

CHAPTER 2

NEAR-JUNCTION THERMAL MANAGEMENT: THERMAL CONDUCTION IN GALLIUM NITRIDE COMPOSITE SUBSTRATES

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The thermal management challenge posed by gallium nitride (GaN) high-electron-mobility transistor (HEMT) technology has received much attention in the past decade. The peak amplification power density of these devices is limited by heat transfer at the device, substrate, package, and system levels. Thermal resistances within micrometers of the transistor junction can limit efficient heat spreading from active device regions into the substrate and can dominate the overall temperature rise. Gallium nitride composite substrates, which consist of AlGaN/GaN heterostructures with thickness of a few microns on a thicker non-GaN substrate, govern the thermal resistance associated with the “near-junction” region. Silicon and silicon carbide have been widely used as a substrate material, but the performance of GaN devices grown on these substrates is still severely limited by thermal constraints and associated reliability issues. The importance of effective junction-level heat conduction has motivated the development of composite substrates containing high-thermal-conductivity diamond, but these composites require careful attention to thermal resistances between the GaN and the diamond. This chapter reviews thermal conduction phenomena in GaN composite substrates containing Si, SiC, and diamond. The review discusses the governing conduction physics and overviews the relevant measurement techniques. The best available experimental data for GaN composite substrates as well as the relevant thermal modeling are presented. The review concludes with an assessment of the potential benefits of the use of diamond on the device thermal performance.

KEY WORDS: gallium nitride (GaN), diamond, high-electron-mobility transistors (HEMTs), thermal boundary resistance (TBR), thermal interface resistance, thermal conductivity, time-domain thermoreflectance (TDTR), micro-Raman thermometry

1. INTRODUCTION

Much progress has been made in the past decade on improving thermal management of power semiconductor devices. This has been aided in part by progress on accommodating increasing power densities and hotspots in relatively low-power CMOS electronics.¹ However, there remain significant opportunities for improvement associated with technologies such as power semiconductor lasers and radar amplifiers that are still severely limited by ineffective cooling.^{2,3} Much attention has been devoted to gallium nitride (GaN) high-electron-mobility transistor (HEMT) technology, for which the peak power density is

NOMENCLATURE

b	heater half-width [m]	V_{out}	out-of-phase voltage of Rf lock-in amplifier
c	phonon propagation speed [m s^{-1}]	x	in-plane coordinates [m]
C or C_V	volumetric heat capacity [$\text{J m}^{-3} \text{K}^{-1}$]	z	cross-plane coordinates [m]
d	layer thickness [m]		
D	thermal diffusivity [$\text{m}^2 \text{s}^{-1}$]		
f_i	fractional concentration of i th atom	Greek Symbols	
$\hbar$	reduced Planck's constant [J s]	α	transmission coefficient
k	thermal conductivity [$\text{W m}^{-1} \text{K}^{-1}$]	γ	Grüneisen parameter
k_B	Boltzmann's constant [J K^{-1}]	θ_D	Debye temperature
L	heater length [m]	η	thermal conductivity anisotropy
$M, \bar{M}$	atomic mass [kg]	Λ	phonon mean free path
n	number of layers in the multilayer system	τ	phonon relaxation time
P	heating power [W]	ω	phonon angular frequency
R	thermal resistance [$\text{m}^2 \text{K W}^{-1}$]	Γ	dimensionless scattering strength
t	time [s]		
T	temperature [K or $^{\circ}\text{C}$]	Subscripts	
v_s	phonon group velocity [m s^{-1}]	B,b	boundary
V_0	unit volume for each atom [m^3]	char	characteristic
V_{in}	in-phase voltage of Rf lock-in amplifier	z	cross-plane

strongly limited by junction self-heating and associated thermal management challenges at the device, substrate, package, and system levels.^{4–7} To address this problem, the complete heat removal path from the heated electronic junction to the ambient air should be investigated to take full advantage of the intrinsic power handling capability of GaN HEMT devices. Among others, a critical challenge for heat removal is conduction of heat from the transistor junction into the substrate. High thermal resistances associated with the “near-junction” region—which is within micrometers of the transistor junction—often fundamentally limit efficient heat dissipation from the active device regions^{5,7} and strongly influence the temperature rise in the device channel.^{8–10} Device-level self-heating and associated high channel temperature rise degrade device performance and reliability.^{11–13}

Thermal transport in the near-junction region heavily relies on the material quality of GaN composites, which typically consist of AlGaIn/GaN heterostructures with thickness of a few microns on a thicker substrate. Due to the limited commercial availability of bulk GaN substrates, AlGaIn/GaN layers are heteroepitaxially grown on non-GaN substrates. The selection of substrate materials is important because (i) the substrate is a key contributor to the total conduction thermal resistance and (ii) the mismatch of the key crystalline properties (e.g., lattice constants and coefficients of thermal expansion) between the GaN and substrate creates a challenge for high-quality GaN heteroepitaxy. Much attention has been paid to SiC due to its higher thermal conductivity ($\sim 400 \text{ W m}^{-1} \text{K}^{-1}$) and lower

lattice mismatch with GaN (3.5%) than those of conventional Si and sapphire; the thermal conductivities of Si and Sapphire are ~ 142 and $\sim 35 \text{ W m}^{-1} \text{ K}^{-1}$, respectively, and the lattice mismatch is 17% for GaN-Si and 14% for GaN-sapphire.^{14–19} Recent efforts have demonstrated high-power operation exceeding 40 W/mm and high-frequency operation exceeding 300 GHz for GaN HEMTs on SiC,^{20,21} but Si is still advantageous over SiC in terms of cost and substrate size, and can also leverage well-established Si fabrication processes.¹⁸

