Anisotropic in-plane thermal conductivity observed in multilayer silicene

The thermal transportation properties of recently synthesized quasi-1D bulk is explored from first principle. The thermal conductivity of this system is found rather low because of the phonon localization caused by the low-dimension nature and large anharmonic scattering of phonons. Detailed analysis of lattice dynamic calculation is applied to explain the origin of the anharmonic effects. The Seebeck coefficients and electric conductance are calculated from first principle and then ZT value is given. We found is actually potential for the application of thermoelectric. This research could be a guidance for further exploring of advanced low thermal conductivity materials.

Keywords: Thermal conductivity, quasi-1D,, thermoelectric, phonons

I.INTRODUCTION

With the development of the existing silicon based circuit industry, the requirements of its integration and miniaturization make a lot of research work focusing on the application of the new two-dimensional materials. The theory and experiments in the last 10 years show that some new two-dimensional materials have many novel and excellent physical properties due to their structure and size. For example, the single atom layer MoS2 has a suitable band gap which makes its field effect transistor switching ratio as large as . Black phosphorus (BP) with thicknesses of several atomic layer have extremely high electron / hole mobility (1000) and leakage current modulation rates ( times of graphene) and the field effect transistor of it has great potential in the application of nano electronic devices. Due to the high thermal conductivity and electron mobility of graphene, it has great potential applications in the field of nano circuits. However, materials prepared in the practical application is often multilayer structure to a few nanometers. Previous studies have focused on the weak Van der Waals interaction (vdW), and there is no surface reconstruction. There have been lots of studies on the electronic and thermal transport properties for this kind of typical layered structure and hetero structures, such as graphene, MoS2, black phosphorus two-dimensional layered structure. The existing preparation technology such as mechanical stripping, molecular beam epitaxy has difficult to produce nano layered structure for the material with strong interaction between layers, and the research of this kind of super thin nano materials has been very scarce. Recently, it has been found that monolayer and multilayer silicon material can be grown on some metal substrates by molecular beam epitaxy. The progress of these experiments ignited the upsurge the two dimensional nanomaterials with strong interaction between layers. In contrast to vdW, the two layer nano materials, which are represented by multi-layer silicon, exhibit special surface reconstructions which are different from the bulk surface and its physical and chemical properties are also very unique, indicating that there is new physics in this kind of ultra-thin nano materials.

Silicon nano is currently the only one system, from its monolayer to multilayer, and then to the bulk structure, that have been prepared by experiment. And it has rich and typical structure in the dimension of zero dimension, one dimension and three dimensions, which have laid a very good foundation for the study of two-dimensional scale multilayer silicon. The study of multilayer silicon is also helpful to understand the physical evolution of matter from low dimension to high dimension. In addition, the preparation process of silicon nano materials is mature and the raw materials are rich, and It has a broad application prospect in the fields of micro nano electronics, energy, information and other important fields in the future.

At present, research of thermal transport properties based on the silicon nano structure mainly includes silicon nanowires, silicon graphene substrate support, silicon thin film and bulk structure. Due to the quantum size effect in the thickness direction and surface reconstruction effect, silicon multilayer structure is expected to have lower thermal conductivity than the bulk and is more suitable for thermoelectric applications. However, the study on the properties of multilayer silicon thermal transport is still very rare, To this end, based on the first principles calculation of Guo, we explored the thermal transport properties of the 2 to 10 layer silicon structure in [108].

II. COMPUTATIONAL DETAILS

In this paper, based on the large scale parallel and efficient LAMMPS molecular dynamics software package, we study the thermal conductivity of multilayer silicon structure by using the non-equilibrium temperature gradient method. Because of the abundant silicon structure model, the phase reconstruction has attracted much attention. In order to well simulate the structures of different phase by MD, the latest Mod potential is chosen, which is able to reconstruct the silicon material elastic constants, the melting point and phase transition. Firstly, we use conjugate gradient method to optimize these structures. All structures are shown in Figure 4-1. For convenience, we define the names of these structures as "nlxs", where n is a pure number, representing the number of layers, l represents layer, x distinguishes different structures (concrete 1, 2, 3 etc. ) and s indicates the type along the length direction with value of a (armchair) or z (zigzag). Table 4.1 lists the structure name, the minimum repeat cell periodicity, the binding energies, the first principle binding energies and the structural properties of the multilayer silicon. The Mod potential is constructed for different type of silicon structures by fitting its bond angle parameter to give correct melting point and elastic constants. It refers to the elastic properties predicted with first principle local density approximation (LDA) and the generalized gradient approximation (GGA). However, these first principle methods tend to overestimate the binding energy of materials and underestimate their equilibrium lattice constants. For this reason, the Mod potential is constructed referring the correction of the equilibrium bond length based on the experimental diamond structure and leads to smaller the binding energy than that predicted by the first principle method.

