Physics-informed neural networks for solving multiscale mode-resolved phonon Boltzmann transport equation

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Overall introduction

Background

Numerically solving phonon BTE is extremely computationally challenging due to the high dimensionality of such problems, especially when mode-resolved properties are considered.

Main work

This work demonstrates the use of physics-informed neural networks (PINNs) to efficiently solve phonon BTE for multiscale thermal transport problems with the consideration of phonon dispersion and polarization.

Main method

A PINN framework is devised to predict the phonon energy distribution by minimizing the residuals of governing equations and boundary conditions, without the need for any labeled training data.

Outline

1. Governing equation
2. Physics-informed neural networks
3. Results and discussions
4. Advantages,limitations and future perspectives

1. Governing equation
   - Phonon boltzmann transport equation (BTE)
   - Dispersion and relaxation time
   - Energy-based phonon BTE
2. Physics-informed neural networks
3. Results and discussions
4. Advantages,limitations and future perspectives

Phonon probability density function

Phonons can be thought of as quantized sound waves, which dominate the heat conduction process in many semi-conductors such as silicon :

$$\epsilon = h\nu = \hbar\omega \quad , \quad \hbar = h/2\pi$$

$$\overrightarrow{\mathbf{p}} = \hbar\overrightarrow{\mathbf{k}} \left(\mathbf{p} = \frac{h}{\lambda}\right)$$

The probability density function is a 6 dimensional function of position and momentum:

$$N = \int_{\text{momenta}} \mathrm{d}^3\mathbf{p} \int_{\text{positions}} \mathrm{d}^3\mathbf{r} f(\mathbf{r}, \mathbf{p}, t)$$

Volumetric average:

$$\langle X(\mathbf{r}) \rangle = \frac{1}{(2\pi)^2} \int X(\mathbf{r}, \mathbf{k}) f \mathrm{d}\mathbf{k}$$

Phonon BTE

Relaxation time approximation:

$$\frac{\partial f_{\omega,p}}{\partial t} + \mathbf{v_g} \cdot \nabla f_{\omega,p} = \frac{f_{0,\omega,p} - f_{\omega,p}}{\tau_{\omega,p}}$$

ω: frequency

p: polarization

$f_{\omega,p}$: phonon density distribution

$f_{0,\omega,p}$: equilibrium phonon density distribution

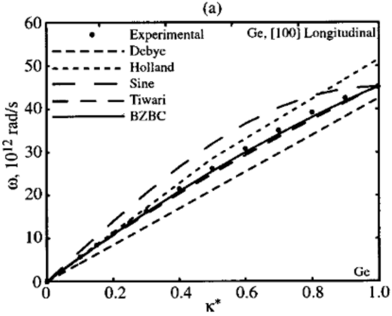
$v_g = \frac{\partial \omega}{\partial k}$: phonon group velocity

$\tau_{\omega,p}$: phonon relaxation time

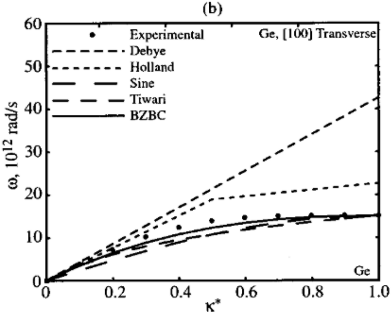
With different polarization and frequency, phonons will have different properties. So called solving mode-resolved phonon BTE is to solve these phonons individually.

Polarization and dispersion relation

Phonon polarization:
Optical branch (contribute little to thermal transport) + Acoustic branch (1 Longitudinal branch + 2 Tranverse branches)



(a) LA branch



(b) TA branch

Figure 1: Germanium phonon dispersion in the [100] direction.

Dispersion relation of acoustic phonons

- The phonon dispersion relation of silicon in the [100] direction is used
- Isotropy is assumed
- Only acoustic phonon branches are considered

$$\omega = c_1 k + c_2 k^2$$

Group velocity:

$$|\mathbf{v}| = \frac{\partial \omega}{\partial k} = c_1 + 2c_2 k$$

LA branch:
$c_1 = 9.01 \times 10^5\,\mathrm{cm\,s^{-1}}, c_2 = -2 \times 10^{-3}\,\mathrm{cm\,s^{-1}}$
TA branch:
$c_1 = 5.23 \times 10^5\,\mathrm{cm\,s^{-1}}, c_2 = -2.26 \times 10^{-3}\,\mathrm{cm\,s^{-1}}$

