Supplementary Information (SI) for Nanoscale.
This journal is © The Royal Society of Chemistry 2026

SUPPORTING INFORMATION

Nanoscale, temporal temperature mapping in AlN/GaN HEMTs via *ab initio* phonon Monte Carlo simulation

Liam Alexis[1], Gangchen Ren[1], Samuel Kielar[2], Jinghang Dai[1], and Zhiting Tian[1,*]

[1] *Cornell University Sibley School of Mechanical and Aerospace Engineering, Cornell University, Ithaca, New York 14853, USA*

[2] *Cornell University Department of Materials Science and Engineering, Cornell University, Ithaca, New York 14853, USA*

* Corresponding author, zt223@cornell.edu

Additional Information Regarding Interatomic Force Constant Fitting

We obtain the interatomic force constants (IFCs) by using data generated from Density Functional Theory (DFT) to train machine-learned linear models of the interatomic forces. The IFCs are then extracted from the parameters of the linear models. All DFT calculations were performed using Quantum Espresso with a plane-wave cutoff of 120 Ry using the local density approximation (LDA) and optimized norm-conserving Vanderbilt pseudopotentials (ONCVPSP) obtained from the pseudo-dojo pseudopotential repository.

First, the pristine wurtzite structures of GaN and AlN were fully relaxed. Several configurations of each of these systems were then obtained by applying small random displacements to the atoms in 6x6x4 supercells for both GaN and AlN. The interatomic forces for all of these configurations were calculated to produce training data for the linear models, which we trained using the hiPhive package. Specifically, we employed linear regression to fit the force-displacement data to obtain the 2nd- and 3rd-order IFCs for each system[1]. For GaN, cutoff lengths used for the force constant fitting were chosen to be 9.5Å and 4.3Å for the 2nd and 3rd-order terms, respectively. For AlN, these cutoffs were 9.2Å and 4.3Å. Long-range coulombic interactions were accounted for by subtracting their contribution from the harmonic IFCs prior to fitting. The long-range contribution was calculated using the Born Effective Charges and Dielectric Constant obtained from the implementation of density functional perturbation theory (DFPT) in QE. The prediction errors of the interatomic forces using these force constants was only a few meV for both wurtzite GaN and wurtzite AlN. These IFCs were then used as input for the Boltzmann Transport Equation (BTE) for phonons, for which we used a 16x16x16 q-mesh.

(**Table S1**). The chosen parameters reproduce the phonon dispersion and thermal conductivity with good agreement, suggesting that the corresponding phonon lifetimes are captured with reasonable accuracy.

Table S1: Details regarding force constant models fit to force-displacement data calculated from DFT for both wurtzite-GaN and wurtzite-AlN.

	wurtzite-GaN	**wurtzite-AlN**
Supercell Dimensions	6x6x4	6x6x4
Supercell Number of Atoms	576 atoms	576 atoms

Average Mean DFT Force per Configuration	0.76 eV/Å	0.79 eV/Å
Average Maximum DFT Force per Configuration	2.07 eV/Å	2.13 eV/Å
RMSE (Training Dataset)	2.7 meV/Å	5.4 meV/Å
RMSE (Test Dataset)	3.0 meV/Å	5.6 meV/Å