From table 4.1, by comparing the binding energy of the first principles calculation of Guo is with that of MD, and from the point of view of stacking, the double layer of silicon is found more likely to form a monolayer of small and medium buckling slip stacking structure. The simulation is doing by velocity Verlet integral algorithm with the timestep to be 1fs. The length of the system in the x direction is 10~100nm, the transverse direction y is in periodic boundary condition with its simulated width to be 5 nm, and free boundary condition is applied in z direction. At the same time the outermost two ends of the x direction are fixed, close to witch a 3nm with Nose-Hoover bath is applied. The left and right ends of the temperature control at 310K and 290K. The simulation is carried out by NVT for 0.4ns, then control the temperature gradient for 10 ns, and finally we statistics the data of the last 10ns. By Fourier's law, the relationship between thermal conductivity and heat flux is

(1)

where stands for thermal conductivity, , is the average heat flux and temperature gradient along x direction respectively. , and means the temperature of the two ends and the sample length between the heat baths. is the total cross area, where is the size in the y direction, the layer number and the thickness of each layer. According to the previous studies, we choose Si (111) layer spacing of 3.14 as the thickness of each layer.

III.RESULTS AND DISCCUSION

We firstly investigate the effect of surface reconstruction on thermal conductivity. 5 kinds of silicon structures of armchair and zigzag were selected to study. The relationship between the thermal conductivity and the length of bilayer silicon in different directions is shown in **FIG.1**. the thermal conductivity of 2l1 structure increases with the length the most significantly, followed by the 2l3 structure and 2lr3 structure, while the least significant is the structure of 2l2 and 2lh. In addition, the structure with the thermal conductivity increasing significantly with the length is obviously anisotropy, different from single layer silicon and bulk silicon, who tend to be isotropic. In the aspect of structural, smooth 2l1 is most favorable for heat conduction, while 2l2 structure whose surface is made of a highly symmetrical and highly buckling pentacyclic ring "bird cage" is most unfavorable for thermal conductivity but suitable for thermoelectric materials. And the edges of the two directions are similar in shape, leading to small difference of heat transport.

When the length of the silicon is smaller than the mean free path of the phonon, the ballistic transport properties of the phonon are obvious. When the length is larger than the mean free path of the phonon, the phonon scattering transport characteristics are obvious. The empirical formula of the John A. Thomas[109] can be used to characterize the thermal conductivity of the phonon transport from ballistic to scattering region, at the same time accurately obtaining thermal conductivity of the infinite long nano materials. Using this formula, we obtain the thermal conductivity of infinitely long multilayer silicon

(2)

where is the fitted full scattering thermal conductance. is the transition length from the ballistic transportation to the scattering transportation. The value is used to measure the thermal conductivity difference in different directions, where stands for the full scattering thermal conductivity (infinite thermal conductivity) in the zigzag (armchair) direction. And is the maximum value of thermal conductivity in the two directions.

The total scattering thermal conductivity and anisotropy of multilayer silicon is shown in table 4.2. It can be seen from the table that the thermal conductivity of the bilayer silicon can reach up to 11.6 W/mK (2l1 structure). In addition, the 2lr3 with small top and bottom buckling possesses the most anisotropy, which can reach 57.3%. The smallest is 2l2 and 2lh (20%). The above results show that surface reconstruction has a significant effect on the thermal transport properties of multilayer silicon. The smooth surface is favorable for heat conduction, while the rough surface can greatly suppress the heat conduction. Meanwhile, the anisotropy of the surface structure leads to the significant anisotropy of the thermal conductivity.

