Phonon Ray-Tracing Monte Carlo Simulation – Principle and Application

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Non-Fourier Heat Conduction

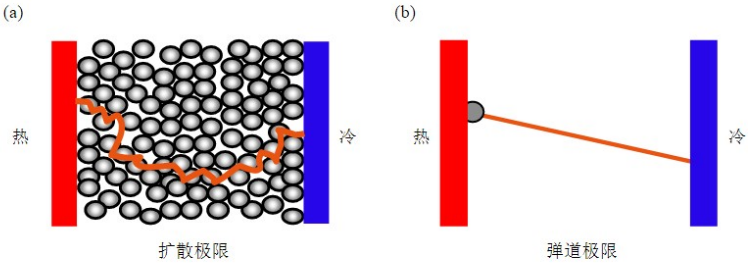


Figure 1: Ballistic-diffusive heat conduction. (a) phonon diffusive heat transport; (b) phonon ballistic heat transport.

When the system size is comparable with phonon MFPs, Fourier's law becomes inapplicable and ballistic-diffusive heat conduction emerges.

Phonon Boltzmann Transport Equation (BTE)

Single mode relaxation time (SMRT) approximation

$$\frac{\partial f_{\omega,p}}{\partial t} + |v_{g,\omega,p}|\vec{s} \cdot \nabla f_{\omega,p} = -\frac{f_{\omega,p} - f^0_{\omega,p}(T)}{\tau_{\omega,p}}$$

$f(t, x, y, z, p_x, p_y, p_z)$ can be 7 dimensional function!

Deterministic methods such as discrete ordinate method (DOM) + finite volume method (FVM) can be extremely time consuming.

Monte Carlo methods: use the sampling to substitute the deterministic solving.

Monte Carlo Simulation

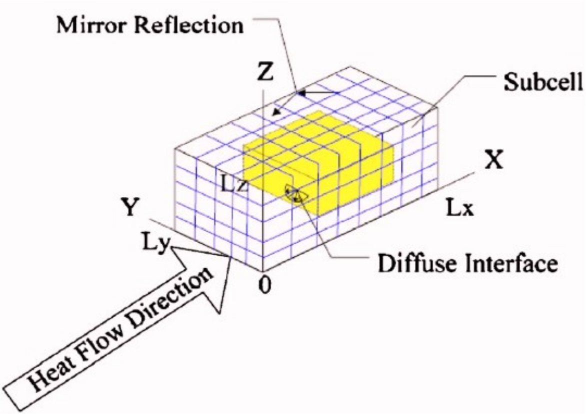
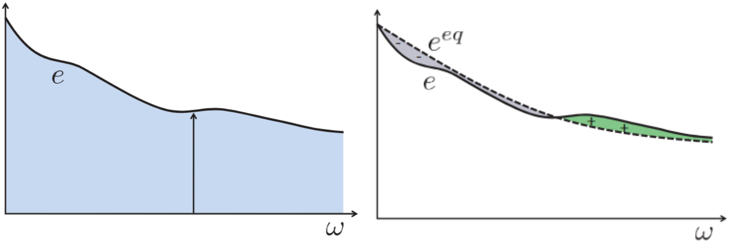


Figure 2: The MC simulation of phonon transport in a nanocomposite with cubic silicon nanoparticles[1].

[1] M.-S. Jeng, R. Yang, D. Song, *et al.*, "Modeling the thermal conductivity and phonon transport in nanoparticle composites using monte carlo simulation," *Journal of heat transfer*, vol. 130, no. 4, 2008.

Energy-Based Variance-Reduced Monte Carlo



(a) Standard particle methods. (b) Variance-reduced methods.

Figure 3: The diagram of Monte carlo methods to approximate the moments of the distribution.

In variance-reduced methods, the stochastic part is reduced to the calculation of the deviation from a known state[2].

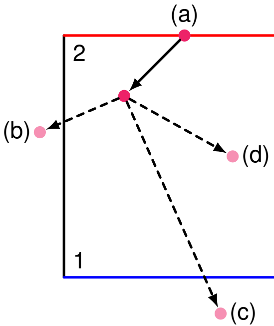
[2] J.-P. M. Péraud and N. G. Hadjiconstantinou, "Efficient simulation of multidimensional phonon transport using energy-based variance-reduced monte carlo formulations," *Physical Review B*, vol. 84, no. 20, p. 205 331, 2011.

