

# Study on the Heat transport and Optimization of Micro/Nano chip

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## Abstract

*In nanostructures whose characteristic lengths are comparable to the phonon mean free path(MFP), the ballistic-diffusive heat conduction leads to the size effect[1], which means the relationship between the heat flux and the temperature becomes complicated. In this work, an effective Monte Carlo(MC) method on the basis of using a model of phonon scattering process is employed to simulate the ballistic-diffusive heat conduction in silicon nanofilms, which is based on the methods proposed by Hua's work to study the effective thermal conductivity of nanostructures with internal heat source in one dimension[1, 2]. To get a clear vision of the temperature distribution of the chip, I first calculated the phonon transport in a two-dimension silicon nanofilm with internal heat source. The simulation agrees with the the diffusive approximation( $Kn \ll 1$ ), and it clearly shows the size effect in two dimensions.*

## I. INTRODUCTION

As the rapid development of microelectronics, an in-depth understanding of nanoscale thermal transport is quite necessary[9, 4]. On one hand, the typical size of the electronic devices have been decreasing at a dramatical speed, just using the example of diode, which is the key component of chips. As is reported in October, 2016,  $MoS_2$  transistors with 1-nanometer gate lengths has been made out[5]. On the other hand, the integration of single chip has been doubling per 18 months since the 1950s, causing the heat flux density arrives at as high as  $10^5 W/cm^2$ , which makes it even harder for the cooling of the chips and electronics. Additionally, when the size of silicon decreases to micro even nano scale, the well-known law of heat transfer, namely Fourier's Law fails. The reliability of electronics, however, is sensitive to the temperature fluctuations. When the temperature reaches 70-80 °C, the reliability will decrease 5% if temperature becomes 1 °C higher[6]. Consequently, great efforts have been devoted to study the phonon transport phenomenon in micro/nano structures, especially the ballistic-diffusive heat

conduction in silicon in recent years.

Speaking of the heat transport in dielectric material, the heat transport is predominant by phonons which are quanta of crystal vibrational energy[7, 8]. In bulk materials, phonons usually undergo several scatterings during the transport and the control law is the Fourier's law,  $q = -k\nabla T$ , where  $q$  denotes the heat flux,  $T$  denotes the temperature and  $k$  is the material constant of heat transfer. While in nanostructures, the characteristic lengths are compatible to the phonon mean free path(MFP), whose physical meaning is the mean distance a phonon can go before scattering occurs, causing some phonons will not undergo scattering before arriving at the boundary, which we call the ballistic transport. Actually, when the size reaches the nano scale, the effect of the boundary becomes quite important and cannot be omitted, and that is the reason why the governing rule and physical picture of nanostructures are so different from in bulk materials. In summary, the heat transport in nanostructures violates the classical rule, and we call the new process the ballistic-diffusive heat conduction. The key point to solve the ballistic-diffusive conduction problem is to solve the famous

equation proposed by Boltzmann[10]:

$$\frac{\partial f}{\partial t} + v_g \nabla f = \frac{f_0 - f}{\tau} + \dot{S}_\Omega \quad (1)$$

In which  $v_g$  is the group velocity of phonon,  $f$  is the phonon distribution function,  $f_0$  is the equilibrium distribution function (since phonons are bosons, the Bose-Einstein distribution[11]),  $\tau$  is the relaxation time and  $\dot{S}_\Omega$  the phonon source per solid angle[12], or more clearly, the internal heat source. What we should notice is that the effect of boundary is not directly included in this equation but its effect will be considered when we impose the boundary conditions when solving that equation.

The temperature profile, which is an important point in this problem, is the focus of my work. Studies to gain the better picture of the temperature profile in silicon with internal heat source have been conducted both theoretically[13, 14] and experimentally[15, 16, 17]. It has been found that in the ballistic-diffusive regime, if we still get an effective  $k$  (which is quite different from the  $k$  in bulk material, we just divide the heat flux by temperature gradient, namely,  $k_{eff} = q/\nabla T$ ), significantly reduces as compared to the bulk material. One direct result is the on the condition of the same heat flux, the nano material will get a higher temperature rise compared to the temperature gradient predicted with the bulk material model, which is an urgent issue in electronic cooling.

Although these both aspects have made great progress these years, the underling mechanism of the size effect is ambiguous and the general model with concrete physical base to predict the size effect and related other things is still lacking. So several simulation methods and techniques have been developed to help solve the problem.

