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Heat Transport in Step-shaped Silicene and Interfacial Thermal Resistance by Molecular Dynamics Simulation

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Abstract: The heat transport characteristics and interfacial thermal resistances (ITRs) in step-shaped silicene are analyzed by the nonequilibrium molecular dynamics simulation in this paper. It is found that the ITRs are independent of width of system when the ratio of widths of two sides is fixed. However, with the increasing ratio of widths, the ITRs decrease, which is mainly blamed to the decreasing asymmetry of system. In addition, the ITRs are larger when the heat flux is from the wider side to the narrower side of step-shaped silicene.
Keywords: Interfacial thermal resistances; Molecular dynamics simulation; Step-shaped silicene.

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1. INTRODUCTION

Graphene, which has outstanding electrical, mechanical and thermal properties, has tremendous application potential in transistor, solar energy battery and thermal management industries [1-8]. Therefore, similar honey-comb two dimensional structure materials have received a lot of interest. Replacing C atoms of Si atoms in graphene, a now structure is created named as silicone. It has been proved the existence by the *ab initio* calculation [9]. Compared with graphene, silicene has better compatibility with traditional silicon-based devices. In the past decades, researchers have successfully fabricated silicene on Ag (011), Ag (111), Ag (110) and Ir (111) surfaces [10-14].

Being different from graphene, the atom bond in silicene is the hybridization of sp^3 and sp^2 bond, leading to a unique bucking structure of silicene and unusual electrical properties. For example, silicene has a non-zero band gap at the Dirac point, leading to a larger Seebeck coefficient [15]. According to the thermoelectric coefficient of merit $ZT=S^2\sigma T/\kappa$, silicene has great application potential in thermoelectric industry. Here, S is the Seebeck coefficient, σ is the electrical conductivity and κ is the thermal conductivity. In terms of electrical conductivity, graphene and silicene have a similar electronic structure and electrical conductivities. Therefore, it is necessary to understand the heat transfer mechanism and thermal properties of silicene. Limited by the difficulty in fabrication and experimental measurement, the molecular dynamics simulation and the *ab initio* calculation has been widely used to study the thermal properties of silicene. Zhang et al. proposed a modified SW potential and worked well on silicene [16]. Compared with graphene, whose thermal conductivity can

exceed 1000 $Wm^{-1}K^{-1}$ [1, 2]; the thermal conductivities of silicene are between 5-70 $Wm^{-1}K^{-1}$ [17-19].

In recent years, the interfacial thermal resistance (ITRs) have been found to have significant effect on thermal management of micro- and nano-devices, since it is comparative with thermal resistance of material themselves [20, 21]. However, the researches about ITRs in silicene are relatively few. In this paper, we discuss the ITRs in step-shaped silicene by the molecular dynamics simulation. Size effect on ITRs is discussed. We also alter the directions of heat fluxes to further investigate the mechanism of ITRs at the step interface in silicene.

2. SIMULATION DETAILS

2.1 Simulation Methods

The nonequilibrium molecular dynamic simulation method is used to analyze the heat transport in step-shaped silicene. Generally speaking, there are two methods to generate heat flux in system and calculate thermal conductivity by nonequilibrium molecular dynamic simulation. The first one is to setting constant heat flux in system and generate corresponding temperature gradient, such as Müller-Plathe method [22]. In Müller-Plathe method, the simulation system is divided into N layers along the heat flow direction, as shown in Figure 1, in which the $n/2$ layer is the "hot layers", and the 0 and N layers are the "cold layers". The exchange of the atom with the lowest velocity in the "hot layers" and the atom with the highest velocity in the "cold layers" causes the temperature of the "hot layers" to rise and the temperature of the "cold layers" to decrease. A stable heat flux can be generated in the system by setting the appropriate exchange time interval and the number of exchange atoms.

$$q = \frac{1}{2tA_R} \sum_{transfer} \frac{M}{2} (v_{hot}^2 - v_{cold}^2) \tag{1}$$

Here, A_R is the cross-sectional area of the system, t is the time, v_{hot} and v_{cold} are velocities of exchange atoms in the "hot layers" and "cold layers", respectively. The coefficient 2 represents the symmetry of both sides of the system. Then the temperature distribution of the system is counted and the temperature gradient $\partial T/\partial x$ is obtained. The thermal conductivity can be obtained by Fourier's law.