Basic Concepts

☼ Simulated particles: Every tracked phonon bundle represents a fixed deviational effective energy $\varepsilon_{\text{eff}}^{d}$.
☼ Local energy: By counting the number of phonon bundles in a cell, the loacl energy and temperature can be evaluated.

$$(N^{+} - N^{-})\varepsilon_{\text{eff}}^{d}/\Delta V = \sum_{p} \int_{\omega=0}^{\omega_m} \hbar\omega D(\omega, p) \times \left[f_T(\omega) - f_{T_{eq}}(\omega) \right]$$

Movement of One Phonon Bundle



(a): phonon emit

(b): phonon-boundary scatter

(c): phonon absorption

(d): phonon-phonon scatter

Figure 4: Possible phonon bundle movements in MC simulation

The movement and the property of a phonon bundle is determined by random sampling based on the probability distribution.

Probability distribution

- Scatter probability:

$$P = 1 - \exp\left(-\frac{\Delta t}{\tau(\omega, p, T)}\right)$$

- Boundary emission frequency:

$$q''_{\omega,b} = \frac{1}{4}\sum_{p} D(\omega,p)V_g(\omega,p)\hbar\omega \times (f_\omega(T_b) - f_\omega(T_{eq}))$$

- Phonon-phonon scatter frequency:

$$P = \frac{D(\omega,p)\hbar\omega}{\tau(\omega,p,T)}(f_\omega(T_{\text{loc}}) - f_\omega(T_{eq}))$$

Simulate multiple phonon bundles together in a timestep to acquire the temperature distribution. It's so called ensemble monte carlo simulation.

Ray-Tracing Phonon Monte Carlo

When ΔT is not large, we can replace the difference by differential to get around to evaluate local T. Therefore, we can track every phonon bundle independently[3].

$$f_\omega(T) - f_\omega(T_{eq}) \approx (T - T_{eq}) \frac{\mathrm{d} f_\omega}{\mathrm{d} T}\Big|_{T=T_{eq}}$$

- Boundary emission:

$$q''_{\omega,b} \approx \frac{1}{4} \sum_p C(\omega, p, T_{eq}) V_g(\omega, p) \times (T_b - T_{eq})$$

- Phonon-phonon scatter:

$$P \approx \frac{C(\omega, p, T_{eq})}{\tau(\omega, p, T_{eq})} (T_{\text{loc}} - T_{eq})$$

[3] J.-P. M. Péraud and N. G. Hadjiconstantinou, "An alternative approach to efficient simulation of micro/nanoscale phonon transport," *Applied Physics Letters*, vol. 101, no. 15, p. 153 114, 2012.

Steady-State Simulation

Scatter probability:

$$P = 1 - \exp\left(-\frac{\Delta t}{\tau(\omega, p, T_{eq})}\right)$$

Sample random number $R \in (0, 1)$, we have

$$t = -\tau(\omega, p, T_{eq}) \ln(1 - R)$$

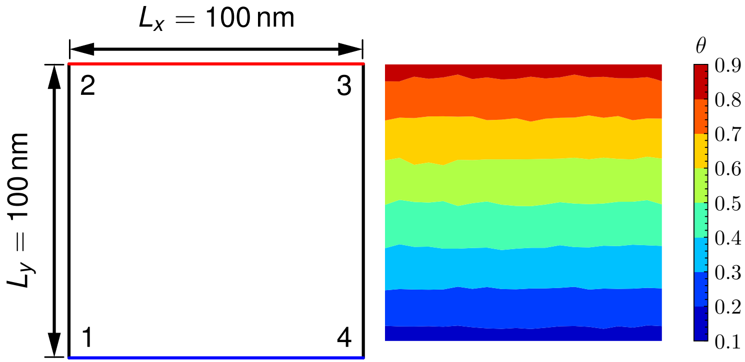
Multiply v_g/L in the equation,

$$l = -Kn(\omega, p, T_{eq}) \ln(1 - R)$$

The Monte Carlo simulation is then time independent![4]

[4] Y.-C. Hua and B.-Y. Cao, "Phonon ballistic-diffusive heat conduction in silicon nanofilms by monte carlo simulations," *International Journal of Heat and Mass Transfer*, vol. 78, pp. 755–759, 2014.