Three types of methods have been adopted to help simulate the phonon ballistic transport using Boltzmann transport equation(BTE): molecular dynamics(MD)[18], Lattice-Boltzmann method(LBM)[19] and Monte Carlo(MC)[20, 21]. Compared with the MC method, MD method is limited in the size for its amount of calculation and LBM is

not suitable for simulation of complicated boundaries. MC method, which is a quite universal method in computational physics, has gained great success in solving many models in quantum and statistical mechanics[22]. In our problem, we trace a great number of phonons (usually greater than  $10^6$  and also depends on the size of the problem), derive the distribution function through statistics and then get the thermal properties of the material. In a nutshell, MC method actually give a discrete solution to the BTE and thus is more powerful when it comes to the effect of scattering and different boundary conditions. Our work aims at getting the temperature profile of the actual electronic chips, and based on that we can consider some methods to do the optimization. Considering most optimization of chips till now are actually conducted in macro scale, the attempt to do that work in nano scale can help better understand and finally solve the cooling problem.

## II. METHODS

### i. Monte Carlo simulation details

#### i.1 The gray approximation

For simplification, we choose the gray approximation in the MC simulation, which has been proved effective and acceptable in past work[1, 2]. The gray media approximation assumes that the phonon properties are frequency-independent, that's to say, the dispersion relationship of phonon is easiest and the  $p$  just equals a constant. On operation, we can first get the dispersion relationship of phonon in silicon by quantum mechanics or doing experiments and then find out the frequency interval of which phonons carry the most of the energy to get the typical frequency we choose in MC simulation. Hence, we finally focus on the phonons traveling with one single velocity and we can study the scattering using one average MFP (These point is quite important for us to get the simplified BTE, namely Equation (1)).

It is well-accepted to choose the phonon MFP of bulk material,  $l_a$ , to do the MC simulation.  $l_a$  can be calculated using the method of the kinetic theory[23].

$$l_a = \frac{2\lambda_b}{C_v v_g} \quad (2)$$

where  $\lambda_b$  is the thermal conductivity of bulk silicon,  $C_v$  is the heat capacity whilst keeping the volume constant,  $v_g$  is the average group velocity. For silicon at room temperature, we list the main data in the following chart[24].

$\lambda_b$	150 W/(m k)
$C_v$	$1.63 \times 10^6 \text{ J}/(\text{m}^3 \text{ k})$
$v_g$	6400 m/s

But if we explore the dispersion model of phonon in silicon more detailed, we will find the phonons in silicon can be divided into two types of phonons: acoustic phonons and optical phonons. If we only consider the acoustic phonons that carry most of the energy(that is acceptable in room temperature or we only need to consider the optical phonons at ultralow temperature), we get a new value of MFP, 260nm[24]. Actually, when we consider that new dispersion model, we need to change the corresponding  $C_v$  and  $v_g$ , finally we choose the value at 43.7 nm[2, 4, 12].

## i.2 Relationship between energy and temperature

We use the MC method to trace the phonons in the nanofilm and we can get the distribution, but we need to know the relationship between the distribution and the temperature to get the temperature profile. Similar to the photon, the phonon intensity emitting from a black boundary has the form of what is famous as Stephen-Boltzmann rule[25](The similarity also lies in the two quasi-particles both being Boses)

$$E = \sigma T^4 \quad (3)$$

where  $\sigma$  is a constant related to the material. As for the internal unit, we can also derive the

phonon intensity emitting imitating the theory of participating media radiation[26], which can be written as

$$dQ_{em} = 4\epsilon\sigma T^4 dT \quad (4)$$

where  $\epsilon$  is the phonon emissivity( $\epsilon=l_a^{-1}$ ). Because we consider the equilibrium state, the phonons received from the boundaries and all the other unit control volumes are equal to those emitting from the internal heat source. Thus, if we accept the local thermal equilibrium assumption, we can then get the local temperature.

## i.3 The sampling method

As we all know, although the MC method is powerful and seems easy to employ, the sampling of particles is of critical importance in the simulation not only because the sampling method differs greatly as the system changes but also because this is important for the feasibility of MC simulation(We can expect a dramatic decrease in the calculation if a suitable sampling method is adopted). So then we will discuss which sampling method we will apply in this problem.

We can define the intensity of each phonon bundle emitting as

$$W = \frac{E}{N_p} \quad (5)$$

It should be pointed out that  $N_p$ , which is the number of the phonon bundles we trace, must be large enough to preserve the simulation accuracy[27](According to the MC method, we can minimize the fluctuation if the number of particles is large enough).

Usually, we discuss the phonon transport in a ball coordinate, so in this coordinate, the traveling direction vector of the phonon bundle is given by

$$\mathbf{S} = [\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta] \quad (6)$$

How to sample the bundles of phonons to set the information of  $\psi$  and  $\theta$  is the key issue in

this step. Since the study on radiation whose energy carries are photons has been detailedly conducted, as we did before, we can get the relationships between the angles and independent random numbers according to Ref[26].