The influence of thickness change on the thermal transport properties was then investigated. Here we study mainly on multilayer silicon structure with 3-10 layers, whose surface has typical Si (111) surface reconstruction. In order to compare, we also calculated the thermal conductivity of Si on its (111) surface and the thermal conductivity of the monolayer. The magnitude of the anisotropy is also shown in table 4.2. From the Figure 4-3 (a), in the case of the medium thickness of the 3~6 layers, the anisotropy of the multilayer silicon with zigzag type is higher than that of armchair. And with the increase of the number of layers, the anisotropy decreases gradually. The reason is that the zigzag direction of the multilayer silicon surface is composed of a smooth zigzag atomic chain (as shown in Figure 4-1). Compared with the bulk silicon structure, the heat conduction along the zigzag direction has no obvious effect on the heat flow. While along the armchair direction, the fluctuation of multilayer silicon surface is very large, the same is its obvious affection on heat flow. This difference is mainly caused by the surface reconstruction effect, and will decrease with the increase of the thickness of the silicon. In order to predict the relationship between the thermal conductivity and the thickness, we calculated the thermal conductivity of the 8-10 layers silicene with the surface reconstruction. In order to compare, the thermal conductivity of the bulk Si (111) surface with no surface reconstruction (9 layers) and the thermal conductivity of the monolayer were calculated. As shown in Table 4-2, with the increase of thickness, the anisotropy decreases gradually. When the thickness is up to 10 layers, the anisotropy of the thermal transport of multilayer silicon can be neglected (only about 1.5%),which is consistent with the results of bulk silicon and single silicon. On the other hand, as shown in Figure 4-3 (b), at the same thickness, in the case of shorter length (10~50nm), the anisotropy is obvious. When the length is about 100nm, the anisotropy difference becomes very small, and the size effect of the thermal conductivity anisotropy is obvious. This is essentially due to the difference in the out-of-plane acoustic branch (LA), the transverse acoustic branch (TA), and the vertical plane acoustic phonon (ZA) of the multilayer silicon structures along different directions. However, with the increase of length, the ballistic transport is gradually saturated, and the difference of the heat transfer caused by the umklapp process is gradually reduced.

In order to understand the relationship between the thermal conductivity and the length of the different structures and different layers, we use molecular dynamics to measure the phonon spectra of several typical structures. The multilayer structure is chosen. The selected high symmetry points are , , , , Take points along as shown in Figure 4-4.According to the supercell structure, the zigzag boundary corresponds to direction in the dispersion, and the armchair boundary corresponds to ’ direction. According to the relationship between the phonon spectrum and heat conduction, in the two-dimensional nano system, the acoustic phonon plays a major role in heat transport. There are a total of 3 acoustic branches, including to the LA mode along the transmission direction , TA along the transverse and ZA mode along the perpendicular direction. Figure 4-4 (a) and (b) corresponds to the calculated spectra of the bilayer structure 2l1 and 2l2. The group velocity of acoustic branch in 2l1 is obviously larger than that of ’, making zigzag direction more heat conducive , which also verifies the difference between 2l1z and 2l1a thermal conductivity and anisotropy. Accordingly, the three phonons in the two direction is almost the same as that in the 2l2, so the 2l2z and 2l2a are the least anisotropic structures with surface reconstruction. Comparing the two graphs, it can be found that all the group velocities of three phonons of 2l2 decrease. At the same time, the low frequency optical branch has the trend of moving down and couple with acoustic ones, which makes it less heat conducive, so that the 2l2 heat transport changes little with the length. The figure (c) (d) (E) is the dispersion of 3l1, 4l1, 6l1 2 x 1 structure, all of whose three phonon group velocity are larger along zigzag than armchair. With the increase of layers, the optical branch participation gradually gathered in the high frequency area (>15THz), having almost no contribution to thermal conductivity while the vibration mode of the low frequency (<5THz) region is almost unchanged. On the other hand, with the increase of thickness, the acoustic velocity of armchair direction increases gradually, which prompts the decrease of anisotropic in multilayer silicon with the increase of layer number. Compared with phonon spectrum of the 6 layer structure(e) , the difference between the 10 layers (f) is mainly the contribution of more atoms in the middle and high frequency (>5THz) region, which has little effect on the thermal conductivity.