Plots of lifetimes of wurtzite GaN and wurtzite AlN

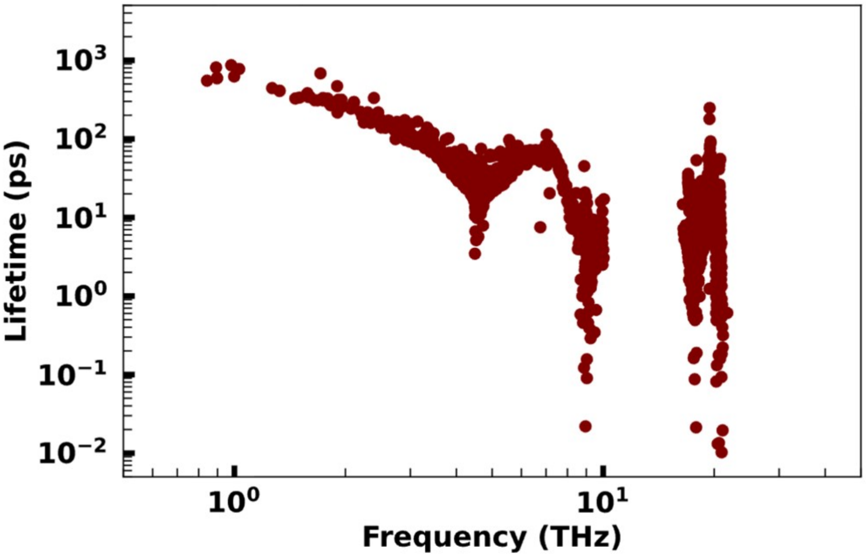

Fig. S1: Lifetimes plot for GaN

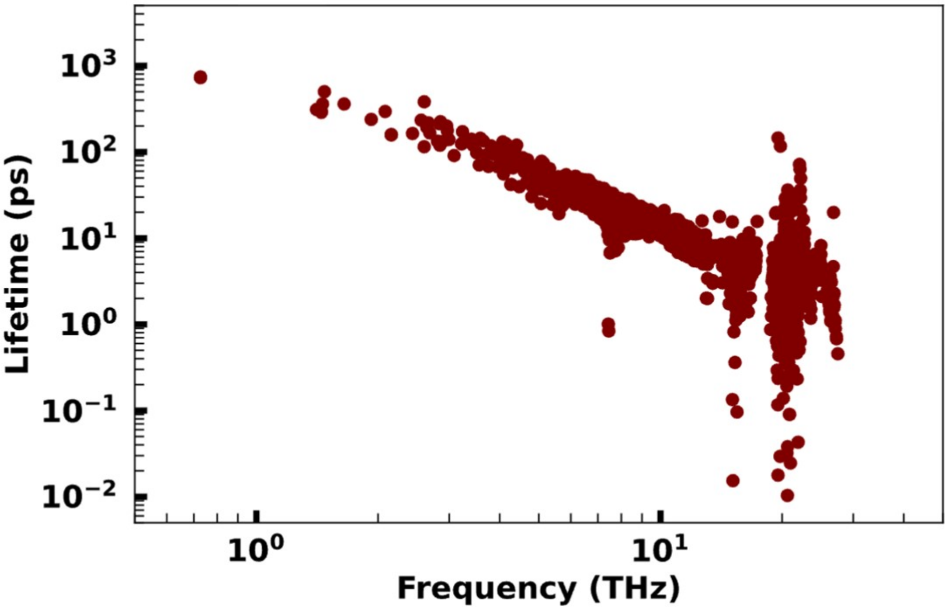

Fig. S2: Lifetimes plot for AlN

Additional information regarding GaN/AlN Interface Calculations

For bulk GaN, the cutoff energy was 60 Ryd, and the k-points mesh was 5 × 5 × 5 for the 4 × 4 × 2 supercell. For bulk AlN, the cutoff energy was 50 Ryd, and the k-points mesh was 5 × 5 × 5 for the 4 × 4 × 2 supercell.

We used the projector augmented-wave method[2] of Perdew, Burke, and Ernzerhof[3] (Al.pbe-n-kjpaw_psl.1.0.0.UPF, Ga.pbe-dn-kjpaw_psl.1.0.0.UPF and N.pbe-n-kjpaw_psl.1.0.0.UPF for the three types of elements). The resulting phonon dispersion and optimized lattice constants of AlN and GaN (**Table 2**) demonstrated strong agreement with experimental data[4].

Table S2: AlN and GaN lattice constants optimized from DFT and Experimental data.

