

Molecular Dynamics Simulations of Kapitza Length for Argon-Silicon and Water-Silicon Interfaces

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A comprehensive understanding of heat conduction between two parallel solid walls separated by liquid remains incomplete in nanometer scale. In addition, the solid/liquid interfacial thermal resistance has been an important technical issue in thermal/fluid engineering such as micro electro-mechanical systems and nano electro-mechanical systems with liquid inside. Therefore, further advancements in nanoscale physics require an advanced understanding of momentum and energy transport at solid/liquid interfaces. This study employs three-dimensional molecular dynamics (MD) simulations to investigate the thermal resistance at solid/liquid interfaces. Heat conduction between two parallel silicon walls separated by a thin film of liquid water is considered. The density distribution of liquid water is discussed with the simulation results to further understanding of the dynamic properties of water near solid surfaces. Meanwhile, temperature profiles appear discontinuous between liquid and solid temperatures due to the dissimilarity of thermal transport properties of the two materials, which validates thermal resistance (or Kapitza length) at solid/liquid interfaces. MD results also investigate the temperature dependence of the Kapitza length, demonstrating that the Kapitza lengths fluctuate around an average value and are independent of the wall temperature at solid/liquid interfaces. Our study provides useful information for the design of thermal management or heat dissipation devices across silicon/water and silicon/argon interfaces in nanoscale.

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NOMENCLATURE

a = Lattice constant (nm)
 N = Number of molecules (liquid or solid)
 σ = Diameter of molecules (zero potential distance) (nm)
 ε = Depth of Lennard-Jones potential (eV)
 ρ = Number density
 R_K = Kapitza resistance (interface thermal resistance)
 L_K = Kapitza length (nm)
 ΔT = Temperature jump (K)
 q = Heat flux
 $\partial T / \partial z$ = Temperature gradient

1. Introduction

Nanostructures and nanomaterials are getting significant impact on

addressing advanced energy science issues, especially in green and renewable energy technologies. The development of disruptive nanotechnology-enabled, low-cost/high-performance solid-state lighting, thermal insulation, and waste heat recapture technologies are typical revolutions in renewable energy by exploiting advances in nanoscale science and technology.¹ On the other hand, low-cost nanostructures with high thermal conductivity, and small contact resistances remain to be explored to improve the performance of thermal insulation materials or thermal management devices. Therefore, understanding the thermal transport mechanism of nanostructures and nanomaterials is a crucial factor for enhancing the efficiency of green energy storage facilities like batteries, super capacitors, or energy-harvesting devices, because the behavior and reliabilities of these devices strongly depend on the way the systems dissipate heat. In particular, the influence of interfacial thermal resistance at solid/liquid interfaces (also known as the Kapitza resistance) is one of the key issues in nanoscale thermal and fluid transport, and has not been explicitly known or fully understood since its discovery by Kapitza in 1941.^{2,3} Indeed, when the system size is reduced to nanometer scale, theoretical models based on continuum

descriptions cannot explain the nanoscale physical phenomena across solid/liquid interfaces due to the intermolecular interactions are more dominant in extremely tiny size conduits; hence, investigations on an atomistic scale are more effective. In addition, the lack of information about thermal transport across the solid/liquid interface is due not only to the limitation of typical continuum approach, but also to the difficulty of experiment in nanoscale.⁴ Under such conditions, the molecular dynamics (MD) simulations approach provides valuable insight into the mechanisms of heat and momentum transport through solid/liquid interfaces according to the interatomic interaction. The MD approach enables simulations with different physical conditions such as: the systems is modeled on an atomistic scale, particles are allowed to interact for a period of time under varying force fields, and the trajectories of all particles are calculated using Newton's equation of motion. Therefore, MD simulations have great potential for investigating such problems as thermal transport across solid/liquid interfaces in nanometer scale.