Effective relaxation time

Matthiessen's rule:

$$\tau^{-1} = \tau_{\text{impurity}}^{-1} + \tau_U^{-1} + \tau_N^{-1} = \tau_{\text{impurity}}^{-1} + \tau_{NU}^{-1}$$

Table 1: Relaxation time formulas and coefficients

$\tau_{impurity}^{-1}$	$A_i\omega^4$, $A_i = 1.498 \times 10^{-45}$ s^3
LA	$\tau_{NU}^{-1} = B_L\omega^2T^3$, $B_L = 1.180 \times 10^{-24}$ K^{-3}
TA	$\tau_{NU}^{-1} = B_T\omega T^4$, $0 \le k < \pi/a$ $\tau_{NU}^{-1} = B_U\omega^2/\sinh(\hbar\omega/k_BT)$, $\pi/a \le k \le 2\pi/a$ $B_T = 8.708 \times 10^{-13}$ K^{-3}, $B_U = 2.890 \times 10^{-18}$ s $a = 0.5431$ nm

Energy-based phonon BTE

$$\frac{\partial e_{\omega,p}}{\partial t} + \boldsymbol{v_g} \cdot \nabla e_{\omega,p} = \frac{e^{eq}_{\omega,p} - e_{\omega}}{\tau_{\omega,p}}$$

Where

$$e_{\omega,p} = \hbar\omega D(\omega,p)[f - f^{BE}(T_{ref})]$$

$$e^{eq}(\omega,p,T) = \hbar\omega D(\omega,p)\left[f^{BE}(T) - f^{BE}(T_{ref})\right] \approx C(\omega,p)(T - T_{ref})$$

$D(\omega,p) = \frac{k^2}{2\pi^2 v_g}$, phonon density of states

1 Governing equation

2 Physics-informed neural networks
- Problem statement
- Framework

3 Results and discussions

4 Advantages,limitations and future perspectives

Problem statement

Governing equation

$$R(e(\boldsymbol{x}, \boldsymbol{s}, k, p, \boldsymbol{\mu})) = 0 :=$$

$$\begin{cases} \boldsymbol{v_g} \cdot \nabla e - \frac{e^{eq} - e}{\tau} = \boldsymbol{v_g} \cdot \nabla e + \frac{e^{neq}}{\tau} = 0 \\ \nabla \cdot \boldsymbol{q} = \nabla \cdot \sum_p \int_0^{\omega_{\max p}} \int_{4\pi} \boldsymbol{v_g} e d\Omega d\omega = 0, \end{cases}$$

$$\boldsymbol{v_g} \cdot \nabla e = |\boldsymbol{v_g}|(\cos\theta, \sin\theta\cos\phi, \sin\theta\sin\phi) \cdot (\nabla_x e, \nabla_y e, \nabla_z e)$$

Boundary conditions

$$\mathscr{B}_i(\boldsymbol{x}, \boldsymbol{s}, k, p, e, \boldsymbol{\mu}) = 0, \quad \boldsymbol{x}, \boldsymbol{s}, k, p \in \Gamma_b, \boldsymbol{\mu} \in \mathbb{R}^d$$

Loss function

$$\mathscr{L}(\boldsymbol{W}, \boldsymbol{b}) = \left\| \boldsymbol{v_g} \cdot \nabla e - \frac{e^{eq} - e}{\tau} \right\|^2 + \|\nabla \cdot \boldsymbol{q}\|^2 + \sum_i \|\mathscr{B}_i\|^2$$

Boundary conditions

Isothermal boundary:

$$e\left(\boldsymbol{x}_b, \boldsymbol{s}, k, p\right) = e^{eq}\left(k, p, T_b\right), s \cdot \boldsymbol{n}_b > 0$$

Diffusely reflecting boundary:

$$e\left(\boldsymbol{x}_b, \boldsymbol{s}, k, p\right) = \frac{1}{\pi} \int_{\boldsymbol{s}' \cdot \boldsymbol{n}_b < 0} e\left(\boldsymbol{x}_b, \boldsymbol{s}', k, p\right) \left|\boldsymbol{s}' \cdot \boldsymbol{n}_b\right| d\Omega, s \cdot \boldsymbol{n}_b > 0$$

Periodic boundary:

$$e\left(\boldsymbol{x}_{b_1}, \boldsymbol{s}, k, p\right) - e^{eq}\left(k, p, T_{b_1}\right) = e\left(\boldsymbol{x}_{b_2}, \boldsymbol{s}, k, p\right) - e^{eq}\left(k, p, T_{b_2}\right)$$