For the heteroepitaxial growth of GaN on SiC and Si substrates, a transition layer is needed to minimize the lattice mismatch stress and enable the growth of a high-quality GaN buffer layer. An AlN transition film with thickness ranging from ~ 30 nm (Ref. 22) to 200 nm (Ref. 10) is common for GaN on SiC grown by metal-organic chemical vapor deposition (MOCVD). Much thicker and more complex transition layers are required for GaN on Si grown by MOCVD due to the much larger lattice and coefficient of thermal expansion mismatches between GaN and Si than those between GaN and SiC.^{23,24} The molecular beam epitaxy (MBE) growth of GaN on Si has recently enabled the use of a thin AlN transition layer (~ 38 nm) between the GaN and Si in contrast to complex AlGaIn/AlN transition layers in MOCVD GaN on Si.²⁵ Although all of these transition layers for GaN on SiC and Si serve to relieve the stress/strain, significant mechanical stress/strain is still present in the transition layer and near-interfacial GaN regions. Therefore, a high density of microstructural defects exists within the volume of the transition layer and near its interface, which impedes heat transport into the substrate.

At present, inefficient heat spreading from active device regions is still the limiting factor in achieving the intrinsic power handling capability offered by GaN, even with SiC substrates.^{5,26} Composite substrates made from chemical-vapor-deposited (CVD) diamond can be a compelling material solution since they can potentially offer local thermal conductivities higher by an order of magnitude than Si and by a factor of nearly five than SiC; thermal conductivity values of high-quality polycrystalline diamonds can be near $2000 \text{ W m}^{-1} \text{ K}^{-1}$ at room temperature and drop to $\sim 1200 \text{ W m}^{-1} \text{ K}^{-1}$ at 500 K.^{27–31} However, the much larger lattice mismatch between GaN and diamond (11%) compared to that between GaN and SiC (3.5%) makes diamond integration very challenging. Therefore, the current GaN-on-diamond composites also incorporate large defect concentrations or fully amorphous regions near the GaN-diamond interface, which contribute an effective thermal resistance between the GaN and the diamond and reduce the potential benefits of using the diamond substrate.

One method to integrate diamond substrates in the near-junction region involves the direct growth of GaN epitaxial layers atop single-crystal or polycrystalline diamond substrates.^{32–34} Recent studies have reported AlGaIn/GaN heterostructures directly grown on single-crystal diamond substrates in (111) or (001) orientation by using MBE³² or MOCVD.^{33,34} These composites incorporated hundreds of nanometers of transition layers—e.g., 680 nm-thick AlN/GaN multibuffer layers for the structure reported by Hirama et al.³⁴—between GaN and diamond for strain compensation. The overall thermal resistance of these composites can be large because these relatively thick transition layers are often highly disordered and therefore exhibit low thermal conductivity. An alternative method is the transfer of the AlGaIn/GaN heteroepitaxial structure to a polycrystalline diamond

substrate.^{26,35–38} In this approach, the AlGaIn/GaN heteroepitaxial layers are first grown on a Si substrate by MOCVD. Then, the Si substrate and highly resistive transition layers are etched away. The next fabrication step involves depositing a disordered adhesion layer thinner than 50 nm onto the exposed GaN buffer and growing CVD diamond of up to 100 μm on the adhesion layer. The final structure is relatively simple; from the top, the layers are an ~ 20 nm thick GaN/AlGaIn device layer, an ~ 1 μm thick GaN buffer layer, a 25–50 nm adhesion layer, and diamond. The success of this approach is governed by the thermal resistance of the disordered adhesion layer as well as the near-interfacial diamond, both of which are subject to optimization at present.^{37–39}

This chapter reviews thermal transport physics and relevant thermal properties in GaN composite substrates containing Si, SiC, and diamond for HEMT applications and predicts the potential improvement available through the use of diamond on the temperature rise of the device channel. Section 2 develops a semi-analytical simulation approach for the temperature rises at different length scales, with the goal of providing a more rapid and flexible simulation process than is available through conventional finite element software. Section 3 covers the fundamental physics involved with thermal transport in GaN composite substrates. Special attention is paid to the phonon transport and scattering phenomena that govern the thermal conductivity of GaN and the thermal resistance at the interface between the GaN and substrate. Section 4 discusses thermal property measurement methods, with a focus on those relevant to GaN composite substrates. The best available experimental data for thermal properties in GaN composites are summarized in Section 5, which also discusses the impact of boundary and imperfection scattering on the intrinsic and interface thermal transport phenomena. The review concludes with comments on the improvements in thermal properties—in particular the GaN-substrate thermal interface resistance—required for future advances.

2. IMPACT OF NEAR-JUNCTION THERMAL TRANSPORT ON THE TRANSISTOR TEMPERATURE

The geometry and thermal properties of the complex multilayer structure in GaN HEMT devices govern the conduction thermal resistance and the device channel temperature rise. The thermal boundary resistance (TBR) at each interface also contributes significantly to the total conduction thermal resistance and can cause a sizeable additional channel temperature rise.^{8–10} Successful design of the GaN HEMT therefore requires a comprehensive understanding of the impact of the constituent layers and interfaces on the channel temperature rise. An additional geometric complication is that modern HEMTs often employ a compact multifinger configuration for high-power operations. Previous experiments have measured the temperature rises in the channel region using photocurrent measurement⁴⁰ and in the multifinger and package level using micro-Raman thermometry.⁴¹ However, a modeling approach is still needed that can be used to examine scaling effects and the impact of substrate material and boundary resistance. This section describes a compact and flexible thermal model that can predict the effect of composite substrates on cooling of HEMT devices with varying lateral length scales. A comparison of the thermal performances of diamond- and SiC-based composite substrates with different configurations suggests the

potential benefits of using diamond to improve the near-junction cooling of GaN HEMT devices.