As shown in **FIG.1**, the optimized configuration of the Bulk possesses C2/m symmetry (space group no. 12) with an monoclinic lattice. The obtained lattice constants along the three lattice vectors are 4.445 ,8.122,11.057, and the volume of unit cell is 370.33 which are in reasonable agreement with the experiment15.

To confirm the dynamical stability of bulk , phonon dispersion is calculated in the framework of the frozen phonon method22. The along the high symmetrical path of the Brillouin zone and phonon states density are plotted in **FIG.2**. No appreciable imaginary modes are found in the first Brillouin zone, suggesting that the bulk is dynamically stable.

To further study its thermal stability at finite-temperature, we performed ab initio molecular dynamics (MD) simulations at typical temperatures and the results of Mean Square Displacement(MSD)23 are shown in **FIG.3**. The MSD is defined as

, (2)

where means the average of all the atoms.

For solids the MSD does not change while for liquids and gas it changes linearly with time. Therefore, the bulk is thermally stable in a wide temperature range from 300 K to 800 K. However, the structure starts melting when heated to 900 K. Thus we only concentrated on the trusted temperature range (300–700 K), and choose 300 K as a typical temperature to perform the thermal conductivity calculations.

To obtain reliable results of thermal conductivity, the convergence dependence to q points density has to be tested. **FIG.4**a shows the convergence of thermal conductivity on q points with N increase from 2 to 8. The TC shows its convergence at N=4, above witch the result changes a little but not the computational effort, so we choose the number of transverse q points to be both 4. Besides, the convergence on q points with N increase from 16 to 1024 is also tested as in **FIG.4**b. The result of could be a good estimate of the converged result and we choose it to calculate TC only for the trends of TC on other properties like temperature et. al to save computer resources. **FIG.4**c shows the convergence on phonon cut off free path. The exact convergence could not be obtained even at due to the abnormally large lifetime of long wave phonons show in **FIG.4**d, which always exist in low dimensional materials. However, a lot of research shows the relation of TC and phonon cut off free path obeys the rules of 24

, (3)

and **FIG.4**e verifies that it also make sense in bulk and the calculated results are over estimated. As the conclusion, the calculated results of thermal conductivity are not converged even in extremely dense q points, however they can be used as upper limited estimates of the exact results.

The thermal conductivity of is extremely low and anisotropic as shown in **FIG.5**. The TC values decreases with increasing temperature and obeys the rule of , and the largest value at 300K is much less than . The TC along the stripes are almost 3 times that of the transverse value which may result from the nature the quasi-1D structure.

Mode localization of phonons is believed to account for low thermal conductivity in this quasi-1D bulk system. To understand the underlying physical mechanism of localization of phonons on thermal conductivity, we have carried out a vibrational eigen-mode analysis. Mode localization can be quantitatively characterized by, the participation ratio25 for each eigen-mode

, (4)

where N is the total number of atoms and is the complex amplitude of atom s for eigen-mode. The participation ratio presents the fraction of atoms participating in a given mode and effectively indicates the localized modes with and delocalized modes with O (1). It can provide a more detailed information about the localization effect to each mode. The eigenvectors and frequencies are obtained using Phonopy20 with and mesh sampling. **FIG.8** shows the participation ratio of . A lot of phonons have participation ratio below 0.5 which means they are strongly localized and lost the capability to carry energy and they have little contribution to thermal conductivity.

C12N

CN

Large anharmonic would be another key factor that account for the low thermal conductivity. **FIG.6** shows the group velocity of the phonons. Although the frequencies are pretty low (phonons are pretty soft), the group velocities are not so small witch can be understood by the steep phonon dispersion, for example, along the path ΓM. The maximum group velocity is comparable to that of graphene witch possesses the largest thermal conductivity so far. So group velocity is not responsible for the low TC. The large Gruneisen parameters26 showed in **FIG.9**b means pretty large anharmonic effects in which suggest strongly three-phonon scattering effects27. **FIG.7**a shows the three-phonon scattering relaxation time of all the phonons. The mean free path are also show in **FIG.7**b.Except for the long wave ones, all the life time are pretty small and this is exactly the origin of the low TC. The scattering strength show in **FIG.9**a also shows large scattering of phonons.