Framework

$$e = e^{eq} + e^{neq}, e^{neq} = e - e^{eq}$$

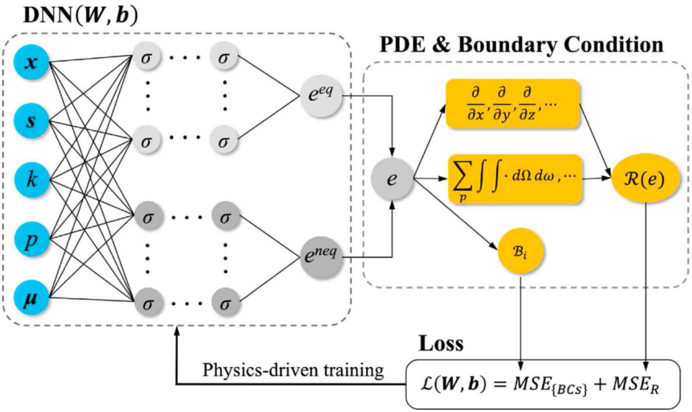


Figure 2: Schematic of PINN framework for solving stationary mode-resolved phonon BTE.

1 Governing equation

2 Physics-informed neural networks

3 Results and discussions
- 1D cross-plane phonon transport
- 2D in-plane phonon transport
- 2D square phonon transport
- 3D cuboid phonon transport

4 Advantages,limitations and future perspectives

Cases for analyses

Table 2: Training and validation losses of numerical experiments

Case	Training Loss	Validation Loss
1D cross-plane	2.0×10^{-4}	1.4×10^{-3}
2D in-plane	5.6×10^{-4}	4.5×10^{-3}
2D square	2.4×10^{-2}	1.6×10^{-2}
3D cuboid[a]	6.5×10^{-3}	8.8×10^{-3}
3D cuboid[b]	9.8×10^{-3}	4.9×10^{-3}

Computational efficiency

Table 3: Training and testing information

Case	Training				L (m)
	N_x	N_s	N_l	Walltime (h)	
1D cross-plane	40	16	5	0.80	$[10^{-8}, 10^{-4}]$
2D in-plane	300	144	5	4.83	$[10^{-8}, 10^{-4}]$
2D square	450	144	4	6.62	$[10^{-8}, 10^{-5}]$
3D cuboid[a]	1200	144	3	15.52	$[10^{-8}, 10^{-6}]$
3D cuboid[b]	1200	64	3	8.68	$[10^{-5}, 10^{-3}]$

(a) Training time

Case	Testing				L (m)
	N_x	N_s	N_l	Walltime (s)	
1D cross-plane	40	64	17	2.11	$[10^{-8}, 10^{-4}]$
2D in-plane	1600	1024	17	24.72	$[10^{-8}, 10^{-4}]$
2D square	2601	576	7	9.57	$[10^{-8}, 10^{-5}]$
3D cuboid[a]	132,651	576	5	344.54	$[10^{-8}, 10^{-6}]$
3D cuboid[b]	132,651	576	5	351.64	$[10^{-5}, 10^{-3}]$

(b) Testing time

1D cross-plane phonon transport

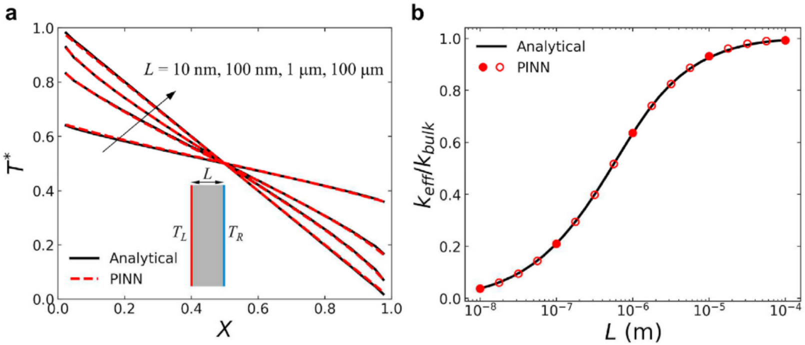


Figure 3: (a) Dimensionless temperature profiles of silicon thin films with different thickness. (b) Effective thermal conductivity normalized by the bulk thermal conductivity at different film thickness. The filled circles represent the parameter points used for training, while the open circles are predicted points not included in training

2D in-plane phonon transport

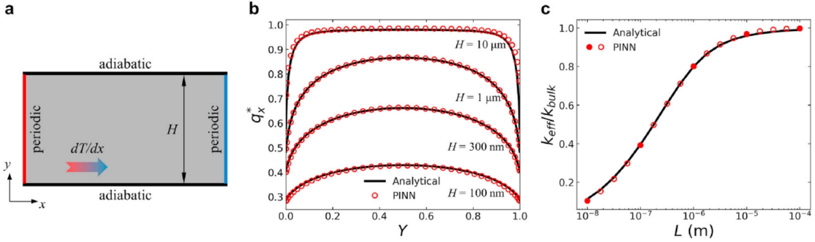


Figure 4: (a) Schematic of 2D in-plane phonon transport case. (b) Distribution of dimensionless x-directional heat flux along the y-axis in thin films with different thickness. (c) Effective thermal conductivity normalized by the bulk thermal conductivity at different length scales.