2.1 Numerical Model

Overall thermal resistances of a GaN HEMT device are dominated by different components in the HEMT multilayer structure, depending on different characteristic lateral length scales of the heated region. In order to study the complex heat conduction at variable lateral length scales, we present here a numerical algorithm that models the multilayer HEMT structure, as shown in Fig. 1, and is based on an extended version of the matrix formulation developed by Feldman.⁴² This quasi-closed-form methodology is better suited for this study than the general-purpose commercial FEA software due to its ability to quickly modify the complex HEMT geometries with anisotropic and temperature-dependent material properties. It performs the thermal simulations for both steady-state and transient conditions using much less computing time.

Layer 1 corresponds to a semi-infinite medium (usually air), and layers 2 to n represent the different compositions of the HEMT structure such as the GaN/AlGaIn device layer, the GaN buffer layer, and the AlGaIn and/or AlN transition layer. The HEMT channel region lies between layers 1 and 2, where an AC heating power is injected into the heated area. The bottom layer $n + 1$ stands for the semi-infinite substrate. This bottom boundary condition recognizes the fact that the substrate is usually much thicker than the other films as well as the channel length. The measured or best-known temperature-dependent material properties are used for each layer, as well as for the thermal boundary resistances (TBRs) in between. We refer the reader to Section 5 for a comprehensive review of the material properties of GaN composite substrates.

The code finds the temperature rise averaged over the heated area by solving the time-domain, 2D heat diffusion equations as follows:

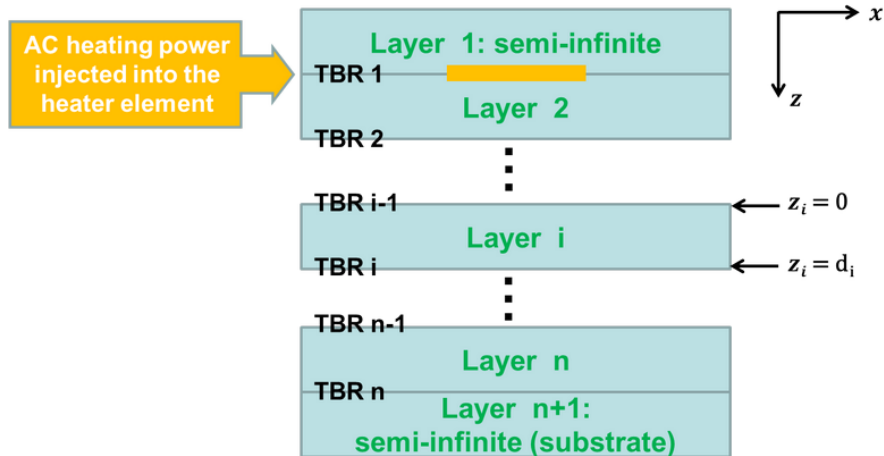


FIG. 1: Multilayer HEMT model for thermal simulation. The heating power is injected into a heater element with varying dimensions.

$$\frac{1}{D_i} \frac{\partial T_i}{\partial t} = \eta_i \frac{\partial^2 T_i}{\partial x^2} + \frac{\partial^2 T_i}{\partial z_i^2} \quad (1)$$

$$k_{1,z} \frac{\partial T_1}{\partial z_1} \Big|_{z_1=d_1} - k_{2,z} \frac{\partial T_2}{\partial z_2} \Big|_{z_2=0} = \frac{P}{2bL} e^{-j2\omega t} \quad (2)$$

$$-k_{i,z} \frac{\partial T_i}{\partial z_i} \Big|_{z_i=d_i} = -k_{i+1,z} \frac{\partial T_{i+1}}{\partial z_{i+1}} \Big|_{z_{i+1}=0} = \frac{T_i|_{z_i=d_i} - T_{i+1}|_{z_{i+1}=0}}{R_{b,i}} \quad (3)$$

In Eqs. (1)–(3), the subscript i denotes the i th layer from the top, and n is the total number of layers. Geometric parameters b and L are the half-width and the length of the heater, respectively; $k_{i,z}$ is the cross-plane thermal conductivity of the i th layer, and $R_{b,i}$ is the TBR for the interface between layer i and $i + 1$. The thermal conductivity anisotropy is defined as $\eta = k_x/k_z$. The heating power P is injected at the boundary between layers 1 and 2. A recursive algorithm solves these equations and finds the average temperature rise ΔT in the heater using an extended version of the matrix formulation method developed by Feldman.⁴² A very low frequency (e.g., 0.1 Hz) essentially simulates the steady-state temperature rise under DC heating.

