A STUDY OF SILICON DIOXIDE NANOWIRE BY MOLECULAR DYNAMICS SIMULATIONS: INFLUENCE OF INTERATOMIC POTENTIALS AND BOUNDARY CONDITIONS

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Abstract : The results of molecular dynamics (MD) simulation depend on the choice of interatomic potentials, force conditions and simulation parameters. Interatomic potential has been used for MD simulations of silicon dioxide, based on properties of heat conduction phenomena. In this method, BKS potential is used .Nonequilibrium molecular dynamics method is used to calculate temperature gradient.

Keywords **- Thermal conductivity, Molecular Dynamics simulation, nanowire**

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I.INTRODUCTION

In the development of nanotechnology, thermal properties of nonmaterial's is essential part. System failure will happen because of excessive temperatures and temperature gradient. At nanometric scales, for thermal conductivity measurements modeling and simulation tools are necessary. In such a system prediction of heat transfer is challenge when the mean free path of heat carriers is of the same order of magnitude as the thickness of the layers in the material. Molecular dynamics (MD) is a convenient tool for studying atomic scale material. For transport properties, MD is well-suited. (1)

In solids, heat conduction can occur through lattice vibrations, electronic excitations and radiative processes. In insulators, electronic contributions to thermal conductivity are small, At very high temperatures, radiative contributions become important because of T3 dependence of the radiative term. (2)

As the size of the electronic circuits decreases, density increases and correspondingly dissipation of heat increases. For the dissipation of heat generated in electronic devices metallic heat sink materials such as copper are used. The thermal conductance at interfaces is low due to effective contact area, however this low effective contact area is due to the fact that solid surfaces are rough at atomic level. To increase the effective contact area and hence the interfacial thermal conductance, in the electronic industry, thermal grease is used which is an extremely flexible material that can form an efficient contact with both solid surfaces under pressure, effectively increasing the contact area between the original two solid surfaces. (3)

Due to nanotechnological advances, there is possibility of synthesizing and designing materials at the atomic level. For optimization of design before synthesis, Prediction of the properties of potent materials is allowed by Molecular dynamics (MD) simulations. In many applications, low thermal conductivity materials are required. By introducing porosity thermal conductivity of a solid can be reduced but it reduces the strength of the material. Amorphous materials have low thermal conductivities, but in some applications it is necessary to use a crystalline solid. (4)

Method: The thermal conductivity **K** is the ratio of the thermal current(heat flux per unit area) to the temperature gradient along the z direction (Fourier's law)

$$\mathrm{K} = \frac{\mathcal{J}_z}{\partial T/\partial z} \qquad \text{Eq. a)}$$

Thermal conductivity is calculated by equilibrium molecular dynamics, Nonequilibrium molecular dynamics In equilibrium molecular dynamics, Heat flux autocorrelation function is used while in Nonequilibrium molecular dynamics, temperature gradient is used. In equilibrium molecular Green-Kubo formalism is used while in Nonequilibrium molecular dynamics, Fourier's law is used.

According to the Kinetic theory, the thermal conductivity is given by the formula (due to Finite size effects)

$$\mathrm{K} = \frac{1}{3} C v \ell \qquad \text{Eq. b)}$$

Where C is heat capacity per unit volume, v is velocity and ℓ is mean free path of the phonons.

Because of localization effect,care should be taken ,while applying the formula to the glasses. As the energy E of the mode increases, the scattering rate increases as E^4 until $\ell^{-1} \sim$ k where k is the wavevector of the mode. (5)

Heat capacity C is due to contribution of transport phonons, v and ℓ are the characteristics of "propagative" phonons which are also contributing to the transport properties. (6)

II.Procedure: A molecular dynamic simulation is performed on a silicon dioxide nanowires using BKS interatomic potential. In simulation box, heat transport coefficients are directly calculated. Heat flux is induced in the system with the help of "hot" and "cold" plate. This creates a temperature gradient and to determine thermal conductivity steady state have to be reached. Plates are compatible with periodic boundary conditions

In this simulation, a long simulation cell is divided into a series of parallel slabs and the temperature is measured. In the center of the simulation cell, Heat is added to the slab and removed from a slab at one end of the simulation cell at fixed rates by rescaling velocities at every time step. After sufficient time, a temperature gradient is established that decreases from center to ends of the simulation cell. Since a heat flux is given, the temperature gradient is measured, we calculate the thermal conductivity through Eq.1.