Square Film (Si)

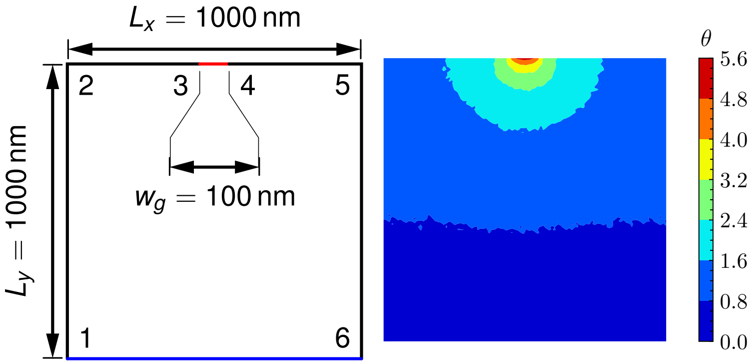


(a) Schematic diagram. (b) Dimensionless temperature field.

Figure 5: MC simulation of a si square film.

- When $L_y \ll L_x$, the case is cross-plane heat conduction.
- When $L_y \gg L_x$, the case is in-plane heat conduction.

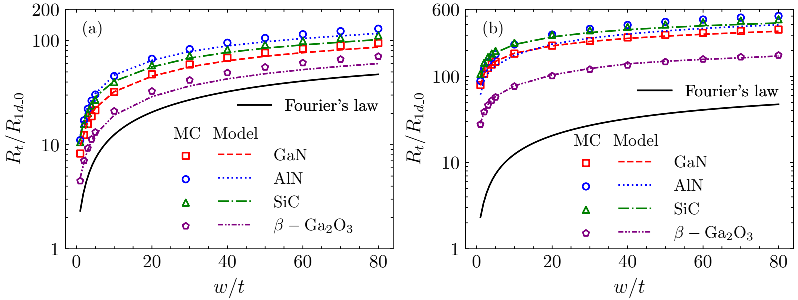
Thermal Spreading (Si)



(a) Schematic diagram. (b) Dimensionless temperature field.

Figure 6: MC simulation of thermal spreading process.

Thermal Spreading Resistance of WBG Materials

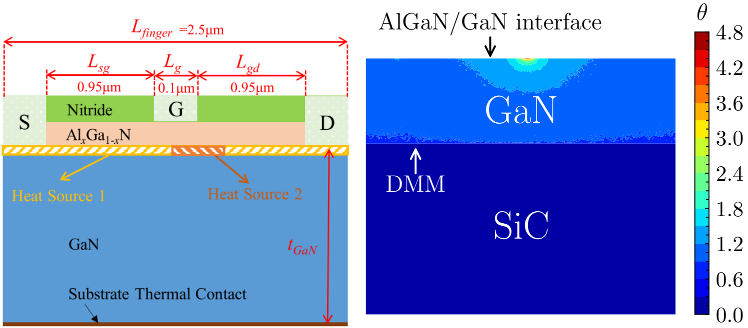


(a) $t = 4\,\mu m$ (b) $t = 0.2\,\mu m$

Figure 7: Dimensionless total thermal resistance of different semiconductors as a function of w/t, $w_g/w = 0.01$[5].

[5] Y. Shen, Y.-C. Hua, H.-L. Li, *et al.*, "Spectral thermal spreading resistance of wide-bandgap semiconductors in ballistic-diffusive regime," *IEEE Transactions on Electron Devices*, vol. 69, no. 6, pp. 3047–3054, 2022.

Multi-layer Device Structure



(a) Device structure of a GaN HEMT.

(b) Dimensionless temperature field.

Figure 8: TCAD simulation + Monte carlo simulation of GaN on SiC HEMTs.

Advantages and Limitations

Advantages

- Meshfree and convenient for complex geometries
- Time independent
- Computationally efficient and easy to parallelize

Limitations

- Can not address temperature dependent properties, *i.e.*

$$\frac{D(\omega, p)\hbar\omega}{\tau(\omega, p, T)} \left(\frac{1}{\exp\left(\frac{\hbar\omega}{k_b T_{\text{loc}}}\right) - 1} - \frac{1}{\exp\left(\frac{\hbar\omega}{k_b T_{eq}}\right) - 1} \right)$$

Thank You!