There are two aspects to consider further in the above-mentioned model. First, the code assumes a semi-infinite substrate, but a more realistic setup would be a finite-thickness substrate with a fixed temperature at its bottom boundary. We therefore need to check the conditions on which this assumption of a semi-infinite substrate is valid. Second, the implementation of the numerical model involves extensive mathematical operations, including recursive matrix transformations. We need to check the correctness of the code in the DC limit of a frequency-domain solution. To determine the accuracy of our model, we compare the results from our quasi-analytic model, calculations using a commercial FEM package (COMSOL), and experimental data from micro-Raman thermometry of a similar structure.⁴¹ We find that they agree reasonably well for length scales of $<100 \mu\text{m}$, as shown in Fig. 2. The semi-infinite assumption of the substrate becomes invalid when the heater length scale is $>100 \mu\text{m}$, resulting in $\sim 20\%$ difference between our simplified model and a full numerical solution using COMSOL. Figure 3 further confirms the accuracy of our modeling approach. Our DC Joule heating and electrical resistance thermometry measurements on a GaN-diamond composite substrate are compared with our model (we refer the reader to Section 4.1 for additional details of the measurement). The GaN buffer dominates the temperature rise in this sample, and reasonable agreement is obtained using thermal conductivity data for the GaN measured by independent time-domain thermoreflectance (TDTR) technique.

2.2 HEMT Thermal Resistance Decomposition

The spatial temperature distribution of HEMT devices depends on the characteristic lateral length scale of the heating source. Although the specific dimensions of current multifinger HEMT devices vary, one can generally divide the characteristic lateral length scales into three levels: (i) $<1 \mu\text{m}$, (ii) $1\text{--}100 \mu\text{m}$, and (iii) $>100 \mu\text{m}$. Because of the difference in characteristic length scales compared to the thickness of the underlying layers, the overall

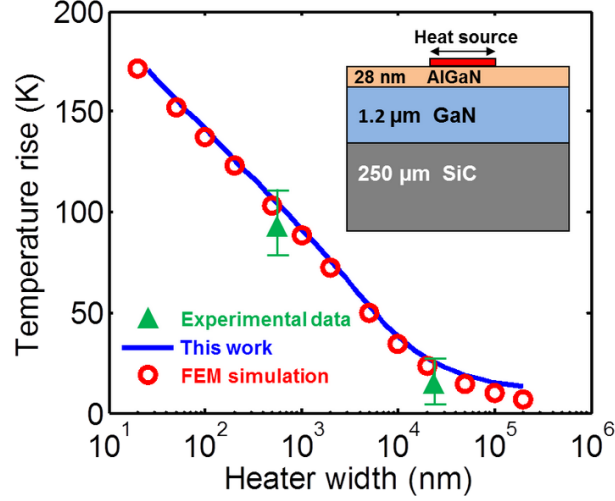


FIG. 2: Comparison of the semi-analytical HEMT thermal model with finite element method (FEM) simulation (COMSOL) and the experimental data from Kuball et al.⁴¹ Our simplified model achieves good agreement for lateral length scales of $<100 \mu\text{m}$.

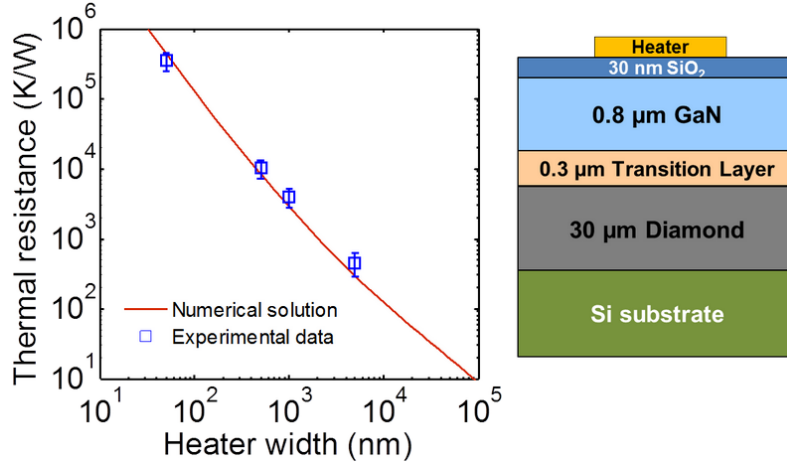


FIG. 3: Simulated and measured thermal resistances seen by different heating sources on a multilayer HEMT test structure. The experimental data are taken by DC Joule heating and electrical resistance thermometry using variable heater widths.

thermal resistance seen by each of these three levels differs significantly. Figure 4 shows the thermal resistance decomposition of the HEMT multilayer stack, and quantifies its contributions to the overall temperature rise in these three levels.

When the heater length scale is $<1 \mu\text{m}$, 2D heat spreading within the GaN buffer dominates the temperature rise of the hotspot in the channel region, as shown in Fig. 4. The volumetric thermal resistance of the GaN buffer accounts for $>50\%$ of the overall thermal resistance seen by a heat source at this length scale. The thermal resistance of the