Low TC means the potential of applications in thermoelectric field and is predicted to be a good thermoelectric material. **FIG.10**a shows Seebeck coefficient at different temperatures. The typical values are in the range of several mV/K and are comparable with that of SnSe. Seebeck coefficient are sensitive to temperature while **FIG.10**b shows that electric conduction are not. The power factor are shown in **FIG.10**c. Although Seebeck coefficient is smaller at 700K, power factor is higher because of the rise and fall of around fermi level. However is also higher at 700K which eliminate the difference. The electric thermal conductivity is comparable at all the temperature and is even higher, which dominant at high temperature as shown in **FIG.11**a. At this point all the factors of figure ZT of merit are collected and the final results are shown in **FIG.11**b. After some n-doping or p-doping, ZT reaches its maximum and the best values could be obtained at high temperature. At 700K this ZT value is around 0.8 and this is not bad for the application of thermoelectric energy translation.

IV. CONCLUSIONS

To summarize, in this work, we propose to study the thermal transportation properties of quasi-1D bulk material from first principle. Our numerical results demonstrate that possess thermal conductivity as low as 0.5 W/mK and its TC are strongly anisotropic and the direction along the 1D blocks is the most thermal conductive. The low thermal conductivity origins from the phonon mode localization caused by the week interaction between the 1D blocks and also origins from large anharmonic effect which accounts for the large three-phonon scatter rate. The potential of in thermoelectric application is also inspected and we found although the Seebeck coefficient is large, the low electric conductance limits the figure of merit ZT to be around 0.8 which is comparable to the current thermoelectric material 28 but not stand for the best catalog in this field. Our research shows that quasi-1D bulk materials have low thermal conductivity with large probability and is a guidance for searching of new thermoelectric materials in the future.

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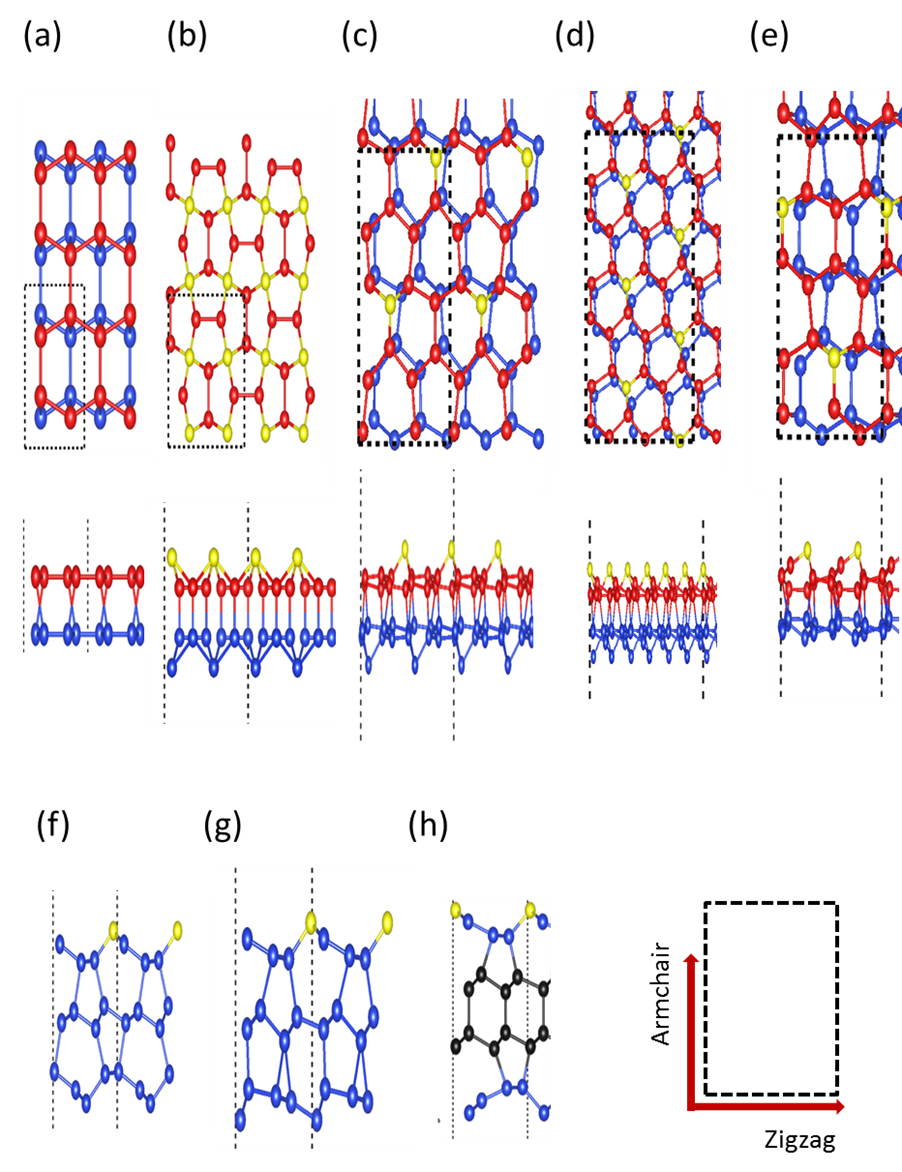
**TABLE.1.** Symmetry of the structures, binding energy Ec(eV/Si) and structure features

