Comparison of Simulation Methods for Thermal Spreading Resistance in GaN HEMTs

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2 Problem Statement and Methodology
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Thermal Issues in GaN HEMTs

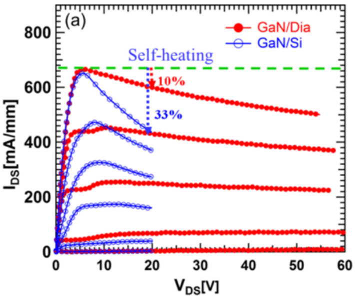

Figure 1: $I_{DS} - V_{DS}$ of GaN/Dia and GaN/Si HEMTs [1].

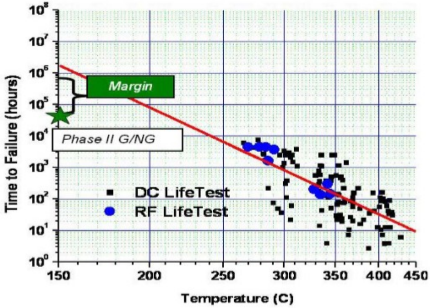

Figure 2: Mean time to failure (MTTF) for TriQuint GaN PAs [2].

Accurate thermal simulation is crucial for near-junction thermal management and electro-thermal co-design of GaN HEMTs.

[1] K. Ranjan, S. Arulkumaran, G. Ng, *et al.*, "Investigation of self-heating effect on DC and RF performances in AlGaN/GaN HEMTs on CVD-diamond," *IEEE Journal of the Electron Devices Society*, vol. 7, pp. 1264–1269, 2019.

[2] M. Rosker, C. Bozada, H. Dietrich, *et al.*, "The DARPA wide band gap semiconductors for RF applications (WBGS-RF) program: Phase II results," *CS ManTech*, vol. 1, pp. 1–4, 2009.

Thermal Spreading in GaN HEMTs

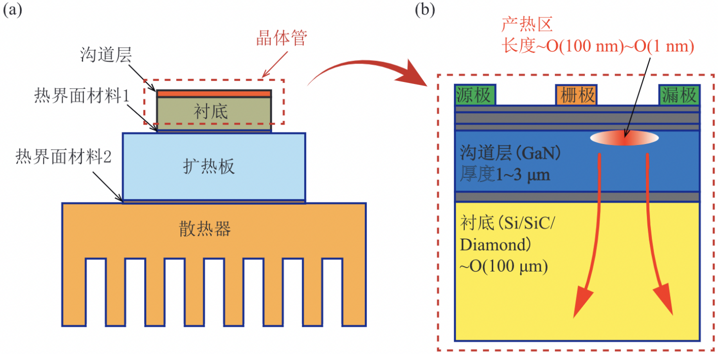

Figure 3: Schemation of the cross-section of GaN HEMTs: (a) overall structure (b) enlarged view in the near-junction region.

Thermal spreading resistance dominates the heat transport in the near-junction region. Many efforts have been made to model the thermal spreading resistance using Fourier's law.

Phonon Ballistic Transport in the Near-Junction Region

Phonon MFPs are comparable with the thickness of the GaN layer and the width of the heat generation area. Phonon ballistic transport can significantly increase the thermal resistance.

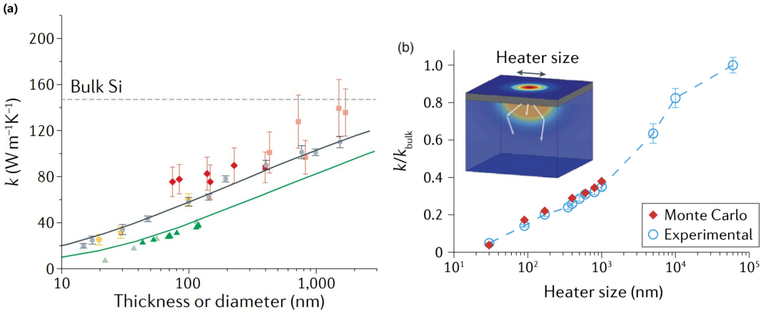

Figure 4: (a)Thermal conductivity versus film thickness or nanowire diameter. (b) Effective conductivity versus varying heater sizes[3].