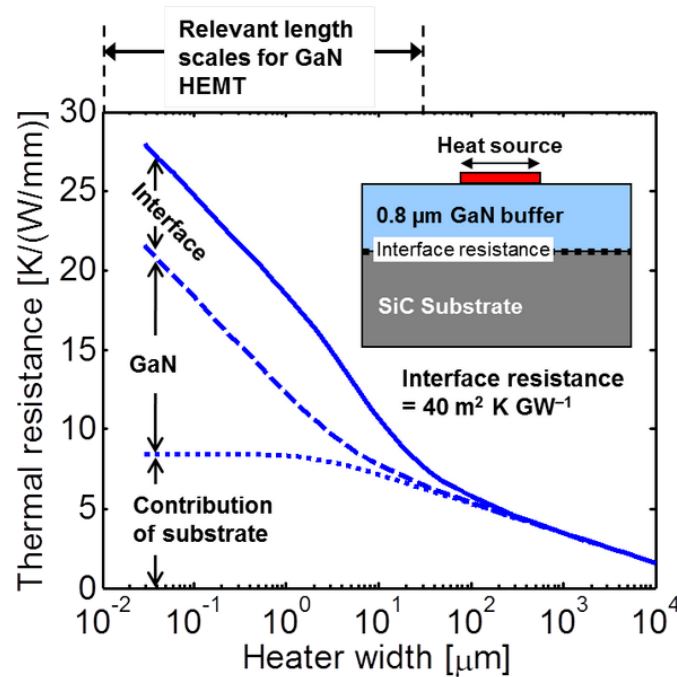


FIG. 4: Thermal resistance decomposition. The GaN layer and thermal interface resistance are the major contributors to the total thermal resistance for lateral length scales (associated with heat source) of $<100\ \mu\text{m}$, while the substrate spreading resistance dominates for length scales of $>100\ \mu\text{m}$.

substrate starts to be comparable to that of the GaN buffer when the heater length scale exceeds $1\ \mu\text{m}$. As the heater length scale becomes very large (i.e., $>100\ \mu\text{m}$), the substrate thermal resistance becomes dominant. The thermal interface resistance between the GaN buffer and the substrate also affects the channel temperature rise for heater length scales of $<100\ \mu\text{m}$ but becomes almost irrelevant for length scales of $>100\ \mu\text{m}$. The relevant length scale of a single-finger hotspot in GaN HEMT is approximately $0.5\text{--}1\ \mu\text{m}$.⁴³ A multifinger GaN HEMT may span $>100\ \mu\text{m}$ but the region of heat generation is several hotspots, each of which is $\sim 1\ \mu\text{m}$ long. Therefore, a lower thermal resistance GaN buffer and a lower thermal resistance at the GaN-substrate interface help reduce the channel temperature in the single-finger and multifinger hotspots below the gates, while a more thermally conducting substrate lowers the average temperature of the overall HEMT package. Since the GaN buffer layer is fairly standard in all GaN HEMT devices, the following section explores the more interesting impacts of the substrate.

2.3 Comparison of SiC and Diamond Substrates

The increasing power density of HEMT devices demands higher thermal conductivity substrates, such as CVD diamond, which are more effective than SiC for heat extraction; thermal conductivity values of high-quality polycrystalline diamonds are near $2000\ \text{W m}^{-1}\text{K}^{-1}$.

K^{-1} at room temperature,^{27–31} whereas SiC thermal conductivity values range from 271 to $390 \text{ W m}^{-1} \text{ K}^{-1}$ at room temperature.^{15–17,19} Figure 5(a) compares the simulated channel temperature rise of a HEMT device on SiC and diamond substrates. Two diamond configurations are considered: one with an $\sim 1 \mu\text{m}$ thick AlGaN/AlN transition layer between the GaN buffer and diamond and one without this transition layer. For the diamond configuration with the transition layer, the thermal conductivity of $16 \text{ W m}^{-1} \text{ K}^{-1}$ is assumed

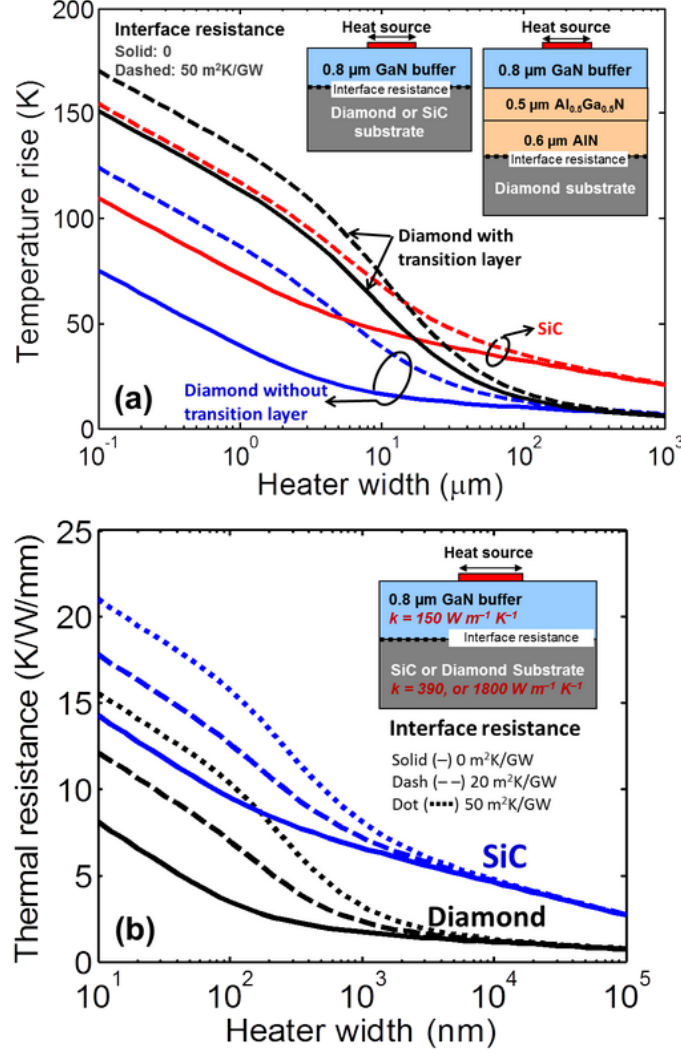


FIG. 5: (a) Simulated channel temperature rises of HEMT devices on SiC, diamond with transition layer, and diamond without transition layer with variable lateral length scales for a power dissipation of 6 W/mm . (b) Simulated thermal resistances of HEMT devices on SiC and diamond without transition layer with variable length scales at the same power dissipation level. (a,b) Inset: schematics of the HEMT structures. Figures are not drawn to scale.