	GaN		AlN	
	a (Å)	c (Å)	a (Å)	c (Å)
DFT optimized	3.23	5.25	3.13	5.02
Experiment data	3.19	5.189	3.11	4.98

To resolve the lattice mismatch at the AlN/GaN interface, we used 3.18 Å for the in-plane lattice constant, which was the average of optimized GaN and AlN DFT lattice constant *a*. The interface IFCs of the center regions were derived from supercells built from GaN and AlN unit cells. The total length of the supercell was 6 cells long. The cutoff energy of the interface supercell was 80 Ryd, and the k-points mesh was 5 × 5 × 1 for the 3 × 3 × 1 supercell. In AGF calculation, to represent the infinitely large transverse direction, the transverse k-points mesh was 20 × 20 in the Brillouin zone to ensure convergence.

The transmittance calculated for the whole frequency range is shown in Fig. S3. The divergence is caused by the gap in the phonon dispersion of GaN and AlN, respectively.

The interface thermal conductance (G) at a certain temperature can be calculated using the interface phonon transmission via this equation:

$$G = \frac{1}{2\pi A}\int_0^{\infty} \hbar\omega \Xi(\omega) \frac{\partial f_{B.E.}(\omega,T)}{\partial T} d\omega$$

where A is the cross-section aera, $\hbar$ is the reduced Planck constant, $\Xi(\omega)$ is phonon frequency distributed transmission plotted in Fig 3(a), ω is the phonon frequency, T is the temperature, $f_{B.E.}(\omega,T)$ is the Bose-Einstein distribution. The conductance as a function is plotted in Fig. S4. Moreover, if we do not integrate it, we can get a spectral weighted interface thermal conductance. Room temperature spectral conductance is depicted in Fig. S4.

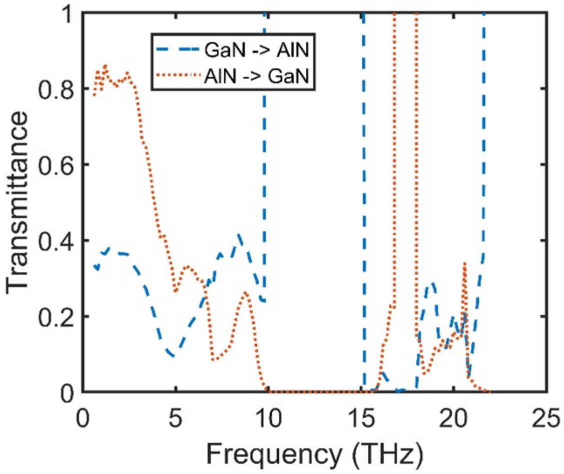

Fig. S3: Transmittance data calculated from the transmission for the full frequency range.

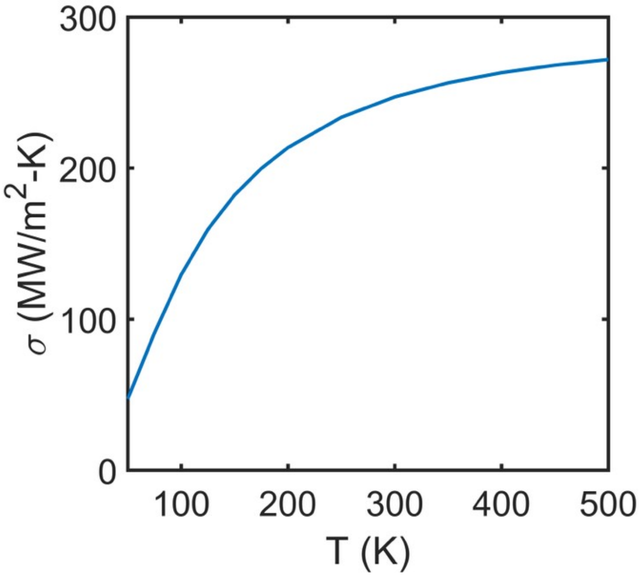

Fig. S4: The 2-probe interfacial thermal conductance of the GaN/AlN interface calculated from our AGF transmission