The classical BKS interatomic potential is given as

$$\Phi_{ij} = q_i q_j / r_{ij} + A_{ij} \exp(-b_{ij} r_{ij}) - C_{ij} / r_{ij}^6 \qquad \text{Eq.1}$$

Where r_{ij} is the separation between atoms i and j

Φ_{ij} is the interaction energy of atoms i and j, which consists of a Coulomb term and a covalent contribution. (7)

The scope of the paper is to find out the capability of NEMD simulation to provide estimation of the thermal conductivity in SiO_2. Thermal transport is calculated along (001) axis of quartz. Periodic boundary condition is applied along x axis only (for nanowire)

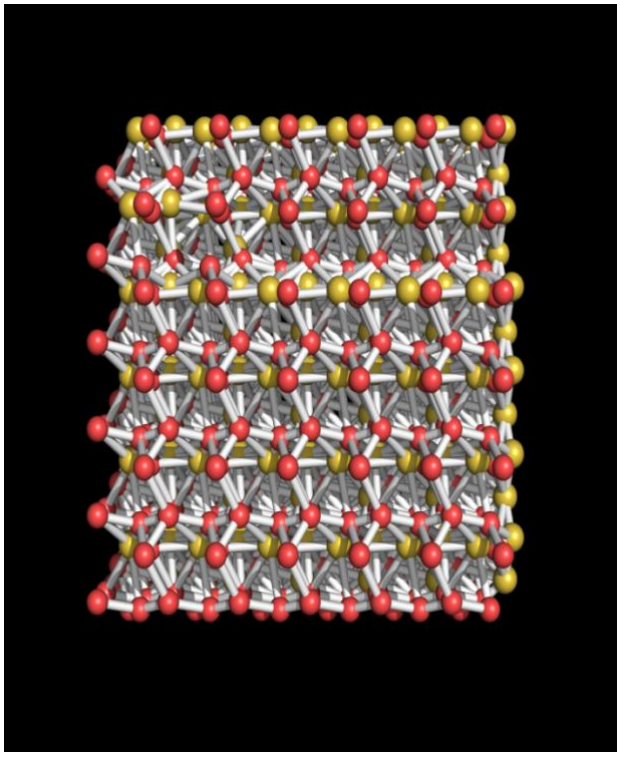

Figure 1: Initial Position of Silicon Dioxide molecule.

III.**The model Set up**: This simulation is carried out using classical Molecular dynamic Simulation in a micro canonical ensemble using 1200 particles of Quartz with the help of BKS potential. These particles are packed in a cubic box of length 25.774548A^0 Periodic boundary conditions are imposed along (001) direction. Due to the periodic boundary condition imposed on system, the heat flows from the hot energy reservoir to cold energy reservoir at the end of the silicon slab.MD steps at a constant temperature of 300 K using Anderson thermostat with a time step of t=1.0 picosecond.

Most commonly used theoretical method for molecular dynamics simulation is Non-equilibrium molecular dynamics (NEMD) to determine thermal conductivity. Ratio of heat flux to temperature gradient gives thermal conduction, There are two approaches to calculate this.

- A known heat flux is imposed and temperature gradient is calculated.
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For the imposition of heat flux, simulation cell is divided into even number of equal of section, one half as hot section and other half as cold section

Heat leaves both sides of the hot sections and enters through both sides of cold sections which leads to generate heat flux and corresponding temperature gradient is measured. (8)

Two temperature gradients of equal in magnitude but having opposite sign which is due to periodic nature of the simulation cell. The difference in average temperature of symmetrically equivalent sections

3.1 Pair radial distribution functions (rdf's): For this, parameter rcut is taken as 5.0 and no of time steps from which output is recognized is taken as 100. In silicon dioxide nanowire Si-O distance is linked at corners and in rings 6 members forming the ribs of fused cage-like structure. From fig ,it is seen that the first Si-O peak is broader in this models. The BKS model shows higher coordination numbers at next nearest neighbor distances which is consistent with the higher density obtained wih this potential