for the 0.5 μm thick AlGaIn transition layer and the thermal conductivity of $30 \text{ W m}^{-1} \text{ K}^{-1}$ is assumed for the 0.6 μm thick AlN transition layer.³⁷ A disordered adhesion layer (thinner than 50 nm) is modeled as a thermal interface resistance for both configurations. The SiC configuration we consider involves an ~ 40 nm thick AlN transition layer between the GaN and SiC; the intrinsic resistance of the AlN layer and the TBRs at its boundaries are lumped into a GaN-SiC thermal interface resistance. The simulation assumes a range of thermal interface resistances from 0 to $50 \text{ m}^2 \text{ K GW}^{-1}$, based on the literature data (see Section 5.2).

When the heater length scale is very large ($>100 \mu\text{m}$), both diamond configurations result in a 70% lower temperature rise than occurs in the SiC. This large characteristic length scale induces almost 1D heat conduction through the layers into the substrate; the performance therefore remains unaffected by the presence/absence of the transition layer. When the heater length scale is $<20 \mu\text{m}$, the diamond substrate with the transition layer yields higher channel temperature rises than the SiC does. This is because the heat is mostly confined within the GaN buffer and transition layers, reducing the effectiveness of the diamond substrate; the relatively low thermal conductivity of the transition layer significantly increases the thermal resistance between the GaN and diamond. Therefore, the benefit of removing the transition layer from the diamond configuration is clear. Comparing diamond composite substrates with and without the transition layer, up to 52% reduction in the temperature rise can be achieved for heater length scales from $<1 \mu\text{m}$ to tens of micrometers (length scales that are relevant for most GaN HEMT devices) by removing the transition layer [see blue and black curves in Fig. 5(a)]. A comparison of the diamond substrate without the transition layer to the SiC substrate suggests that a GaN-diamond thermal interface resistance below $\sim 30 \text{ m}^2 \text{ K GW}^{-1}$ allows the diamond substrate to outperform the SiC substrate even with zero interface resistance on all the characteristic length scales [see Fig. 5(b)]. Therefore, the interface resistance of $30 \text{ m}^2 \text{ K GW}^{-1}$ should be a target resistance to achieve for diamond composite substrates.

3. GOVERNING CONDUCTION PHYSICS AND THERMAL MODELING

Thermal conduction in GaN composite substrates is predominantly due to phonon transport and, more specifically, to those phonons in the acoustic branches. Gallium nitride composites contain semiconductor layers with multiple interfaces, which add scattering sites for phonons and render the interpretation of heat conduction data far more challenging. The conduction resistances of GaN composites include (i) the thermal resistance of the GaN buffer layer, (ii) the thermal resistance at the GaN-transition layer interface, (iii) the thermal resistance of the transition layer, (iv) the thermal resistance at the transition layer-growth substrate interface, and (v) the spreading resistance of the growth substrate. Resistances ii–iv are grouped into a single resistance associated with the transition layer, and what has been reported in the literature is actually the sum of boundary and internal resistances; this lumped resistance is often referred to as the (effective) thermal boundary resistance of the GaN-substrate interface,^{8–10} the effective resistance of the transition film,⁴⁴ or the GaN-substrate thermal interface resistance.²² In this context, it is referred to as the latter. In this approach, the total conduction resistance of GaN composites can be

divided into three contributions: the intrinsic GaN thermal resistance, the GaN-substrate thermal interface resistance, and the substrate thermal resistance. This section provides a brief overview of conduction physics and thermal modeling for both the GaN thermal conductivity and the GaN-substrate thermal interface resistance.

3.1 GaN Thermal Conductivity

Kinetic theory provides a simple model of the lattice thermal conductivity k , which considers the volumetric heat capacity C , the average acoustic phonon velocity v_{avg} , and the phonon mean free path (MFP) Λ or phonon relaxation time τ

$$k = \frac{1}{3} C v_{\text{avg}} \Lambda = \frac{1}{3} C v_{\text{avg}}^2 \tau \quad (4)$$

Although this simple model lumps together the contribution of all phonons (the phonon MFPs are all assumed to take the same value, which is known as “the gray approximation”), it clearly indicates the important role played by the MFP (or the relaxation time) of phonons in the lattice thermal conductivity. Phonons in crystalline semiconductors do not follow the gray approximation because they have a broad distribution of MFPs (e.g., at room temperature, the MFPs of phonons in bulk GaN range from tens of nanometers to a few micrometers).⁴⁵ Because the GaN buffer layer is $\sim 1 \mu\text{m}$ thick in typical GaN composites, this implies that the GaN film in composite substrates possess lower thermal conductivity than bulk GaN due to phonon boundary scattering. Therefore, knowledge of the phonon MFP spectrum—the MFP dependent contributions of phonons to thermal conductivity^{45,46}—is important to accurately predict the impact of boundary scattering (i.e., the size effect) on the thermal conductivity of the GaN buffer layer.