[3] G. Chen, "Non-fourier phonon heat conduction at the microscale and nanoscale," *Nature Reviews Physics*, vol. 3, no. 8, pp. 555–569, 2021.

Phonon Boltzmann Transport Equation

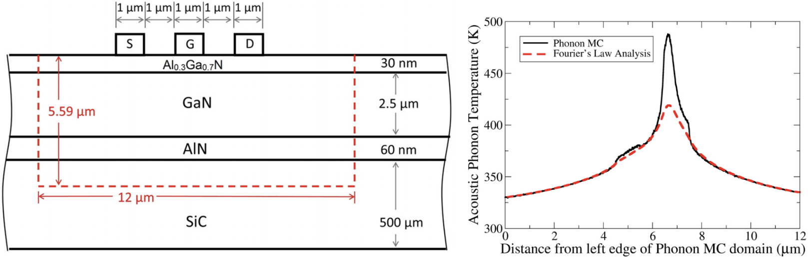

Figure 5: Schematic diagram of the cross section of the GaN HEMT and the simulated channel temperature[4].

To account for the influence of phonon ballistic transport on the thermal spreading process, the phonon Boltzmann transport equation (BTE) should be solved in the near-junction region.

[4] Q. Hao, H. Zhao, and Y. Xiao, "A hybrid simulation technique for electrothermal studies of two-dimensional GaN-on-SiC high electron mobility transistors," *Journal of Applied Physics*, vol. 121, no. 20, p. 204 501, 2017.

Existing Simulations for GaN HEMTs

Various methods have been adopted in GaN-based device simulations,

- Isotropic MC with empirical phonon dispersion, Hao *et al*. (2017, JAP, IJHMT, TED), shen *et al*. (2022, TED)
- Gray MC, Donmezer *et al*. (2014, TED), Bikramjit *et al*. (2020, JAP)
- FEM with k_{eff}, Song *et al*. (2020, IJHMT)

There has not been a thorough examination of the performance and reliability of the different methods, making it challenging to utilize the results and findings from different studies.

This Work

- First-Principle based steady-state full-band phonon tracing Monte Carlo simulations are developed to investigate the near-junction thermal spreading process in GaN HEMTs.
- The reliability, accuracy, and computational efficiency of isotropic MC, gray MC, and FEM with k_{eff} are compared thoroughly.

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- Full-band Phonon Monte Carlo Simulation
- Simplified Simulation Methods

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Thermal Spreading Process in GaN HEMTs

- The c-axis (polarization axis) of GaN is aligned with the thickness direction
- Substrate and interfacial thermal resistance are not considered in the current study
- A uniform heat flux is modeled at the top of the GaN layer to represent the heat source

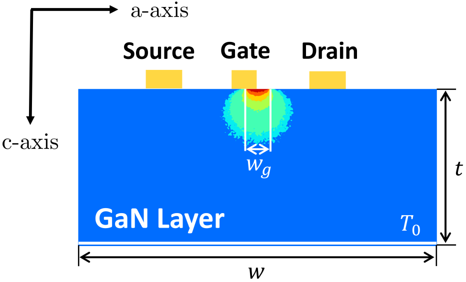

Figure 6: Schematic of thermal spreading process in the GaN layer.

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First-pinrciple Calculation

The third-order anharmonic calculation of wurtzite GaN is performed with $15 \times 15 \times 15$ **q**-point grids, generating 3375 discrete **q**-points. With 12 phonon branches there are total 40500 available phonon states for MC simulations.