Over the last decade, the MD method has been extensively used to examine the thermal resistance at solid/liquid interfaces. In particular, Torri et al.⁵ found that the thermal resistance at solid/liquid interfaces increases significantly with the weakened interaction strength between solid and liquid molecules, while the energy transfer across solid/liquid interfaces is strongly affected by the number of liquid molecules in contact with solid surfaces. One effective way to enhance heat transfer across solid/liquid interfaces is to increase the wetting behavior of solid surfaces by assigning hydrophilic head-groups or self-assembled monolayers with different chain lengths onto solid surfaces.⁶ On the other hand, Hu et al.⁷ developed a simple way to reduce the Kapitza resistance at solid/liquid interfaces by increasing the interaction energy per unit area of water/gold contact surfaces. The effect of vibration mismatch between solid and liquid on interfacial thermal resistance has been discussed as well; Kim et al.⁸⁻¹¹ reported that interfacial thermal resistance is proportional to the 4th power of the thermal oscillation frequency ratio, which was modeled by changing the crystal bonding stiffness of the lattice crystal walls. The authors also characterized the thermal resistance length as a function of relative thermal oscillation frequencies, solid/liquid interaction strength, temperature gradient, and wall temperature. Despite the many achievements enhancing heat transfer through solid/liquid interfaces, there are still few data pertaining to solid/liquid interfacial resistance, especially the temperature dependence of solid/liquid interfacial thermal resistance.¹² Stevens et al.¹³ found that interface conductance has linear dependence on temperature, which indicates that interfacial transport is directly related to the thermal vibration states of molecules near the interface. However, their research only focused on Lennard-Jones (LJ) solid/solid interfaces. Recently, Shi et al.¹⁴ reported that Kapitza length increases linearly with the temperature of solid surfaces in the case of argon-silver and argon-graphite interfaces. The author indicated that local density profiles of liquid argon increase as temperature decreases, which directly enhances the momentum exchange between solid and liquid molecules at lower temperature walls.

As evidenced through this review, there are numerous issues needing further investigation in this area. Our study investigates heat conduction between parallel silicon walls separated by a thin film of liquid water or argon via three dimensional molecular dynamics simulations. Non-equilibrium molecular dynamics simulations are utilized to perform

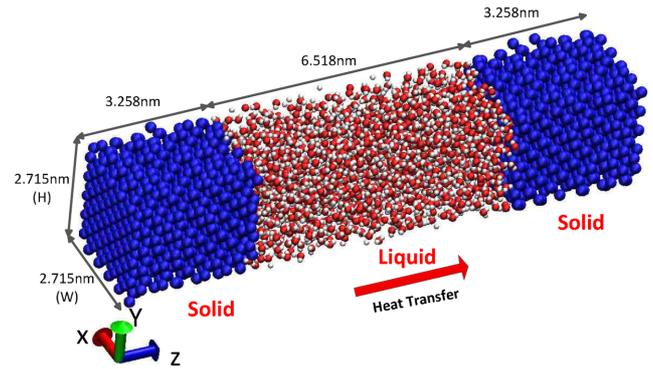


Fig. 1 Schematic and dimensions of MD simulation domain

thermal transport by setting thermostats with different temperatures at solid regions that not only create heat flux and temperature gradients, but also validate Fourier's Law in nanochannels. Temperature jumps are observed under such conditions due to the interfacial thermal resistance, which also characterizes the Kapitza length at solid/liquid interfaces. We found that Kapitza length is independent of wall temperature at silicon/water and silicon/argon interfaces. In addition, Kapitza length at a silicon surface in the case of liquid water is greater than in the case of liquid argon. This difference demonstrates the thermodynamic properties of water, which are not only sensitive to van der Waals forces like liquid argon, but are also affected by long-range Coulombic forces that lead to weaker interaction with silicon walls.

This paper is organized as follows: In section 2, we summarize the setup for our MD simulations with detailed explanation of the liquid water/argon and silicon model employed. In section 3, we discuss the investigation of density distribution, temperature distribution, and the determination of Kapitza length at solid/liquid interfaces. Finally, section 4 presents summaries of our findings and our conclusion.