$$\kappa = -q / (\frac{\partial T}{\partial x}) \tag{2}$$

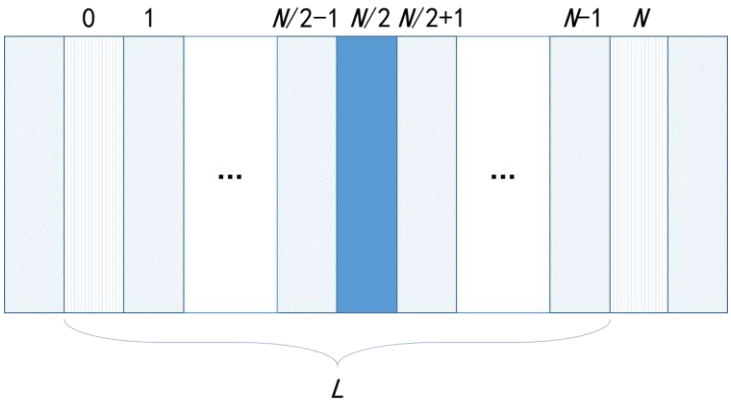

Figure 1. The demonstration of Müller-Plathe method

The second method is to set a constant temperature difference ΔT in the system, that is to set the temperature of the hot bath area and cold bath area at both ends as $T+\Delta T/2$ and $T-\Delta T/2$, respectively.

Due to the existence of temperature difference, a certain amount of heat flux J will be generated in the system, so the heat flux density is

$$q = \frac{J}{A_R} \tag{3}$$

Next, similar to the first method, the thermal conductivity can be calculated by Fourier's law by calculating the temperature distribution of the system and obtaining the temperature gradient. In this paper, the second method is used.

2.2 Modeling

The simulated step-shaped silicene is as shown in Figure 2 with the length of 80 nm. The width of the wide side and the narrow side are named as W_{wide} and W_{narrow}, while $W_{narrow}=W_{wide}/2$ is set and the length of both sides equals. And the narrow side is in the middle of the wide side. Two ends of system along the direction of heat flux with the width of about 0.5 nm are the fixed regions, leading to the fixed boundary in x direction. Next to the fixed regions are the thermostats regions with the width of about 5.0 nm. The temperatures of heat source and heat sink regions are set as $T+\Delta T/2$ and $T-\Delta T/2$ by Nose-Hoover thermostat [23, 24], in which T is the average temperature of the system and ΔT is the temperature difference. Opposite directions of heat fluxes can be obtained by altering the temperature of thermostats. When the heat flux is from the wide side to the narrow side, it is called $q_{wide\text{-}narrow}$; on the contrary, it is called $q_{narrow\text{-}wide}$ as shown in Figure 2. Free boundary conditions are applied in y and z directions. Along the direction of heat flux, we build both of armchairs and zigzag silicene and compare them with each other.

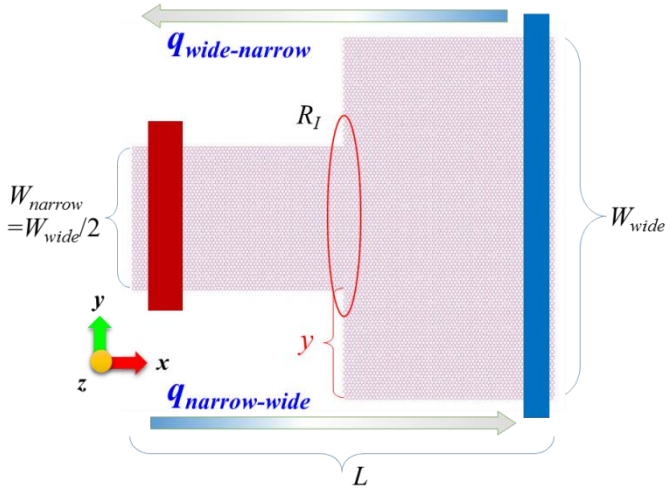

Figure 2. Schematic of the simulation system of step-shaped silicene

The optimized SW potential is applied to describe the interactions between Si atoms in silicene nanosheets [16]. It can reproduce the bulking structure and phonon dispersion curves of silicene from the *ab initio* calculation [25, 26]. The original bucking distance and bond length of silicene is 0.04269 nm and 0.2242 nm, respectively. The thickness of silicene nanosheets is considered as the van der Waals diameter of Si atom 0.42 nm [27]. The whole simulation is operated by the large-scale atomic/molecular massively parallel simulator (LAMMPS) in this paper.

3. RESULTS AND DISCUSSIONS

We firstly discuss the influence of width of silicene. With the width ratio W_{narrow}/W_{wide}=0.5 fixed, W_{wide} increases from 24 nm to 280 nm. Figure 3 is the variation of ITRs under opposite directions of heat fluxes with T=100 K and ΔT=30 K. The temperature jump and interfacial thermal resistances are observed at the step interface and the ITRs are named as $R_{wide\text{-}narrow}$ and $R_{narrow\text{-}wide}$ under opposite directions of heat fluxes.