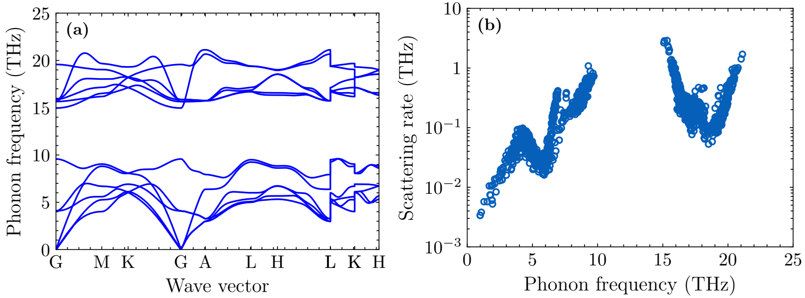

Figure 7: First-principle-calculated phonon peroperties of GaN at 300 K (a) Phonon dispersion along high-symmetry points. (b) Phonon scattring rates.

Full-band Phonon Monte Carlo Simulations

- Steady-state phonon tracing MC simulations
- Energy-based variance-reduced techinque

The number of emitted phonon bundles of a boundary with temperature T_b can be expressed as

$$N(T_b) = \frac{1}{\varepsilon_{\text{eff}} V} \sum_{\text{state } j} \vec{v}_j \cdot \vec{n} \hbar\omega_j \left[f_{\mathrm{BE}}(\omega_j, T_b) - f_{\mathrm{BE}}(\omega_j, T_{\mathrm{ref}}) \right], \vec{v}_j \cdot \vec{n} > 0$$

The flight distance before scattering is drawn as

$$\vec{l} = -\vec{v}_j \tau_j \ln(R_l)$$

After scattering, the phonon mode is redrawn with probabilities proportional to

$$\hbar\omega \left[f_{\mathrm{BE}}(\omega_k, T_{\mathrm{loc}}) - f_{\mathrm{BE}}(\omega_k, T_{\mathrm{ref}}) \right] / \tau_k$$

Interface Scattering

In the case of a collision with an adiabatic boundary, the phonon bundle is diffusively scattered to its iso-energy state. The probabilitity of drawing the j-mode phonon is proportional to

$$\left(\vec{v}_j \cdot \vec{n}\right) \delta(\omega - \omega_{\text{in}}), \vec{j}_k \cdot \vec{n} > 0$$

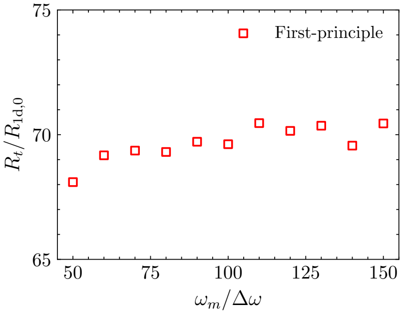

Figure 8: Dimensionless total thermal resistance calculated with different $\Delta\omega$, $t = 1\ \mu$m, $w_g/w = 0.01$, $w/t = 40$.

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Validation of the Simulation

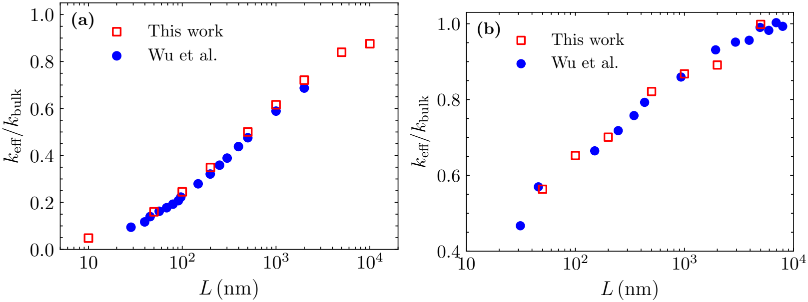

Figure 9: Effective thermal conductivity varying with the characteristic length in (a) cross-plane heat conduction and (b) in-plane heat conduction. Other numerical results come from Wu *et al.*[5]

[5] R. Wu, R. Hu, and X. Luo, "First-principle-based full-dispersion Monte Carlo simulation of the anisotropic phonon transport in the wurtzite GaN thin film," *Journal of Applied Physics*, vol. 119, no. 14, p. 145 706, 2016.