1. When the phonon bundle emits from the boundary,  $\sin \theta = (R_{\theta b})^{1/2}$ ,  $\phi = 2\pi(R_{\phi b})^{1/2}$
2. When the phonon bundle travels in the media,  $\cos \theta = 1 - 2R_{\theta m}$ ,  $\phi = 2\pi(R_{\phi m})^{1/2}$

We need notice that  $R_{\theta b}$   $R_{\phi b}$   $R_{\theta m}$   $R_{\phi m}$  are independent random numbers ranging from 0 to 1 and can be generated by computer programs. Because we mainly consider the stable status which is also the normal state in actual chips, we can divide the scattering of phonons into only two parts, one is phonon-interface scattering and intrinsic scattering. We need to note that the boundary scattering is actually quite complicated and I will discuss it in later paragraphs. Now we just need to know, we have two types of boundaries in this simulation, one the black-body where the phonons will be completely absorbed, the other adiabatic where we assume phonon scattering can be equivalent to a diffuse reflection process which means phonon will be absorbed and then randomly remitted. Furthermore, speaking of the intrinsic scattering, such as phonon-impurities, phonon-phonon and phonon-electron scattering, can be treated wholly in the relaxation time approximation. According to Hua's work[28], the average travel distance of phonon bundle can be calculated as

$$\Delta l = -LK n \ln(1 - R_s) \quad (7)$$

Based on the definition of kn number ( $kn = \frac{MFP}{l_{typical}}$ ), we can know if the scattering the phonon bundle undergo is the same as in the bulk material,  $l = MFP$ . In nano structures, the scattering is quite stronger than in bulk material so the actual traveling distance will be quite different.

The last item is the tracing algorithm which is shown in Fig 1 .

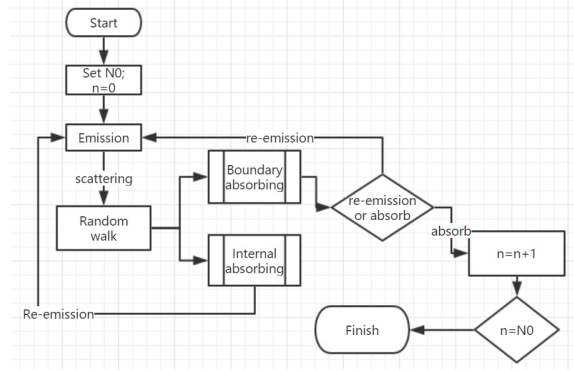


Figure 1: Block diagram of the tracing algorithm

## ii. Monte Carlo simulation steps

### ii.1 Problem formation

The Two dimensional thermal transport in silicon films with internal heating can be characterized by the two dimensional BTE,  $\partial f / \partial t + V_{gx} \partial f / \partial x + V_{gy} \partial f / \partial y = (f_0 - f) / \tau + \dot{S}_{\Omega}$ .

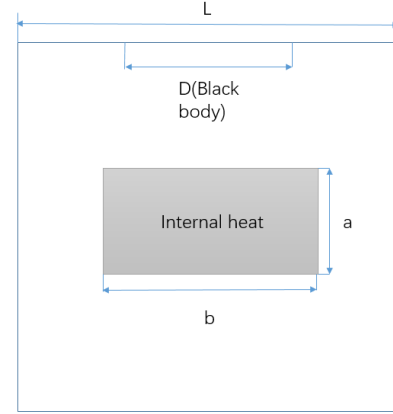


Figure 2: Two dimensional thermal transport in silicon films with internal heating

The schematic of simulating object is illustrated in Fig 2. The upper boundary with the length of D is considered as phonon black-body, that is to say, phonon are completely absorbed there, which means heat will only conduct to outer space there, while all the other boundaries are adiabatic and the phonon-boundary scattering at them is assumed to be completely diffusive. The internal heat source

is implemented by setting the phonon source inside the nanofilms, which is clearly shown in the Fig, and phonons with definite energy will originate within the zone. Then, all the phonon bundles will be traced until they exit through the black-body boundary.

The temperature profile then can be obtained from the phonon distribution calculated by our MC simulation[2]. More importantly, we should note that since our system is comparable with the phonon MFP, the local thermodynamic equilibrium cannot be established, and the temperature is more a parameter than its conventional meaning of representing a thermal equilibrium state.

One famous theory proposed that in that case, the temperature calculated is actually a representation of the average energy of all phonons around a local point[29]. And we will adopt that explanation and will give our temperature profile according to that.