2D square phonon transport

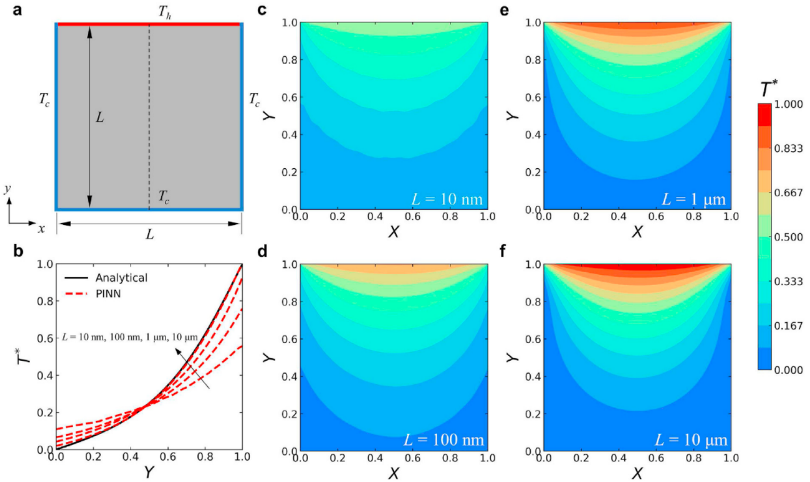


Figure 5: (b) Non-dimensional temperature profiles along the vertical centerline (dashed line in (a)) at different length scales. (c-f) Contours of dimensionless steady-state temperature at different length scales.

3D cuboid phonon transport

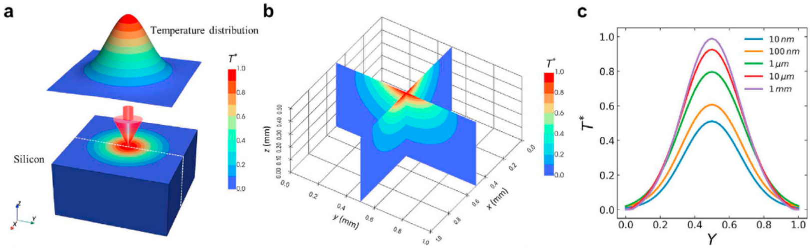


Figure 6: (a) Gaussian temperature distribution is applied to the top surface, while all the other surfaces are maintained at lower temperature. (b) Dimensionless steady-state temperature distribution (c) PINN-predicted dimensionless temperature distributions along the centerline on the top surface at different length scales.

3D cuboid phonon transport

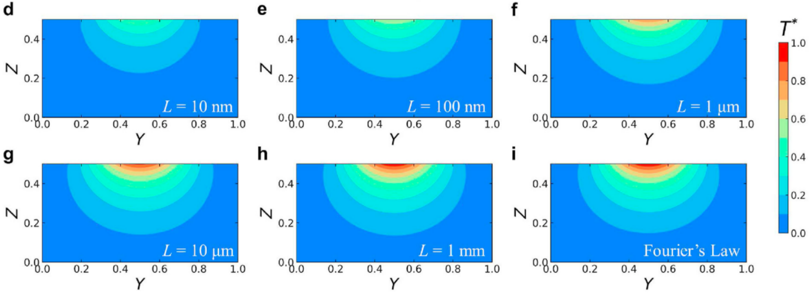


Figure 7: (d-h) PINN-predicted contours of dimensionless steady-state temperature in the central plane (i) solution under fourier's law

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Advantages,limitations and perspectives

Advantages

- computationally efficient especially for 3D problems
- can parameterize the solution to phonon BTE with geometric variations
- data-free training

Limitations

- current only for steady-state phonon BTE
- small temperate difference assumption
- the training cost will increase for complex problems

Perspectives

- employ the LSTM neural network to predict the dynamics
- adopt the distribution function f-based BTE with space-dependent relaxation time
- adopt CNN for complex geometries

Thank You!