In addition to boundary scattering, phonon scattering on crystalline imperfections can be particularly important in GaN composites, since the GaN heterostructure is often highly defective. Heteroepitaxy of GaN on SiC, Si, and diamond often involves significant mechanical stress/strain and the associated high densities of defects in the GaN and transition layer; this is due to the large lattice mismatch and differing thermal expansion coefficients between GaN and the substrate as discussed in Section 1. Several transmission electron microscopy (TEM) investigations of GaN/AlN/SiC structures have revealed high densities of dislocations on the order of 10^8 – 10^9 cm^{-2} in the GaN and 10^{10} – 10^{12} cm^{-2} in the AlN.^{47–50} These studies observed that highly defective regions exist near the GaN/AlN and AlN/SiC interface and within the AlN transition layer and that the density of dislocations in the near-interfacial GaN can be higher than near the top. Reitmeier et al.⁴⁷ argued that the initial AlN layers on the SiC substrate are non-stoichiometric and thus contain a very high density of point defects, which leads to a high density of dislocations in the AlN transition layer and in the near-interfacial volume of the GaN layer. Faleev and Levin⁵¹ also suggested that point defects (e.g., vacancies or interstitial atoms) are generated near the growth surface during epitaxial growth and that their inward diffusion and structural transformation lead to the creation of clusters of point defects, dislocations, stacking faults, or other types of defects in the volumes of the epilayers. Their transmission electron microscopy examination of two GaN/AlN/SiC composites

—prepared using metal-organic chemical vapor deposition (MOCVD) and hydride vapor phase epitaxy (HVPE), respectively—revealed that no planar defects exist in the MOCVD-grown sample whereas in the HVPE-grown sample high densities of stacking faults exist in both GaN and AlN layers.

Phonon scattering on film boundaries and various types of imperfections can be taken into account in the framework of the semiclassical phonon thermal conductivity integral, which was originally developed by Callaway⁵² from an approximate solution to the phonon Boltzmann transport equation (BTE). Many modeling efforts have used modifications to the Callaway⁵² phonon conductivity integral model to compute the lattice thermal conductivity of wurtzite GaN.^{44,49,53–58} Unlike the simple model in Eq. (4), these models consider the phonon dispersion relations and the frequency-dependent phonon relaxation times. In some variations of the Callaway model,^{54,56,57} the mode-dependent phonon relaxation times are considered; the contributions of longitudinal and transverse phonons are separately treated. Equation (5) shows one implementation of the Callaway model assuming a Debye dispersion relation (isotropic and linear) for a single, triply degenerate acoustic-phonon branch^{44,53,55}

$$k = \left(\frac{k_B}{\hbar} \right)^3 \frac{k_B}{2\pi^2 v_s} T^3 \int_0^{\theta_D/T} \frac{\tau x^4 e^x}{(e^x - 1)^2} dx \quad (5)$$

Here, k_B is the Boltzmann constant, $\hbar$ is Plank's constant divided by 2π , v_s is the phonon group velocity, θ_D is the Debye temperature, τ is the phonon relaxation time, and $x = \hbar\omega/k_B T$ is the dimensionless phonon frequency. Callaway's k_2 correction term⁵² is often neglected since this term is only important for very pure, defect-free materials.^{44,46,53,55} The total phonon scattering rate τ^{-1} is determined by combining the relevant scattering rates through Matthiessen's rule (i.e., $\tau^{-1} = \sum_i \tau_i^{-1}$, where τ_i^{-1} represents the scattering rate corresponding to the i th process relevant to a given material system). As discussed above, boundary scattering (τ_B), point defect scattering (τ_P), dislocation scattering (τ_D), as well as Umklapp scattering (τ_U) should be considered for GaN buffer films in composite substrates at temperatures relevant to the operation of power transistor devices.

The Umklapp phonon scattering rate is modeled using

$$\tau_U^{-1} = BT\omega^2 \exp\left(-\frac{C}{T}\right) \quad (6)$$

where B and C are adjustable parameters determined by fitting to bulk GaN data.^{44,54–57} Here, B is given by

$$B = \frac{\hbar\gamma^2}{Mv_s^2\theta_D} \quad (7)$$

where γ is the Grüneisen parameter and M is the average mass of an atom in the crystal. Phonon scattering by point defects is typically treated using the Rayleigh model, where the scattering rate scales with the fourth power of the phonon frequency (the inverse fourth power of the phonon wavelength). Localized impurities and vacancies are therefore highly effective at scattering high-frequency phonons but are much less effective at scattering

low-frequency phonons. In this treatment, the point defect scattering rate can be approximated using

$$\frac{1}{\tau_P} = \frac{V_0 \Gamma \omega^4}{4\pi v_s^3} \quad (8)$$

where V_0 is the unit volume for each atom and Γ represents the strength of the point defect scattering.^{44,53,54,59,60} The most commonly used form for the point defect scattering strength is based on Klemens' perturbation theory⁵⁹ and mainly considers the difference between the mass of the substitutional atom and the average atomic mass^{54,58,60}

$$\Gamma = \sum_i f_i \left(\frac{M_i - \bar{M}}{\bar{M}} \right)^2 \quad (9)$$

where f_i is the fractional concentration of the i th species, M_i is the atomic mass of the i th species, and $\bar{M} = \sum_i f_i M_i$ is the average atomic mass. In addition to the mass-difference-induced scattering, the above form of the scattering strength can also include the impact of the elastic strain field of point defects.^{53,55,56} Phonon scattering by dislocations includes the scattering either by the elastic strain field of the dislocation lines or by the cores of the dislocation lines.⁵³ The phonon scattering rate by the strain field of the dislocations is linearly proportional to the phonon frequency, while the scattering rate at the cores of the dislocations scales with the third power of the frequency.⁵³ Su et al.⁴⁹ assumed in their thermal conductivity model that the MFP of phonons due to dislocations is limited to the average distance between dislocations (i.e., is independent of the phonon frequency). One simple but commonly used model for the boundary scattering rate is given in the Casimir limit as $\tau_B^{-1} = v_s/L$, where L is the sample dimension; for GaN buffer films in composite substrates, the film thickness defines L . We refer the reader to a review by Marconnet et al.⁶¹ for a more fundamental and broad treatment of phonon boundary scattering in several nanostructures, including thin films. Equations (5)–(9) and the above form of the boundary scattering rate together can account well for both the magnitude and the temperature dependence of the thermal conductivity of GaN buffer films in composite substrates as well as the bulk GaN thermal conductivity.⁴⁴