## ii.2 Monte Carlo simulation

The MC technique simulates phonon transport process by random number samplings, equivalent to directly solving the phonon BTE. The phonon tracing algorithm is as follows:

1. Draw the initial properties (by randomly choose a point in heat source zone), for example,  $r_0$  of phonon bundle.
2. Calculate the traveling length using the Eq(7), and renew the position of the phonon,  $r_{new} = r_0 + \Delta r$ .
3. If a phonon collides with a boundary, if it is the black-body boundary, set  $n=n+1$  ( $n$  denotes the number of phonons which emit), or at the adiabatic boundary then set the position value at the boundary and let the phonon re-emit from the boundary.
4. If a phonon does not collide with the boundaries, the phonons just re-emit at  $r_{new}$ , and we set  $r_0 = r_{new}$ .
5. Record the frequency phonons get absorbed at each control body (each grid) and when  $n$  equals  $N_p$  ( $N_p$  is the number of the

phonon bundles we trace in simulation), the whole process is finished.

Just one thing should be noticed, although we choose a large number of phonon bundles, we trace only one at a time. When a phonon exits at the black-body boundary, we emit another and repeat till all the phonon bundles has been traced and recorded.

## III. RESULTS

## IV. CONCLUSIONS AND DISCUSSIONS

### i. Results and discussion

The dimensionless temperature profiles in Si nanofilms are shown in Fig 8, Fig 4, Fig 5. As  $Kn = 0$ , the phonon transport is purely diffusive and the corresponding temperature profile can be calculated by the classical law. With the increase of the Knudsen number, phonon ballistic transport becomes stronger. The temperature jumps occur at the boundaries and the temperature gradient becomes smaller. And we can find there exists a temperature jump between at the boundaries and increase with the Knudsen number.

We can conclude that when the  $kn$  gets closer to  $\infty$ , there will be no temperature gradient in the nanofilm and will result a highest temperature jump on the boundaries.

And we can know when the  $kn$  Number becomes bigger, the scattering decreases and thus it gets harder to reach the equilibrium, so we increase the sampling number from 50,000 to 5000,000 as the  $kn$  ranges from 0.05 to 5.

One thing should be added is the perturbation at the boundary is mainly caused by the truncation error of the computer and we just give up some units to correct and that won't affect the whole temperature profile.

### Boundary condition changes

If we narrow the width that the phonons can pass, which are shown in Fig 6 and Fig 7 namely the black-body boundary, we can find the temperature profile will change and

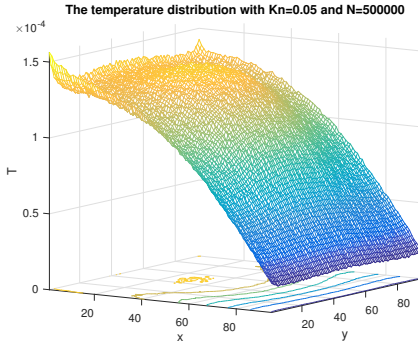


Figure 3:  $Kn=0.05$

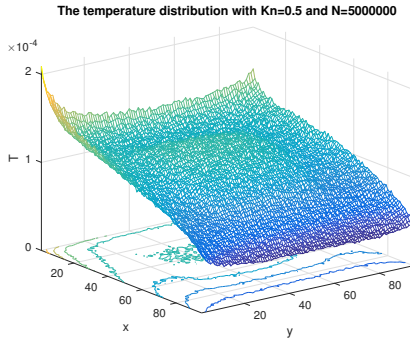


Figure 4:  $Kn=0.5$

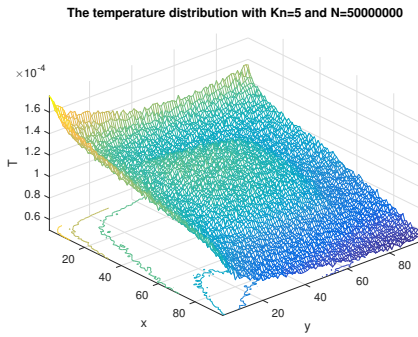


Figure 5:  $Kn=5$

the temperature around the exit will be lower. That calculation means this method can be applied to more complex boundary conditions.

## ii. Conclusion

- Based on Hua's work on one-dimension study on conductivity which focuses on the mechanism in the ballistic-diffusive transport, we develop this method to two-dimension and in the future to real devices by considering more complicated boundary conditions and influence.
- The MC technique can help solve the BTE and gives a valid temperature profile in different Knudsen numbers which is the same with different MFPs in reality. And this will help us understand the heat conduction in nano-films and then develop the optimization.