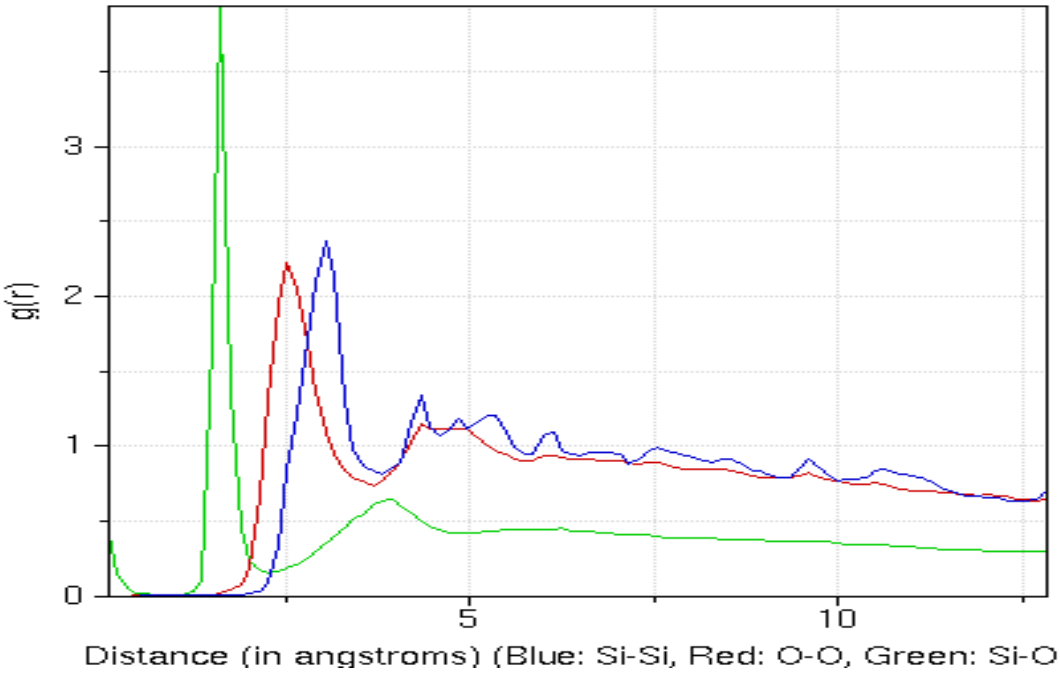

Figure 2: Radial distribution function versus no. of time steps of MD

3.2Temperature versus no of time steps of MD: For the calculation of temperature profile, Temperature gradient is calculated. Heat is added to the slab from the center of simulation cell and removed from slab from other end by Anderson thermostat. This simulation is carried by using microcanonical ensemble (NVE) which shows constant number of atoms, constant volume and constant energy. Total number of time steps is 1500 and equilibrium is attained after750 time steps. initially it shows more fluctuations in temperature but after some 200 time steps it goes down and then attain equilibriums.