2. Molecular Dynamics Simulations Details

In this study, we simulated three dimensional nanochannel as shown in Fig. 1, the system consists of two $5a \times 5a \times 6a$ unit cells diamond structure of silicon lattices crystal walls with lattice constant $a = 0.543$ nm, which corresponds to 1250 silicon atoms at each wall. The silicon walls were separated by 6.518 nm in length and filled by liquid water or argon. The outermost layer at both sides of the simulation domain was fixed to maintain constant volume. Thermostats were imposed at the next four layers for both hot and cold walls, while the remaining atoms throughout the domain were free to move. Periodic boundary conditions were applied in x and y directions for whole systems. For more accurate silicon/silicon interaction potential, we utilized the Stillinger-Weber model, which employs two-body and three-body interactions to enforce the correct coordinate tetrahedral bonded structure of silicon.¹⁵ In this study, liquid argon and water will be considered as the fluid confined in silicon nano-channel. Argon atoms behave approximately like soft spheres, they attract and repulse one to another with weak van der Waals forces, which commonly used in computer simulation with simple LJ potential.⁸⁻¹⁰ While liquid water not only sensitive with simple LJ interactions to model van der Waals forces, but

also Coulombic interactions between charge particles, which characterize polarization properties of liquid water. Hence, the simulations of both liquid argon and water were conducted to investigate different impact of LJ interaction added to long-range Coulombic interaction in liquid water on interfacial thermal resistance compared with pure LJ interaction in liquid argon. In addition, the common use of water nano-confinements in numerous applications such as coolant devices in Micro and Nano Electro Mechanical System (MEMS and NEMS) is still ambiguous understanding of the temperature dependence of thermal resistance at the solid/water interface. In such case, further study heat transfer cross the interfaces is critical to thermal management design. In the case of liquid argon, a total of 974 molecules were simulated in a three-dimensional channel corresponding to the number density ($\rho = N\sigma^3/\Omega$) of liquid argon (approximately 0.8). The simplified and most commonly used interaction potential, namely the Lennard-Jones (LJ) 12-6 was utilized to model the van der Waals interactions between silicon/argon and argon/argon molecules with a cutoff distance of 1.0 nm. The LJ potential is given as

$$V_{ij} = 4\varepsilon \left[\left(\frac{\sigma_{ij}}{r_{ij}} \right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}} \right)^6 \right] \quad (1)$$

where r_{ij} is the intermolecular distance, ε is the depth of the potential ($\varepsilon_{Ar} = 0.0103eV$), and σ is the molecular diameter between sites i and j ($\sigma_{Ar} = 0.3405$ nm). In order to simulate liquid water, we chose the simple point charge/extend (SPC/E) model¹⁶, which is commonly used to model water molecules with LJ and Coulombic terms. This water model has three interaction sites corresponding to the three atoms of a water molecule, in which the LJ interactions are carried by an oxygen atom with a cutoff distance of 1.0 nm, while oxygen and hydrogen atoms are assigned point charges to model the long-range Coulombic interactions. In the three sites of the model, water molecule has partial charges $q_O = -0.8476e$ and $q_H = 0.4238e$ at the positions of oxygen and hydrogen atoms, respectively. The binding energy and molecular diameter of oxygen were $\varepsilon_O = 0.00674eV$ and $\sigma_O = 0.3166$ nm. Bond lengths and angle in the water molecule were kept rigidly constrained using the SHAKE algorithm.¹⁷ Due to the electrostatic interactions, we used particle-particle particle-mesh (PPPM) solver which can handle long-range interactions for a periodic system with slab geometry more efficiently than the common Ewald sum algorithm.¹⁸ We simulated with 1696 water molecules in liquid domain, corresponding to an approximate bulk density of 1.0 g/cm³. The Lorentz-Berthelot mixing rule was employed to calculate the LJ parameters for solid/liquid interaction in both types of liquid.¹⁸ With the empirically determined lattice spacing and atomization energy of crystalline silicon, its molecular diameter is $\sigma_{Si} = 0.21$ nm, and the depth of the potential is $\varepsilon_{Si} = 2.168eV$. Therefore, the binding energy for silicon/oxygen is $\varepsilon_{O-Si} = 0.12087eV$. However, in order to model the hydrophobic behavior of the bare silicon surface with water as measured by previous experiments,¹⁹ we modified the value of the binding energy of oxygen and silicon to $\varepsilon_{O-Si} = 0.015eV$, which matches the microscopic contact angle calculated by MD simulations with the macroscopic contact angle of 88° measured experimentally as the study by Barisik et al.²⁰ Meanwhile, we adjusted the binding energy of silicon/argon from its original value of $\varepsilon_{Ar-Si} = 0.149eV$ to the value at which temperature jumps at silicon walls are similar to those in the silicon/water system. This was done to evaluate