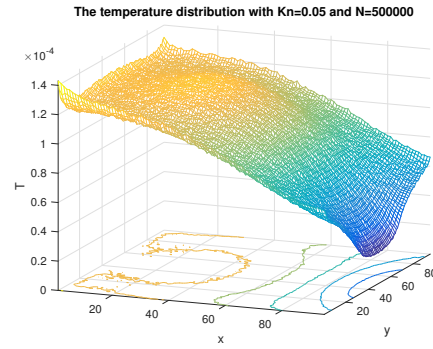


Figure 6:  $Kn=0.05$

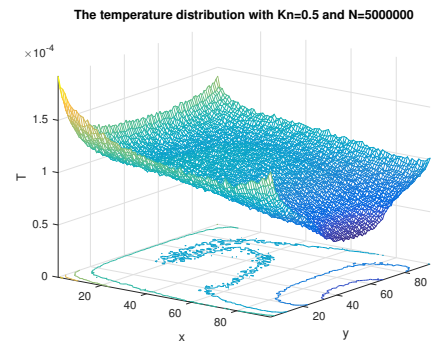


Figure 7:  $Kn=0.5$

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### iii. Forecast and prospects

Rapid progress in the synthesis and processing of materials with structure on nanometer length scales has created a demand for great understanding of thermal transport in nanoscale devices[30]. The most important devices, in terms of worldwide sales, are the integrated circuits used in computer circuits and memories. As I mentioned at the beginning of the article, engineers have been maintaining Moore's Law, which states that the individual device components get smaller every 18 months. Apart from most cases where nanostructures are widely used, in devices, for example, the semiconductor lasers, we want to get away the heat generated as efficiently as we can, the thermal management is of vital importance.

Based on my studies and the forecast of the development of the thermal transport in nanostructures, I mainly choose and focus on three points for my further research in my later Oric study.

- Interface
- MC for multi-structured simulation
- heat hotspots in devices

#### Interface

On small length scales, interfaces between materials become increasingly important. The thermal conductance of many solid-solid interfaces have been studied experimentally but the range of observed interface properties is much smaller than predicted by simple theory.

The idea that an interface should produce a thermal resistance is intuitively appealing, since an interface constitutes an interruption in the regular crystalline lattice on which phonons propagate[30]. According to the exhaustive review by Swartz and Pohl[31], for an interface between dissimilar materials, the different densities and sound speeds result in a mismatch in the acoustic impedance; this is directly analogous to the mismatch in the refractive indices of two optically different

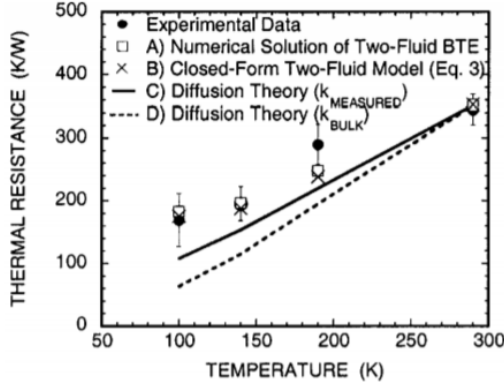
materials[30]. Although the existence of a thermal boundary resistance between a solid and superfluid helium was first detected by Kapitza in 1941[32], and the studies on that issue[33, 34] have been catching people's attention, we still know little about the mechanisms behind the phenomena and cannot get a universal theory or model to describe and predict what happens at the boundary.

#### Multi-structured

Modern Si microelectronics are now firmly in the nanoscale regime. Experiments have demonstrated that the close proximity of interface and the extremely small volume of heat dissipation strongly modifies thermal transport, thereby aggravating problems of thermal management[35]. However, microelectronic devices are too large to do atomic level simulation in the foreseeable future and, therefore, calculations of thermal transport must rely on solutions of the Boltzmann transport equation. But one main problem is microscopic phonon scattering rates needed for predictive models are poorly known, even for silicon[30].

When we consider bulk or thin film materials that contain a collection of nanostructured units, we may find the collective behavior of a large number of units can add to more complexity. Obviously and intuitively, there can be some collective models which are not found if we just consider single units.

With the size of electronic devices shrinking it is necessary to use materials with low dielectric constants, but normal materials with low dielectric constants such as amorphous or nanoporous materials usually have very low thermal conductivities, thus causing a poor thermal management. So comes the question, can we design materials with low dielectric constants and high thermal conductivities? To answer and solve that problem, we need to have a better and more fundamental understanding of phonon transport and electron dynamics in such materials[35].