We can see that with the increasing W_{wide}, $R_{wide\text{-}narrow}$ fluctuates within 3.0-3.4×10^{-10} m^{2}KW^{-1}, while $R_{narrow\text{-}wide}$ varies between 2.1-2.4×10^{-10} m^{2}KW^{-1}, which can be neglected. Therefore, the width is considered to have no influence on ITRs with fixed width ratio W_{narrow}/W_{wide}.

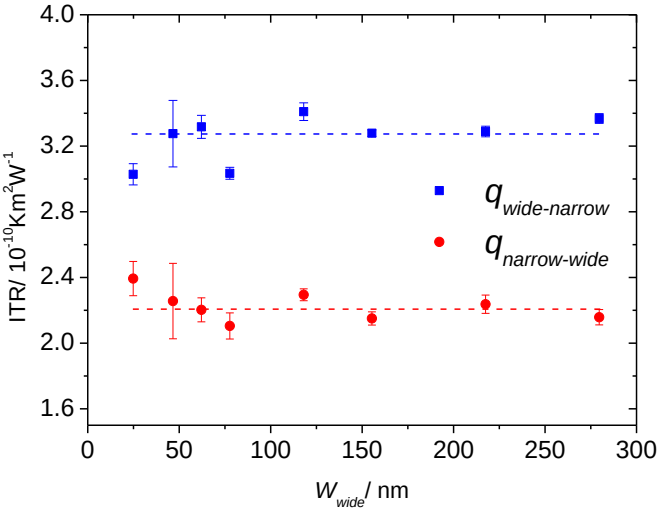

Figure 3. Variation of ITRs with W_{wid}

The influence of width ratio W_{narrow}/W_{wide} on ITRs is further discussed. With W_{wide} is fixed at 47 nm, W_{narrow}/W_{wide} increases from 0.1 to 0.8. The variation of ITRs with W_{narrow}/W_{wide} in armchair and zigzag silicene nanosheets are as shown in Figure 4. We can see that whatever the structure of silicene or direction of heat flux is, ITRs decrease with the increasing W_{narrow}/W_{wide}. In addition, the variation of ITRs in armchair and zigzag silicene nanosheets are similar to each other.

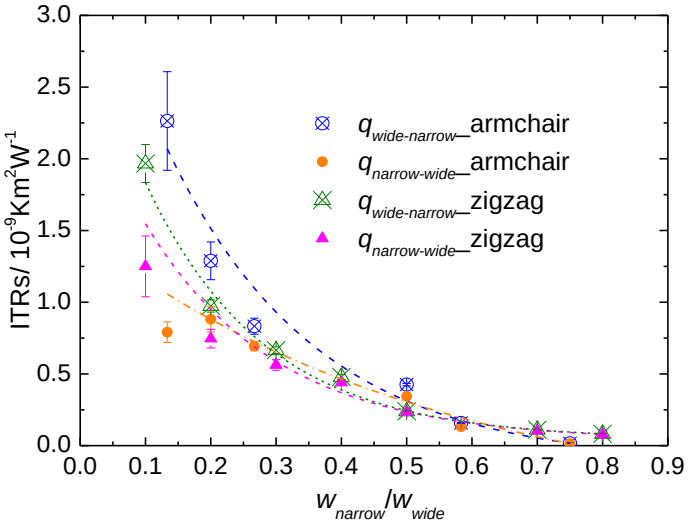

Figure 4. Variation of ITRs with W_{narrow}/W_{wide}

In order to explain the variation of ITRs, the two sides of step-shaped silicene are assumed as tubes with different diameters and the heat transfer in silicene is considered as the fluid motion in tubes. When the fluid flows between tubes with different diameters, the fluid velocity changes while the

flow rate remains unchanged, leading to an inevitable flow resistance, which is relates to the ITRs in heat transfer. With the increasing W_{narrow}/W_{wide}, the difference of diameters between tubes decreases as well as the flow resistance, resulting in the decreasing ITRs.

In Figure 4, we can also see that $R_{wide\text{-}narrow}$ is always larger than $R_{narrow\text{-}wide}$. When the heat flux is from the wide side to the narrow side, the diameters of tubes decrease suddenly and the fluid velocity is accelerated. Some part of fluid cannot pass through the interface and flow congestion happens, leading to flow resistance at the interface. When the direction of heat flux is opposite, the fluid velocity changes gently. And the flow resistance is relatively smaller.

4. SUMMARY

In this paper, heat transport and the interfacial thermal resistance in step-shaped silicene nanosheets is investigated by the non-equilibrium molecular dynamics simulation and the influences of width on ITRs are discussed.

With the width ratio W_{narrow}/W_{wide}, fixed, the ITRs at the step interface are independent of width. With the increasing W_{narrow}/W_{wide}, ITRs decrease demonstrating similarity to fluid flow theory. In addition, the ITRs are found to be larger when the heat flux is from the wide side to the narrow side, which can also be explained by the fluid flow theory.

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