the effect of LJ interaction added to long-range Coulombic interaction in liquid water on interfacial thermal resistance compared with pure LJ interaction in liquid argon.

We started our simulation with NVT (constant number of the molecules, constant volume and constant temperature) ensemble for the entire system to establish an equilibrium state, in which the Maxwell-Boltzmann velocity distribution for all molecules and the Nose-Hoover thermostat were applied to keep the systems temperature at 300 K. In order to induce a heat flux across the simulation domain, different temperatures were assigned on those two thin hot and cold reservoirs using the Langevin thermostat, while the rest of silicon lattices and fluid were in NVE (constant number of the molecules, constant volume and constant energy) ensemble for thermal transport. The simulation time step was 1.0 femtosecond (fs) for both systems. Heat transfer simulations were performed for 10 nanoseconds (ns): 2ns for entire systems to reach steady state, and another 8ns for averaging. Longer time averaging has also been performed to confirm the convergence of results to steady state.

3. Discussion and Results

3.1 Density distribution of liquid water and argon confined in silicon nanochannel

The dynamics and structural properties of a liquid are closely related to its density distribution at the near solid wall; hence, density profiles of silicon and liquid were observed to elucidate their impact on thermal resistance at solid/liquid interfaces. Due to the similarity of solid and liquid characteristics at both interfaces, Fig. 2 shows a typical density distribution of their molecules at the hotter interface.

Fig. 2(a) shows a density profile of silicon crystal, which is periodic fluctuation in a bulk crystal due to the repetition ordering of solid molecules in their lattice positions. This detailed fluctuation was observed when we divided the whole domain into 200 slab bins that are smaller than the molecular diameter of silicon atoms. Fig. 2(b) shows density profiles of oxygen, hydrogen, and argon molecules after normalizing density values. With the effects of wall force field and liquid/liquid interaction, liquid density profiles exhibit oscillatory behavior over several atomic distances from the solid surface, because the interactions between the liquid and solid molecules are much stronger than liquid/liquid interactions at the near interface. This fluctuation is called the layering structure of solid-liked liquid molecules, which increases with the wettability of solid surfaces. Meanwhile, the density distribution of liquid reveals almost no fluctuation far from the solid wall due to the high density of amorphous liquid molecules, these density values converge to the bulk density for both types of liquid water and argon.

In our study, liquid water density profiles illustrate the penetration of hydrogen and oxygen atoms into the first and second layers of solid silicon. The dashed lines in Fig. 2(b) represent the first and second layers of silicon, and water density profiles reveal a small number of density values in this region. This observation consistent with the diffusion of water molecules in the silicon substrate in the study by Barisik et al.^{20,21} Meanwhile, liquid argon densities are adjacent to the