**Figure 8:** Data and predictions for the membrane thermal resistance as a function of temperature. Prediction A is a numerical solution to the phonon Boltzmann transport equation with a simplified two-fluid model. B is a closed-form correction to diffusion theory based on the two-fluid phonon model. C and D, are based on diffusion theory, using the measured membrane thermal conductivity and the bulk thermal conductivity, respectively. Ref.40

### Heat hotspots

Apart from that size effect which describe a phenomenon that the heat conduction rule strongly violate the classical Fourier's law, an additional nanoscale effect resulting from the small size of the region of electron energy transfer to the lattice[30] should also be noticed.

Electrons traveling between the source and drain are accelerated by the electric fields and generate primarily optical phonons[36]. Several past simulations of electron transport using drift diffusion and the more rigorous Monte Carlo or other ways[37, 38, 39] illustrate that rates of phonon generation are sharply peaked on the drain side. And the effect was also examined by Sverdrup[40] experimentally by using a dedicated microstructure and theoretically by breaking the phonons into two propagating and stationary groups.

As is shown in the Fig8, the region with strong lattice heat generation has dimensions near tens of nanometers and is much smaller than the channel length(50-150nm) and the MFP of phonon. This effect will cause the temperature

of phonon "hotspot" to be larger than that predicted using diffusion theory[41].

In summary, all the above three problems are very important for the understanding of nano heat transfer, and MC simulation can play an important role in helping solving these puzzles which is what I will focus on in next steps of my ORIC work.

### iv. About the MC solutions of BTE

Monte Carlo simulation, which is the core of my work, has been proved as the most efficient and effective way to simulate physical systems, especially systems with high degrees of freedom or complexity[42]. As we have discussed above, the BTE, though powerful in describing the phonon transport phenomenon, is difficult to solve analytically in its most general form[43]. Although in recent works[45, 46, 47], analogies from radiative heat transfer have been successfully used to solve both the diffusive and ballistic limit, in such calculations, phonon dispersion was neglected and just a single 'average' polarization branch was considered. What's more, such calculation strategies is only true when the geometries are simplified[44]. And if we just remove the simplifying relaxation approximation, phonon-phonon scattering events are very hard to incorporate.

Monte Carlo simulations are considered as one approach to capture the complexity of phonon transport in the particle regime to solve the BTE. Actually, if we look back on the developments on the MC solution techniques for the BTE over the past 40 years, we may find that tremendous advancements and achievements have been made for electrons and holes in semiconductors[48, 49]. However, there have been very few reports of using Monte Carlo simulations for phonon transport. Studies[50, 51] either assumed the Debye approximation for density of states or did not consider phonon-phonon interactions. Recently, phonon dispersion as well as various phonon scattering mechanisms were considered to study heat transport and to predict the thermal



conductivities[52].Despite the success achieved, one must be aware of the challenges in applying this MC approach to solve more general problems in nano scale heat transport.

- First, it must be realized that it is quite difficult to capture all the selection rules for transitions between polarizations during phonon-phonon interactions[30].In Mazumder and Majumdar's work[52], they ignored the selection rules and thus obtained local phonon distributions in different polarizations based on a quasi-equilibrium condition. However, in highly non-equilibrium cases, this simplified approach fails. Hence, it is urgent to develop schemes for capturing transitions between polarizations during phonon-phonon interactions.
- Second, the relaxation times for phonon-phonon interactions have been used only for bulk materials in the past. In most cases, these data was obtained by approximate analytical solutions requiring fitting parameters[53, 53]. Correctly speaking,these data can no longer be used when it comes to nanostructures, and for some materials, even relaxation times are not available for bulk materials. Hence, there is a need for approaches to predict the relaxation times for arbitrary phonon dispersion relations.

We need to point out if we can solve the main two obstacles above, Monte Carlo simulations will truly become a extremely powerful and effective tool for studying nanoscale energy dissipation and thermal transport[30].

### Next Work

Based on that calculation of two-dimension problem, I will next conduct studies on devices and will introduce more complicated and real boundaries conditions which are actually a very important point in the whole problem.

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### REFERENCES

- [1] Hua, Y. C., and Cao, B. Y. (2016). The effective thermal conductivity of ballistic-diffusive heat conduction in nanostructures with internal heat source *International Journal of Heat and Mass Transfer*, 92, 995-1003.
- [2] Hua, Y. C., and Cao, B. Y. (2014) Phonon ballistic-diffusive heat conduction in silicon nanofilms by Monte Carlo simulations *International Journal of Heat and Mass Transfer*, 78, 755-759.
- [3] Toberer, E. S., Baranowski, L. L. and Dames, C.(2012) Advances in thermal conductivity *Annual Review of Materials Research*, 42, 179-209.
- [4] Hua, Y. C., and Cao, B. Y. (2016) Ballistic-diffusive heat conduction in multiply-constrained nanostructures *International Journal of Thermal Sciences*, 101, 126-132.
- [5] Desai, S. B., Madhvapathy, S. R., Sachid, A. B., Llinas, J. P., Wang, Q., Ahn, G. H., ... and Wong, H. S. P. (2016). MoS2 transistors with 1-nanometer gate lengths *Science*, 354(6308), 99-102
- [6] Flik, M. I., Choi, B. I., and Goodson, K. E. (1992). Heat transfer regimes in microstructures *ASME J. Heat Transfer*, 114, 666-674
- [7] Landau, L. D., Lifshitz, E. M., and Pitaevskii, L. P. (1980). Statistical physics. *Oxford University Press*, part I