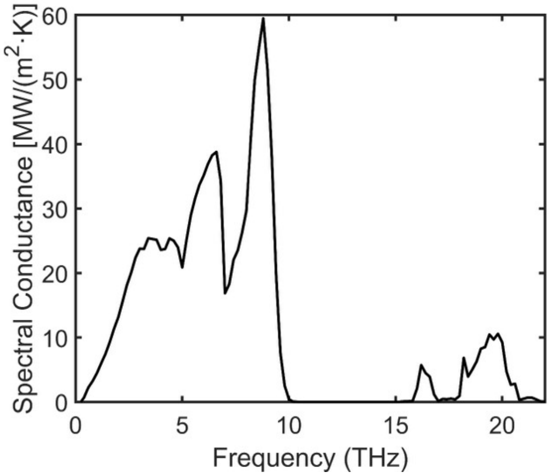

Fig S5: Room temperature spectral conductance

Additional information regarding TCAD and Monte Carlo

Our MC code was written in Python, utilizing the Numba, Scipy, and Sympy libraries. The framework was also formatted to take advantage of Numba's just-in-time (jit) parallelization functionality, increasing analysis speed.

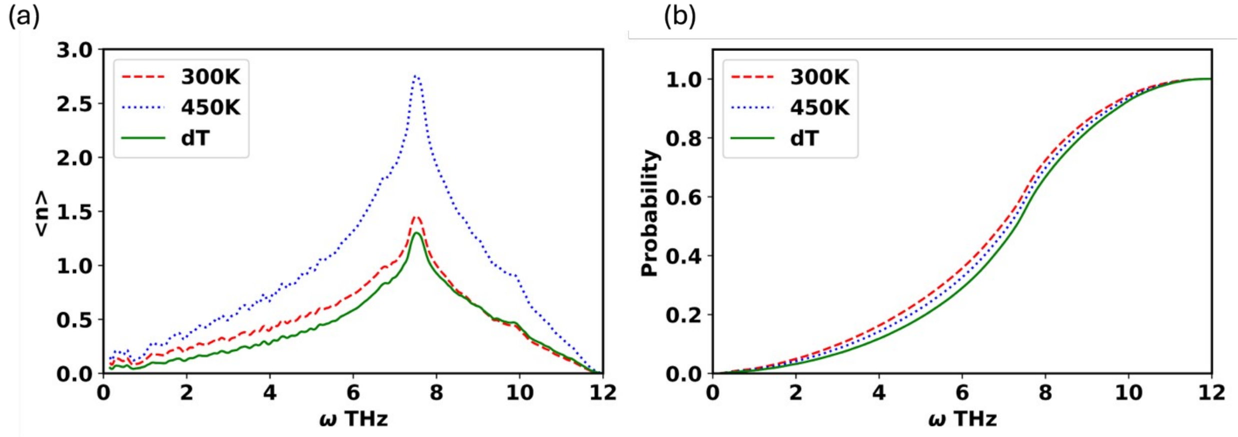

Fig S6: 300K and 450K (a) number densities and deviational number density with (b) calculated probability density function showing statistical change between original probabilities and deviational probability

TCAD workflow yields a heat flux generation volume and attached volumetric heat flux which is combined to produce the rate of heat injection into our system. Phonons are injected into the system according to the probability distribution produced via the Bose Einstein Distribution and the Density of States and until the target heat is achieved. Phonons are then oriented randomly according to the volume provided by TCAD and iterated in time undergoing drift, scattering etc.