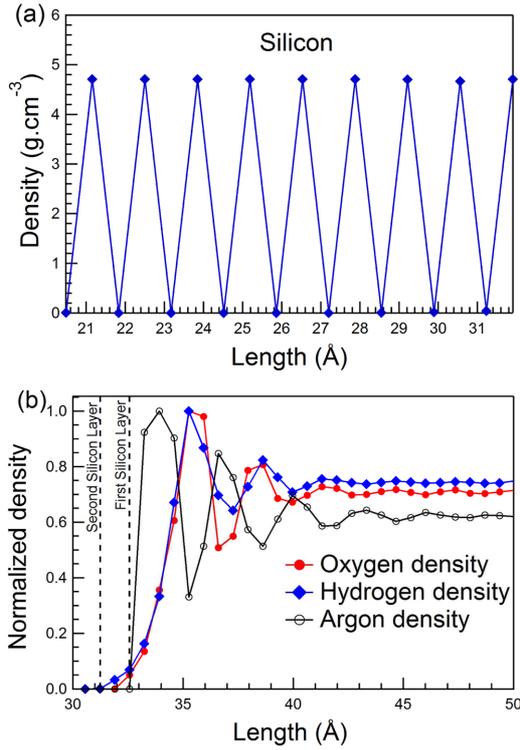


Fig. 2 Density profiles of solid silicon (a), liquid water and argon molecules near silicon wall after normalization (b). For both types of liquid, the left surface was kept at 323 K, while the right surface was kept at 283 K. The interaction strength between solid and liquid was set at $\varepsilon = 0.015eV$

solid wall without any depletion zone in contrast with the observations of Shi et al.¹⁴ and Barisik et al.²² which demonstrate a depletion thickness layer near the solid surface and a significant increase in local liquid density with decreasing wall temperature. In both studies, the higher local density layering effect has a higher probability of solid/liquid momentum exchange, which in turn decreases the temperature jump at the interface with lower temperature. Our simulation results contrastingly indicate that there are almost symmetric density profiles at both interfaces and liquid molecules are strongly adsorbed by silicon walls, while the depletion layers vanish near silicon surfaces; therefore, the momentum exchange and temperature jumps at both interfaces are comparable. In addition, the first and second peaks of liquid argon are 1.34 Å and 4.03 Å away from the silicon wall, respectively, while those of water are 2.01 Å and 5.37 Å, respectively. This predicts a strong interaction of liquid argon with the silicon wall compared to liquid water despite the same interaction strength and cutoff distance used for both types of liquid with the silicon wall. This difference demonstrates the thermodynamic properties of water, which not only are sensitive to van der Waals forces like liquid argon, but also are affected by long-range Coulombic forces that lead to weaker interaction with silicon walls.

3.2 Determination kapitza length

When the thermal transports from liquid to solid, the temperature is discontinuous at the interface between two dissimilar materials, which is known to result in a temperature jump across the interface (ΔT). This

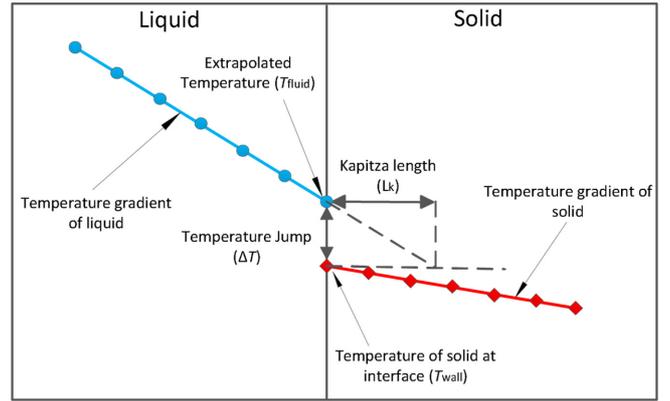


Fig. 3 Description of the temperature jump (ΔT) and Kapitza Length at solid/liquid interface

temperature jump can be expressed as a function of heat flux (\vec{j}) and thermal resistance R_K :

$$\Delta T = -R_K \vec{j} \cdot \vec{n} \quad (2)$$

where \vec{n} is the outward unit normal from the wall. The thermal resistance R_K is also known as Kapitza resistance.^{2,3}