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- [8] Ziman, J. M. (1972). Principles of the Theory of Solids. *Cambridge university press*
- [9] Jiji, Latif M.(2009). Heat Conduction. *Springer*
- [10] Harris, S. (2004). An introduction to the theory of the Boltzmann equation. *Courier Corporation*
- [11] Chandler, D. (1987). Introduction to modern statistical mechanics. *Oxford University Press*
- [12] Hua, Y. C., and Cao, B. Y. (2016) Transient in-plane thermal transport in nanofilms with internal heating *In Proc. R. Soc. A*, Vol. 472, No. 2186, p. 20150811
- [13] Lu, X., Shen, W. Z., and Chu, J. H. (2002). Size effect on the thermal conductivity of nanowires. *Journal of applied physics*, Vol. 472, 91(3), 1542-1552.
- [14] McGaughey, A. J., Landry, E. S., Sellen, D. P., and Amon, C. H. (2011). Size-dependent model for thin film and nanowire thermal conductivity. *Applied Physics Letters*, 99(13), 131904.
- [15] Li, D., Wu, Y., Kim, P., Shi, L., Yang, P., and Majumdar, A. (2003). Thermal conductivity of individual silicon nanowires. *Applied Physics Letters*, 83(14), 2934-2936.
- [16] Hsiao, T. K., Chang, H. K., Liou, S. C., Chu, M. W., Lee, S. C., and Chang, C. W. (2013). Observation of room-temperature ballistic thermal conduction persisting over 8.3 microm in SiGe nanowires. *Nature nanotechnology*, 8(7), 534-538.
- [17] Johnson, J. A., Maznev, A. A., Cuffe, J., Eliason, J. K., Minnich, A. J., Kehoe, T., ... and Nelson, K. A. (2013). Direct measurement of room-temperature nondiffusive thermal transport over micron distances in a silicon membrane. *Physical review letters*, 110(2), 025901.
- [18] Rapaport, D. C., Blumberg, R. L., McKay, S. R., and Christian, W. (1996). The art of molecular dynamics simulation. *Computers in Physics*, 10(5), 456-456.
- [19] Jiaung, W. S., and Ho, J. R. (2008). Lattice-Boltzmann modeling of phonon hydrodynamics. *Physical Review E*, 77(6), 066710.
- [20] Klitsner, T., VanCleve, J. E., Fischer, H. E., and Pohl, R. O. (1988). Phonon radiative heat transfer and surface scattering. *Physical Review B*, 38(11), 7576.
- [21] Mittal, A., and Mazumder, S. (2010). Monte Carlo study of phonon heat conduction in silicon thin films including contributions of optical phonons. *Journal of Heat Transfer*, 32(5), 052402.
- [22] Landau, D. P., and Binder, K. (2014). A guide to Monte Carlo simulations in statistical physics. *Cambridge university press*
- [23] Tong, D. Lectures on kinetic theory. *note, unpublished*
- [24] Chen, G. (1998). Thermal conductivity and ballistic-phonon transport in the cross-plane direction of superlattices. *Physical Review B*, 57(23), 14958.
- [25] Kaviany, M. (2014). Heat transfer physics. *Cambridge university press*
- [26] Howell, J. R., Menguc, M. P., and Siegel, R. (2010). Thermal radiation heat transfer. *CRC press*
- [27] Newman, M. E. J., and Barkema, G. T. (1999). Monte Carlo methods in statistical physics. *Oxford University Press*.
- [28] Yu-Chao, H., Yuan, D., and Bing-Yang, C. (2013). Monte Carlo simulation of phonon ballistic diffusive heat conduction in silicon nanofilm. *Acta Phys. Sin.*, 62(2013) 244401
- [29] Chen, G. (1998). Thermal conductivity and ballistic-phonon transport in the cross-plane direction of superlattices. *Physical Review B*, 57(23), 14958.