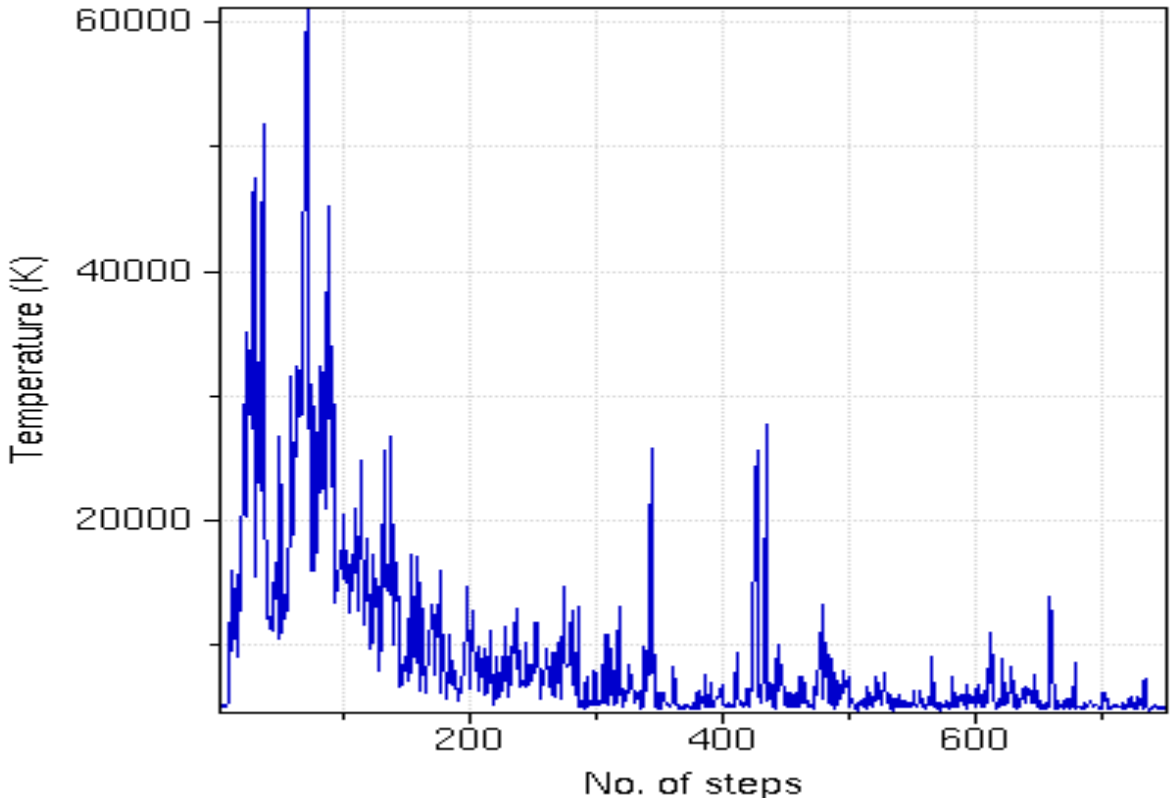

Figure 3: Graph of temperature versus No of timesteps of MD

IV.Results and Discussion: Figure 1 shows initial position of silicon dioxide structure in which 1200 atoms are there in which 400 are of silicon(coloured yellow) and 800 are of oxygen(coloured light red).this structure has 25.774548e-10 x 25.774548e-10 x 25.774548e-10 lengths along x,y and z axis respectively. In this simulation interatomic potential used is BKS which is very effective at low pressures. Figure 2 gives radial distribution function because number of bins used to study are 100 and there are 6 cell-list linked cells. Radial distribution of Si-O bond is wider (green color) in the sense that it gives higher density. Figure 3 shows temperature profile of silicon dioxide with respect to number of time steps. Because of temperature gradient initially it shows maximum temperature but as equilibrium is attained it goes down.

V.Conclusion: A study of molecular dynamics simulation is done with the help of software MD simulation. (9) In this simulation, parameters which are necessary to calculate thermal conductivity are studied here temperature gradient is imposed. Noneqilibrium molecular dynamics simulation method

(NEMD) method is most powerful, At the level of nanostructure, properties of materials are changed because of reduction in surface to volume ratio but the properties of silicon remained as it is so as to further use of silicon in nanoelectronics, many nanostructures are to be under study.

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REFERENCES

1. *Molecular dynamics simulations for the prediction of thermal conductivity of bulk silicon and silicon nanowires: Influence of interatomic potentials and boundary conditions.* **Carolina Abs da Cruz, Konstantinos Termentzidis, Patrice Chantrenne.** s.l. : AIP, 2011, Vol. 110, p. 034309.
2. *Thermal conductivity of crystalline quartz from classical simulations.* **Young-Gui Yoon, Roberto Car and David J. Srolovitz.** s.l. : PHYSICAL REVIEW B, 2004, Vol. 70, p. 012302.
3. *Molecular dynamics simulations of carbon nanotube/silicon interfacial thermal conductance.* **Jiankuai Diao, Deepak Srivastava and Madhu Menon.** s.l. : The Journal of Chemical Physics, 2008, Vol. 128, p. 164708.
4. *MOLECULAR DYNAMICS CALCULATIONS OF THE THERMAL CONDUCTIVITY OF SILICA BASED CRYSTALS.* **Kaviany, A. J. H. McGaughey and M.** s.l. : American Institute of Aeronautics and Astronautics.
5. *Thermal conductivity of a-Si:H thin films.* **David G. Cahill, M. Katiyar, and J. R. Abelson.** s.l. : PHYSICAL REVIEW B, 1994, Vol. 50. 9.
6. *Molecular dynamics calculation of thermal conductivity of vitreous silica.* **Jullien, Philippe Jund and Remmi.**
7. *Force Fields for Silicas and Aluminophosphates Based on Ab Initio Calculations.* **B. W. H. van Beest, G. J. Kramer,R. A. van Santen.** s.l. : PHYSICAL REVIEW LETTERS, 1989, Vol. 64. 16.
8. *Theoretical Methods for Calculating the Lattice Thermal Conductivity of Minerals.* **Stephen Stackhouse, Lars Stixrude.** s.l. : Reviews in Mineralogy & Geochemistry, 2010, Vol. 71, pp. 253-269.
9. **Mahajan, Sanket S; Subbarayan, Ganesh; Wang, Xufeng.** *MD Simulation.* s.l. : https://nanohub.org/resources/mdsim, 2014.