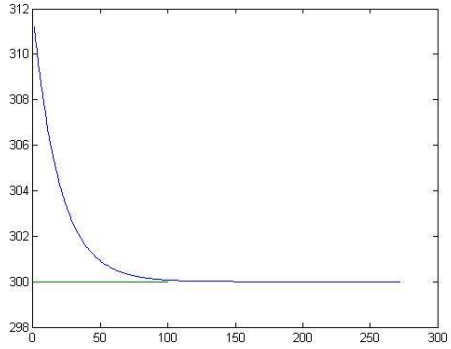
| SR NO | MEAN | STANDARD DEVIATION | THERMAL CONDUCTIVITY |
|---|---|---|---|
| 1. | 61.9973 | 25.9777 | 3.3571 |
| 2. | 62.7332 | 26.0818 | 3.9069 |
| 3. | 67.7217 | 26.4540 | 3.5991 |
| 4. | 51.0162 | 21.2843 | 10.0546 |
| 5. | 59.1648 | 27.0038 | 3.4675 |

## Temperature plot:

Temperature is stabilized using thermostat as shown in fig below

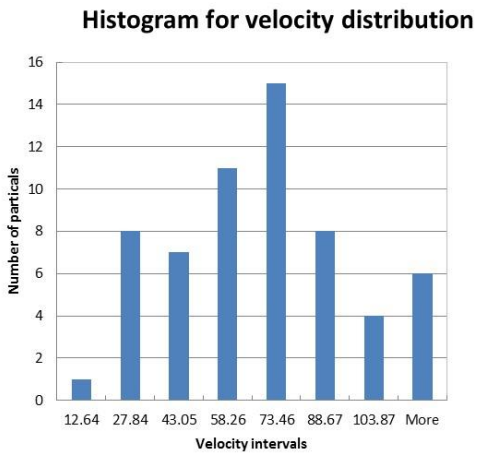



1st run temperature variation

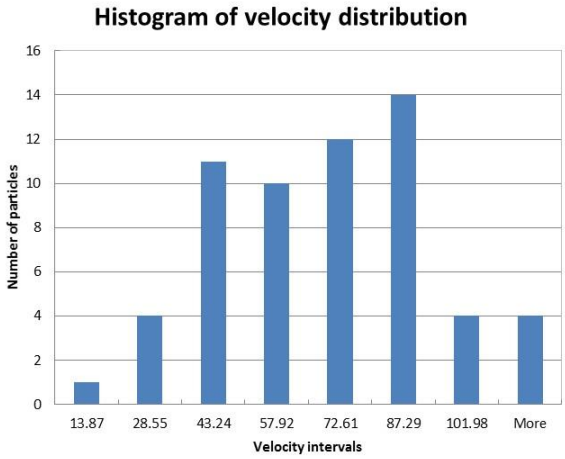



2nd run temperature variation.

## Velocity Distribution at the end of simulation:




(a) Velocity distribution for first run




(b) Velocity distribution for second run

## Conclusion:

It was observed that the value of the thermal conductivity value is sensitive to $\delta t$ and $\tau$.