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- [30] Cahill, D. G., Ford, W. K., Goodson, K. E., Mahan, G. D., Majumdar, A., Maris, H. J., ... and Phillpot, S. R. (2003). Nanoscale thermal transport. *Journal of Applied Physics*, 93(2), 793-818.
- [31] Swartz, E. T., and Pohl, R. O. (1989). Thermal boundary resistance. *Reviews of modern physics*, 61(3), 605.
- [32] Kapitza, P. L. (1941). The study of heat transfer in helium II. *J. Phys.(USSR)*, 4(1-6), 181-210.
- [33] Challis, L. J. (1974). Kapitza resistance and acoustic transmission across boundaries at high frequencies. *Journal of Physics C: Solid State Physics*, 7(3), 481.
- [34] Weber, J., Sandmann, W., Dietsche, W., and Kinder, H. (1978). Absence of anomalous Kapitza conductance on freshly cleaved surfaces. *Physical Review Letters*, 40(22), 1469.
- [35] Cahill, D. G., Goodson, K. and Majumdar, A. (2002). Thermometry and thermal transport in micro/nanoscale solid-state devices and structures. *Journal of Heat Transfer*, 124(2), 223-241.
- [36] Ziman, J. M. (1960). Electrons and phonons: the theory of transport phenomena in solids. *Oxford university press*.
- [37] Lai, J., and Majumdar, A. (1996). Concurrent thermal and electrical modeling of submicrometer silicon devices. *Journal of Applied Physics*, 79(9), 7353-7361.
- [38] Mahan, G. D. (1985). Hot electrons in one dimension. *Journal of Applied Physics*, 58(6), 2242-2251.
- [39] Mahan, G. D., and Canright, G. S. (1987). Hot electrons in one dimension. II. Backscattering. *Physical Review B*, 35(9), 4365.
- [40] Sverdrup, P. G., Sinha, S., Asheghi, M., Uma, S., and Goodson, K. E. (2001). Measurement of ballistic phonon conduction near hotspots in silicon. *Applied Physics Letters*, 78(21), 3331-3333.
- [41] Chen, G. (1996). Nonlocal and nonequilibrium heat conduction in the vicinity of nanoparticles. *Journal of heat transfer*, 118, 539-545.
- [42] Landau, D. P., and Binder, K. (2014). A guide to Monte Carlo simulations in statistical physics. *Cambridge university press*.
- [43] Guyer, R. A., and Krumhansl, J. A. (1966). Solution of the linearized phonon Boltzmann equation. *Physical Review*, 148(2), 766.
- [44] Cahill, D. G., Braun, P. V., Chen, G., Clarke, D. R., Fan, S., Goodson, K. E., ...and Maris, H. J. (2014). Nanoscale thermal transport. II. 2003-2012. *Applied Physics Reviews*, 1(1), 011305.
- [45] Tien, C. L., Wu, X., and Smith, J. S. (1994). Thermal diffusivity measurement of GaAs/AlGaAs thin-film structures. *Journal of Heat Transfer*, 116, 325.
- [46] Goodson, K.E. (1996). Thermal Conduction in Nonhomogeneous CVD Diamond Layers in Electronic Microstructures *ASME Journal of Heat Transfer*, Vol. 118, pp. 279-286.
- [47] Chen, G., Zhou, S. Q., Yao, D. Y., Kim, C. J., Zheng, X. Y., Liu, Z. L., and Wang, K. L. (1998, May). Heat conduction in alloy-based superlattices. *Proceedings ICT 98. XVII International Conference on Thermoelectrics*, pp. 202-205
- [48] Mogilestue, C. (1982). Thermal Conduction in Nonhomogeneous CVD Diamond Layers in Electronic Microstructures. *ASME Journal of Heat Transfer*, Vol. 118, pp. 279-286.
- [49] Fischetti, M. V., and Laux, S. E. (1993). Monte Carlo study of electron transport in silicon inversion layers. *Physical Review B*, 48(4), 2244.

- 
- [50] Klitsner, T., VanCleve, J. E., Fischer, H. E., and Pohl, R. O. (1988). Phonon radiative heat transfer and surface scattering. *Physical Review B*,38(11), 7576.
- [51] Peterson, R. B. (1994). Direct simulation of phonon-mediated heat transfer in a Debye crystal. *J. Heat Transfer*,116, 815-815.
- [52] Mazumder, S., and Majumdar, A. (2001). Monte Carlo study of phonon transport in solid thin films including dispersion and polarization. *J. Heat Transfer*,123(4), 749-759.
- [53] Holland, M. G. (1964). Phonon scattering in semiconductors from thermal conductivity studies. *Physical Review*,134(2A), A471.
- [53] Holland, M. G. (1964). Phonon scattering in semiconductors from thermal conductivity studies. *Physical Review*,134(2A), A471.