Isotropic MC

Isotropic Born-von Karman dispersion:

$$\omega(k) = \omega_m \sin(\pi k / 2k_m)$$
$$\tau^{-1} = \tau_I^{-1} + \tau_U^{-1} = A\omega^4 + B\omega^2 T \exp(-C/T)$$

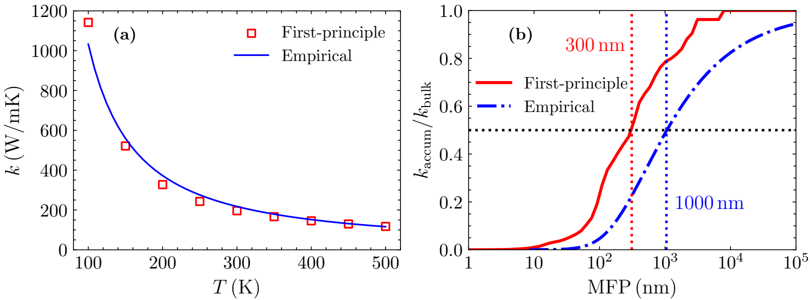

Figure 10: Comparison between first-principle-based predictions and the empirical model for GaN. (a) Bulk thermal conductivity varying with temperature. (b) Thermal conductivity accumulation functoin.

Gray MC

Li *et al*. compared different methods for calculating the average MFP, and found that extracting the average MFP from the fitting of size-dependent effective thermal conductivities well reflects the phonon ballistic effects.

$$\mathscr{L}\left(l_{\text{ave}}\right)=\sum_{t}\left|\frac{1}{3}\sum_{j}\int_{0}^{\omega_j}\frac{C_j v_{g,j} l_j}{1+\frac{4}{3}\frac{l_j}{t}}\mathrm{d}\omega-\frac{1}{1+\frac{4}{3}\frac{l_{\mathrm{avc}}}{t}}\right|^2$$

The fitted average MFP for the phonon properties of GaN calculated in this work is equal to 300 nm.

FEM with k_{eff}

$$k_{\text{eff}} = \frac{1}{3}\sum_j \int_0^{\omega_j} \hbar\omega \frac{\partial f_0}{\partial T} \text{DOS}_j(\omega) v_{g,\omega,j} l_{m,j} d\omega$$

$$l_{m,j} = \frac{l_{0,j}}{\left(1+\frac{2}{3}Kn_{t\_\omega,j}\right)\left(1+A_w\left(\frac{w_g}{w},\frac{w}{t}\right)Kn_{w\_\omega,j}\right) r_t r_{wg}}$$

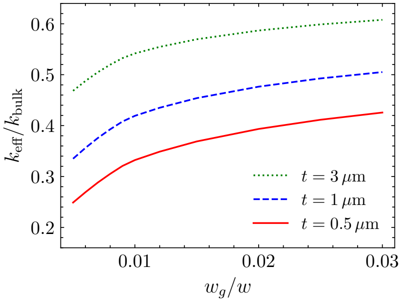

Figure 11: Model-predicted effective thermal conductivity as a function of w_g/w, with $w/t = 20$.

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Thermal Spreading Resistance

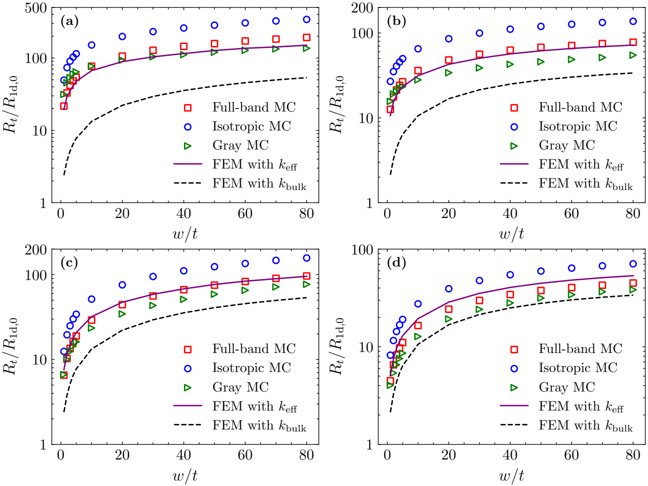


Figure 12: Dimensionless total thermal resistance as a function of w/t with (a) $t = 0.5\,\mu\text{m}$, $w_g/w = 0.005$, (b) $t = 0.5\,\mu\text{m}$, $w_g/w = 0.02$, (c) $t = 3\,\mu\text{m}$, $w_g/w = 0.005$, and (d) $t = 3\,\mu\text{m}$, $w_g/w = 0.02$.

