

# The effective thermal conductivity of ballistic-diffusive heat conduction in nanostructures with internal heat source

Heat transport and Optimization of Micro-nano chip

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# Introduction: Heat conduction in silicon

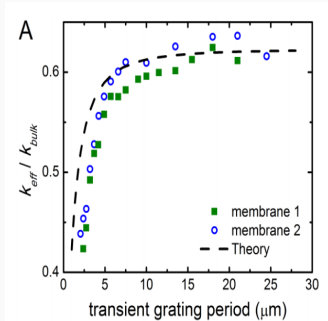
As the typical length of electronic chip arrives at micro even nano scale, the typical heat flux density can reach  $10^5 \text{ W/cm}^2$ , causing the rising of temperature in chips. Because the reliability of chips is greatly influenced by temperature, the study on nanoscale heat conduction in silicon nano-films is especially important.


**MFP** phonon  
mean free  
path

**ballistic transport**  
phonons  
flying directly  
from one  
boundary to  
another

**diffusive transport**  
phonons  
transport  
dominated  
by Fourier's  
law

# Introduction: size-dependent thermal conductivity



 **1:** Thermal conductivity decreases dramatically as the size becomes small (Johnson, Jeremy A ,2013)

As shown in the picture, when the length of the film becomes small and gets close to the MFP of phonon in silicon, Fourier's law won't work. In this region, the transport is both influenced by ballistic and diffusive transport, which is called ballistic-diffusive conduction.

**定理** (BTE with the relaxation time approximation)

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

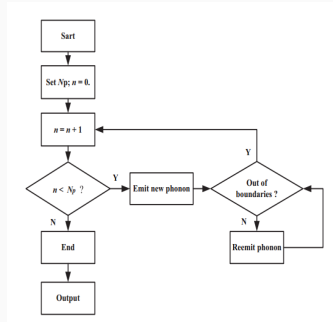
There are mainly several ways to solve or study on this equation.

- Experiments
- Mathematical way
- Simulation
  - MD
  - Lattice Boltzmann
  - MC

# MC Method

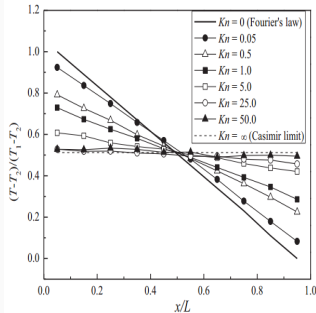
Some key points

- Gray body Approximation
- Debyu Approximation(Assume the lattice elastic)
- local thermal equilibrium assumption



**图 2:** MC Tracing Method  
(Yu-Chao Hua, Bing-Yang Cao ,2014)

# Cross-plane



**Fig 3:** Dimensionless temperature profiles of Si nanofilms (Yu-Chao Hua, Bing-Yang Cao ,2014)

The temperature profiles within the nanofilms are *linear*. As  $Kn=0$ , the phonon transport is purely diffusive and that's just the Fourier's law; as  $Kn \rightarrow \infty$ , since the phonon ballistic transport is dominant, the temperature gradient vanishes and the temperature jump reaches maximum.

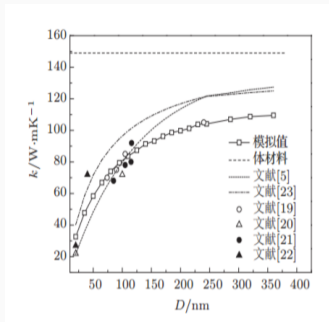
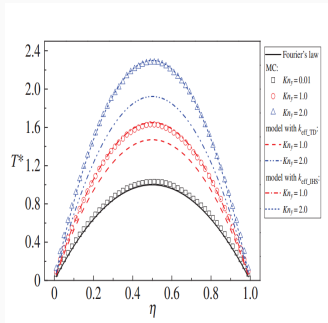


图 4: The thermal conductivity in different depth (Yu-Chao Hua, Dong Yuan ,2013)

As shown in the picture, the size effect is fully displayed as the size of nanofilm is near the MFP. And the Conductivity increases as the depth increases, while the slope decreases.

# In-plane and with internal heating

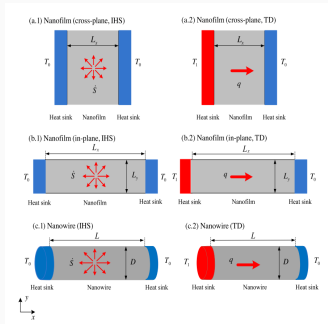


**Fig 5:** Transient in-plane thermal transport in nanofilms with internal heating (Yu-Chao Hua, Dong Yuan, 2013)

In the MC simulations, phonons emit within the nanofilms uniformly and can scatter with the lateral boundaries from the beginning. Therefore, the temperature rise can be significantly larger when compared with the heat diffusion equation based on Fourier's law even at the initial heating stage.



# The effective thermal conductivity



**Fig 6:** The effective thermal conductivity of ballistic–diffusive heat conduction in nanostructures with internal heat source (Yu-Chao Hua, Dong Yuan ,2013)

It is found that the effective thermal conductivity in the IHS scheme is significantly lower than that in the TD scheme. The diffusive heat conduction equation with the effective thermal conductivity is applied to characterize the temperature distributions in the nanostructures with internal heat source.

# Analysis and Next step work

## Next steps

1. From  
One-dimensional to  
two-dimensional and  
three-dimensional
2. Transient transport
3. Complex boundary  
conditions and  
different geometry  
structures
4. Improve the algorithm  
and lower the expense

## Main nodi

- Interface
- Complexity in actual  
device
- How to conduct  
optimization (Without  
no mathematical  
method and quite  
different from Macro  
problems)



Johnson, Jeremy A (2013)

**Direct measurement of room-temperature nondiffusive thermal transport over micron distances in a silicon membrane**

*Physical review letters* 110(2), 025901.



Hua, Yu-Chao and Cao, Bing-Yang (2014)

**Phonon ballistic-diffusive heat conduction in silicon nanofilms by Monte Carlo simulations**

*International Journal of Heat and Mass Transfer* 78,755–759.



华钰超, 董源, 曹炳阳 (2013)

**硅纳米薄膜中声子弹道扩散导热的蒙特卡罗模拟**

物理学报 62(24),244401-244401.



Hua, Yu-Chao and Cao, Bing-Yang (2016)

**The effective thermal conductivity of ballistic-diffusive heat conduction in nanostructures with internal heat source**

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92,995-1003.



Hua, Yu-Chao and Cao, Bing-Yang (2016)

**Transient in-plane thermal transport in nanofilms with internal heating**

*Proc. R. Soc. A* 472(2186),20150811.