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Name | Minimal  period | Symmetry | Ec in Guo | Ec in MD | Buckling Feature |
| 2l1 | 1×1 | Cmme | 5.000 | 4.145 | Smooth |
| 2l2 | √2×√2 | C12/m1 | 4.991 | 4.204 | Large buckling and symmetric |
| 2l3 | 2×2 | C12/m1 | 5.063 | 4.257 | Large buckling and tilt symmetric |
| 2lh | 2×2 | P1 | 5.073 | 4.216 | Large buckling |
| 2lr3 | √3×√3 | P1 | - | 4.225 | Small buckling and symmetric |
| 3l1 | 2×1 | P121/m1 | 5.138 | 4.337 | - |
| 3l2 | 2×1 | P1 | 5.135 | 4.298 | - |
| 4l1 | 2×1 | P1 | 5.225 | 4.368 | - |

**TABLE.2.** The thermal conductivity and anisotropic ratio of different multi-layer silicene.



**FIG.1.** (color online) Some typical structure of multilayer silicon. Within which (a) to (e) are top view and side view of bilayer structures. (f) to (g) are side view of trilayer structures and (h) is that of four-layers. The buckling atoms on the top surface are labeled as yellow while the read atoms represent the others on the top surface. All the atoms on the bottom surface are labeled as blue. The blacks represent those that are inside the structure. The top view of the cells is shown in the last.



3l1

2l22

2l3

2lr3

2lh

3l2

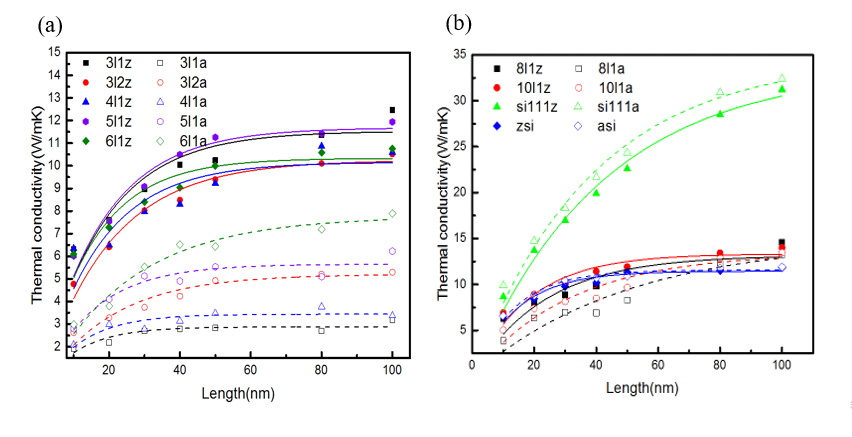
4l1

2l1

**FIG.2.** (color online) The thermal conductivity dependence on length for five types of bilayer silicon. The scatters are the results of MD simulations while the lines are fitted with Eq.1. The letter z/a in the legend mean the transport direction is zigzag/armchair.



**FIG.3.** (color online) The dependence on length of thermal conductivity for silicon with variable layers.



**FIG.4.** (color online) The phonon dispersion of multilayer silicon along high-symmetry points. (a)2l1 and (b) 2l2 are bilayer structure (c) 3l1 is trilayer structure,(d) 4l1 is four-layer structure and (e) 6l1 width six layers,(f)10l1 with ten layers.