In order to determine thermal resistance at the solid/liquid interface, we calculated the Kapitza length (an analogous definition of Kapitza resistance). First we obtained the local temperature gradient from MD simulation results in both solid and liquid domains, and then matched that temperature with the slope of fitting linear curves to the temperature in the bulk of the channel. We then defined the temperature jump by extrapolating the temperature profile from the liquid side into the solid wall as shown in Fig. 3. Kapitza length is therefore given as a function of the temperature jump and temperature gradient of liquid at the interface as

$$\Delta T = L_K \left. \frac{\partial T}{\partial n} \right|_{\text{liquid}} \quad (3)$$

where $\partial T / \partial n$ is the temperature gradient on the liquid side, and the temperature jump is $\Delta T = T_{\text{Fluid}} - T_{\text{Wall}}$.

As shown in Fig. 4, the middle shows temperature gradient profiles in a steady state of heat transfer, in which liquid temperature decreases linearly from hot wall to cold wall. The temperature gradient in liquid regions drops more rapidly than in solid regions, since the thermal conductivity of silicon crystal is much higher than that of liquid. Temperature jumps reveal the discontinuity between liquid and solid temperature due to the dissimilarity of thermal properties of the two materials, which validates the Kapitza length at solid/liquid interfaces. As we expected, the temperature jumps at the hot and cold wall are similar, indicating that the effect of temperature walls on thermal resistance at interfaces is negligible for either monoatomic liquid argon or polar liquid water. Meanwhile, the difference temperature jumps at silicon surfaces between silicon/water and silicon/argon system confirm the impact of LJ interaction added to long-range Coulombic interaction in liquid water on interfacial thermal resistance compared with pure LJ interaction in liquid argon. In the case of liquid argon, we decreased the interaction strength between silicon and argon from the original value

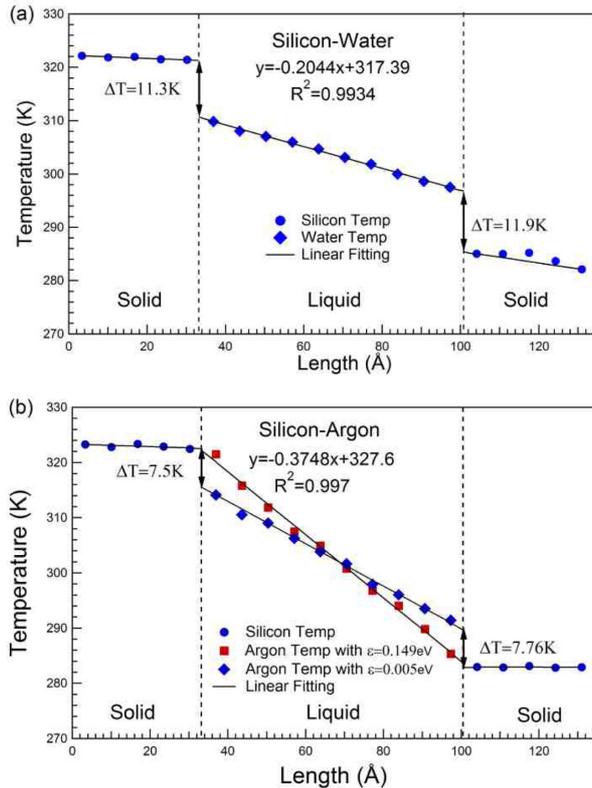


Fig. 4 Temperature profiles with 20 slab bins for both systems: silicon/water (a) and silicon/argon (b). The left silicon surface is kept at 323 K and the right surface is kept at 283 K. The dashed lines indicate solid/liquid interfaces