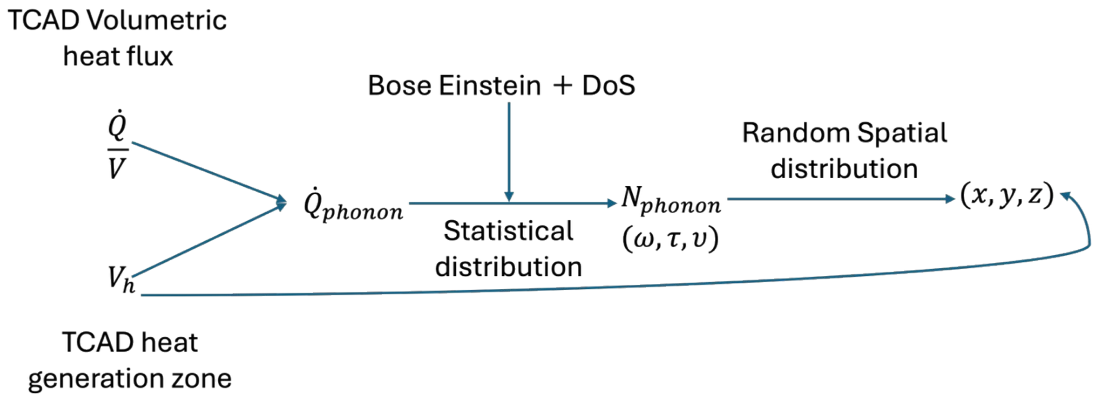

Fig S7: TCAD to MC heat flux mapping schematic

Various voltage conditions were simulated with a consistent increased temperature seen in the MC simulations compared to the TCAD. The central heating zone was always centered around the upper boundary with a steep drop off noted in the MC case but not TCAD.

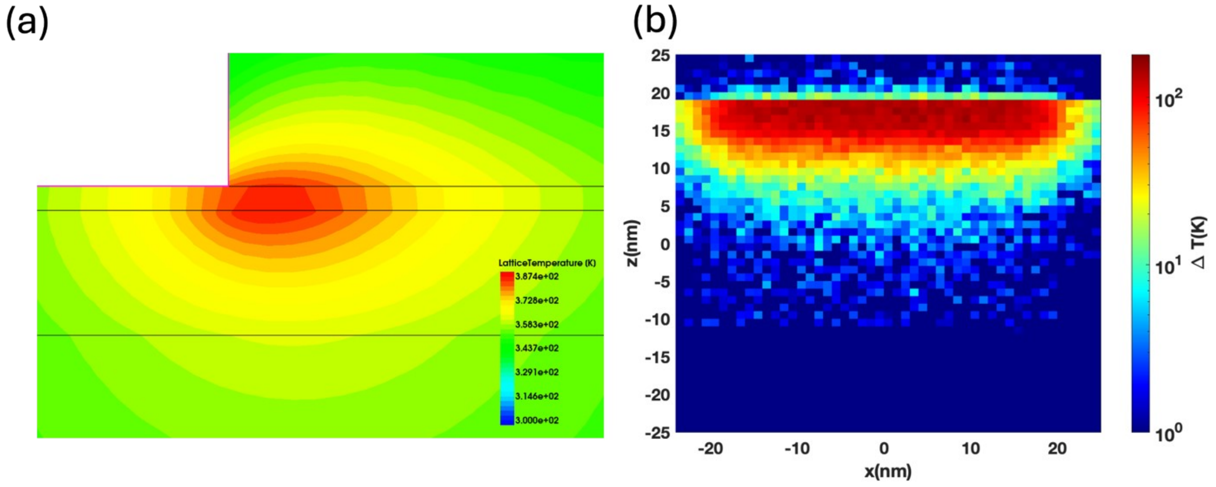

Fig S8: 6V case with **a)** a central maximum temperature of 387K observed in the TCAD case while in **b)** the MC simulation a maximum temperature of 480K was observed centered around the upper interface.

References

1. Kielar, S. *et al.* Anomalous lattice thermal conductivity increase with temperature in cubic GeTe correlated with strengthening of second-nearest neighbor bonds. *Nat. Commun.* **15**, (2024).
2. Blochl, P. E. *Projector Augmented-+rave Method*. *PHYSICAL REVIEW B VOLUME* vol. 50.
3. Perdew, J. P., Burke, K. & Ernzerhof, M. *Generalized Gradient Approximation Made Simple*. (1996).
4. Schulz, H. & Thiemann, K. H. *CRYSTAL STRUCTURE REFINEMENT OF AIN AND GaN*. *Solid State Communications* vol. 23 (1977).