Cross-Plane Ballistic Effect

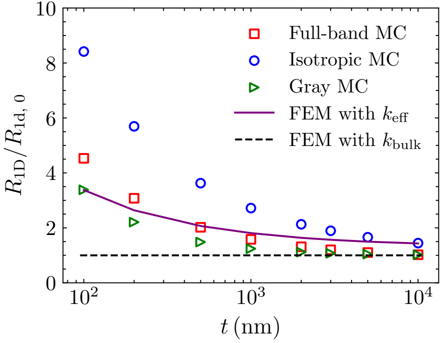
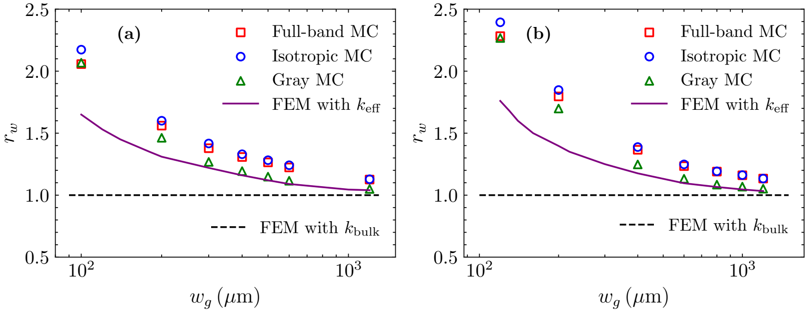


Figure 13: Dimensionless one-dimensional thermal resistance varying with layer thickness.

Lateral Ballistic Effect

$$\frac{R_t}{R_{1d\_0}} = \frac{R_F}{R_{1d\_0}} \cdot \frac{R_{1d}}{R_{1d\_0}} \cdot \left[\frac{R_t}{R_{1d}} \left(\frac{R_F}{R_{1d\_0}} \right)^{-1} \right]$$



(a) $w/t = 20$ (b) $w/t = 40$

Figure 14: Thermal resistance ratio r_w varying with the heat source width w_g, $t = 1$ µm.

Computational Efficiency

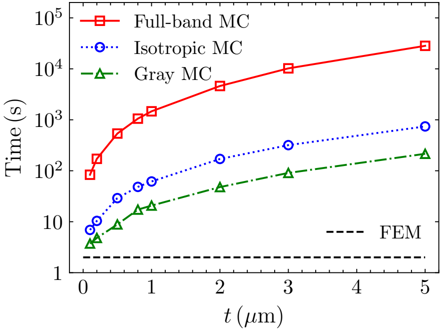


Figure 15: Computation time as a function of t, with $w/t = 40$, $w_g/w = 0.01$.

The phonon number is chosen as 10^6, which guarantees the convergence after verification.

All the simulations are programed in Python with Numba and carried out with a single processor on Apple M1 Pro chip.

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Conclusion

The first-principle-based steady-state full-band phonon tracing MC simulations are developed to investigate the thermal spreading resisatnce in GaN HEMTs.

It is found that in predicting the thermal spreading resistance,

- The empirical isotropic model can reflect the influence of phonon MFP spectrum but overestimate phonon MFPs.
- By choosing the average MFP properly, the gray-medium approximation can approximate first-principle-based predictions roughly.
- Despite the diffusive nature of Fourier's law, FEM with k_{eff} can be used as a fast approach for junction temperature predictions to guide device thermal designs.

Outlook

Finished Work

- phonon dispersion
- Bias-dependent heat generation
- First-principle-based phonon properties

On-going Work

- Hybrid Monte Carlo-diffusion simulation of GaN-on-SiC devices with full-band phonon properties and interface transmissivities

Perspective Work

- Non-equilibrium between electrons and phonons (EMC)
- Transient Simulation

Thank You!