to adjust the same temperature jumps at interfaces compared with silicon/water systems. We observed almost no temperature jump with the original interaction strength from the Lorentz-Berthelot mixing rule for silicon/argon ($\epsilon_{Ar-Si} = 0.149eV$), and the largest temperature jump values could be obtained as shown in Fig. 4(b) with a very weak interaction strength value of $\epsilon_{Ar-Si} = 0.005eV$. The stronger solid/liquid interactions have smaller temperature jumps compared with the weaker solid/liquid interactions due to the better matching vibrational coupling between the absorbed liquid and solid surface, which occurs when the thermal motion of liquid molecules is less influenced by the adjacent liquid molecules than by the adjacent silicon molecules.⁸ In addition, despite the large decay of binding energy of silicon/argon, the temperature gradient of liquid argon decreases more rapidly than in the case of liquid water, which leads to smaller temperature jumps at silicon surfaces. Smaller temperature jumps predict the lower Kapitza length values in the case of liquid argon at silicon surfaces, while larger temperature jumps at silicon/water interfaces are consistent with weaker interaction of water molecules with silicon walls due to the dominance of liquid/liquid LJ interactions added to Coulombic interactions in liquid water.

In order to investigate the temperature dependence of the Kapitza length at silicon/water and silicon/argon interfaces, we performed a series of MD simulations and calculated the Kapitza length using Eq. (3). At first, hot and cold wall temperatures were set at 323 K and 283 K, respectively. Both walls temperature were then increased by 10 K to increase the average system temperature by 10 K while maintaining the

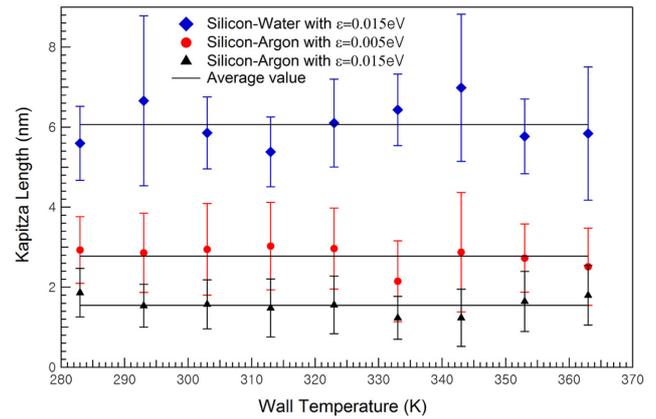


Fig. 5 Kapitza lengths versus wall temperature at solid/liquid interface for both liquid water and argon confined in silicon walls

temperature difference between the two reservoirs. The temperature range for the simulation was from 283 K to 363 K, which mostly applied on cooling systems of computer microprocessor or other heat electronic devices.²³ In order to validate the Fourier's law ($q = -K\partial T/\partial z$) of the heat transfer across the interfaces, we calculated heat flux (q), temperature gradient ($\partial T/\partial z$), and thermal conductivity (K) of liquid water to compare with other studies. With temperature gradient was kept constant during the simulations, the heat flux calculated were found to be 5.438×10^8 W/m² and 1.174×10^9 W/m² corresponding to liquid argon and water systems, respectively. Thermal conductivity of liquid in those cases were 0.146 W/mK and 0.71 W/mK, which approximately equal to Borgelt et al.²⁴ and Muscatello et al.²⁵ for argon and water at the certain temperature, respectively. Due to the vast range of binding energy between silicon and argon, Fig. 5 shows two typical Kapitza length values corresponding to the similar binding interaction strength for both types of liquid $\epsilon = 0.015eV$, and the largest Kapitza length could be obtained in the silicon/argon system with very small interaction strength $\epsilon = 0.005eV$. We found that Kapitza length is not affected by wall temperature in either the silicon/water or silicon/argon system, in which Kapitza lengths fluctuate around an average value with varying temperature walls within the range 283-363 K. This observation indicates that the coupling thermal vibration of solid and liquid molecules relates directly to the strong absorption of the silicon wall with liquid molecules which reduces the impact of temperature on liquid densities and temperature jumps at solid interfaces. In addition, Kapitza length increases with decreasing solid/liquid interaction strength, confirming the correlation of the solid/liquid coupling vibration with the solid/liquid interaction strength. As we expected, the temperature independence of Kapitza length from silicon interfaces is consistent with the behavior of water and argon density distribution at interfaces, as discussed in Fig. 2, and the convergence of temperature jumps at hot and cold walls in Fig. 4. Note that the Kapitza length at silicon/water interfaces is approximately three times greater than that at the silicon/argon interfaces despite the similar binding energy with silicon for both types of liquid. This difference in Kapitza length is due to the different thermodynamic properties of liquid water and argon. Liquid water is affected by the combination of LJ potential and long-range Coulombic interactions, while pure LJ interactions are more dominant in the liquid argon system.

Therefore, solid/liquid interactions in the case of liquid water generate greater deficit momentum exchange than the case of liquid argon with silicon walls.

We compared our results for Kapitza length at silicon/water and silicon/argon interfaces with those of other research, which focused on the interaction between solid and monoatomic liquid. Kim et al.⁸ developed an interactive thermal wall in which lattice crystal walls were assigned by simple mass-spring vibration. In the aforementioned study, the author characterized Kapitza length as a function of solid/liquid interaction strength, the ratio of the thermal oscillation frequency of wall to that of liquid, temperature gradient, and wall temperature. Kapitza length can reach significant values by uncoupling the thermal oscillation frequency between solid and liquid atoms. Under such conditions, the interactive thermal wall model also showed the greater Kapitza length on the higher temperature surfaces. The study by Shi et al.¹⁴ shared the same results; Kapitza length at the argon-graphite and argon-silver interfaces increased linearly with increasing surface temperature. In their observation, solid walls tend to create thin depletion zones near interfaces, while the peak density values of liquid are shown to increase with decreased wall temperature, corresponding to a high local density of liquid near the colder surface, which leads to the higher probability of solid/liquid momentum exchange and the decay of temperature jump in this region. In contrast, our results strongly support the idea that Kapitza lengths are independent of the wall temperature in both cases of monoatomic liquid argon and polar liquid water confined in silicon walls. This is because water and argon molecules are significantly adsorbed by silicon walls and liquid molecules tend to penetrate or adhere to the silicon walls, which reduces the effect of wall temperature on the momentum exchange between solid and liquid. Our results also show that the solid model is quite complex for realistic surfaces like silicon rather than a single spring vibration assigned to the wall with the same mass and diameter as liquid argon.⁸

4. Conclusions

This study performs non-equilibrium molecular dynamics simulations to investigate thermal transport across solid/liquid interfaces with thin liquid water or argon confined between two reservoirs of solid silicon walls. The results of our simulations illustrate the strong adsorption of the silicon wall with liquid molecules, which reduces the effect of wall temperature on the temperature jump at interfaces. Therefore, Kapitza lengths are not affected by the wall temperature and fluctuate around an average value with various temperature walls within the range 283-363 K for liquid water and argon. The independence of Kapitza length on temperature is technologically important for applications where very high heat dissipation is necessary. Kapitza length at the silicon/water interfaces is approximately three times greater than that at the silicon/argon interfaces despite the similarity of binding energy between the silicon wall and water or argon molecules. This means that solid/liquid interactions in the case of liquid water generate greater deficit momentum exchange than the case of liquid argon with silicon walls, which corresponds to the lesser coupling vibration of liquid water with silicon walls. This difference is due to the thermodynamic properties of water,

which are not only sensitive to van der Waals forces like liquid argon but also are affected by long-range Coulombic forces that lead to weaker interaction with silicon walls. Our results verify that the Kapitza length decreases with increasing interaction strength between solid and liquid, which is consistent with the literature.^{8,14} Our study provides useful information for the design of thermal management or heat dissipation devices across silicon/water and silicon/argon interfaces in nanoscale.

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