Beyond the above-mentioned semiclassical BTE approach, there have been recent successes in using atomistic simulations (e.g., first principles calculations) to predict the thermal conductivity of simple bulk crystals such as Si, GaN, and GaAs.^{62–66} These calculations have also shown that the phonon MFPs relevant to thermal conductivity at room temperature range from a few nanometers to as large as 100 μm (i.e., span five orders of magnitude) in Si⁶³ and from a few nanometers to several micrometers (i.e., span three orders of magnitude) in GaAs.⁶⁶ A theoretical study on MFP spectra of bulk Si has shown that phonon MFP distributions predicted by molecular dynamics and first principles calculations differ from those predicted by the semiclassical BTE approaches.⁴⁶ Many attempts have been made to apply such atomistic approaches to thermal conduction phenomena in material systems relevant to GaN composite substrates; we refer the reader to Section 3.4 for a review of these efforts. Such atomistic calculations complement the semiclassical BTE methods and with further advances should allow rigorous treatment of the impacts of defects and boundaries on thermal conductivity in nanostructures.

3.2 Thermal Boundary Resistance

Thermal boundary resistance (TBR)—which occurs due to incomplete transmission of heat carriers across an interface—can contribute significantly to conduction thermal resistance in thin film electronic devices, including GaN-based transistor devices. Since a comprehensive review of TBR by Swartz and Pohl⁶⁷ for solid-solid interfaces, there have been extensive efforts to model TBR, including the acoustic mismatch model (AMM) and the diffuse mismatch model (DMM)^{67,68} and their modifications.^{69–74} The AMM and DMM are the most commonly used theoretical models for predicting TBR. Both models assume that phonons dominate the boundary thermal transport, which is strictly valid for nonmetal interfaces (e.g., interfaces between dielectrics or lightly doped semiconductors). Both models also assume elastic phonon boundary scattering and Debye linear phonon dispersion.⁶⁷ The AMM assumes specular phonon reflection and transmission at the interface, an assumption that is valid at low temperatures (when the dominant phonon wavelength is long) and at perfect interfaces.^{67,69} Thus, the AMM provides reasonable agreement with experimental data at temperatures of <10 K,^{67,69} where specular scattering is probable. The DMM is more forgiving of the interface quality and assumes diffuse phonon reflection and transmission at the interface, and hence provides better agreement with experimental data at higher temperatures.^{67,69} However, at room temperature and above, DMM predictions are typically lower than experimental data for both high-quality interfaces^{71,75} and disordered interfaces.^{22,73}

For GaN composites, it is of interest to determine the theoretical lower limits of the TBR for GaN on various substrates. The DMM provides a realistic lower bound at room temperature and above where phonons have wavelengths in the sub-nm range.⁷⁶ Bellis et al.⁶⁹ modified the original DMM to account for the actual density of states (DOS)—the original model assumes the Debye DOS in both contacting solids—by using the measured volumetric heat capacity data. This form of the model has found its utility in modeling TBR at room temperature and above for a variety of interfaces,^{22,77–79} and is given by

$$R_b = \left(\frac{\alpha_{1 \rightarrow 2}}{12} c_{1D}^3 \sum_j c_{1,j}^{-2} \right)^{-1} C_1(T)^{-1} \quad (10)$$

where R_b is the TBR, $C_1(T)$ is the measured heat capacity of material 1 at temperature T , $c_{i,j}$ is the phonon propagation speed through material i for the j th phonon mode, and c_{1D} is the average phonon propagation speed in material 1.⁶⁹ The transmission coefficient $\alpha_{1 \rightarrow 2}$ quantifies the percentage of phonons that transmits from material 1 to material 2, and hence transfer thermal energy, and is given by a ratio of the phonon speeds in each material,

$$\alpha_{1 \rightarrow 2} = \frac{\sum_j c_{2,j}^{-2}}{\sum_j c_{1,j}^{-2} + \sum_j c_{2,j}^{-2}} \quad (11)$$

Table 1 summarizes the room temperature lower limits of the TBR between GaN and three different substrates (Si, SiC, and diamond), predicted by Eqs. (10) and (11).

TABLE 1: Room temperature thermal boundary resistances (TBRs) between GaN and three different substrates (Si, SiC, and diamond), predicted by the diffuse mismatch model (DMM) with the measured heat capacity modification [see Eqs. (10) and (11)]. These values set the theoretical lower limits of the TBR for three GaN composite substrates

Composite substrate	DMM prediction [$\text{m}^2 \text{ K GW}^{-1}$]
GaN on Si	0.8
GaN on SiC	1.1
GaN on diamond	3.0

3.3 GaN-Substrate Thermal Interface Resistance

The actual interface in GaN composites involves the transition layer between the GaN buffer layer and the substrate (Si, SiC, and diamond). The GaN-substrate thermal interface resistance is therefore not the discrete interface resistance discussed in Section 3.2, but rather involves intricate resistance mechanisms. Figure 6 illustrates the mechanisms

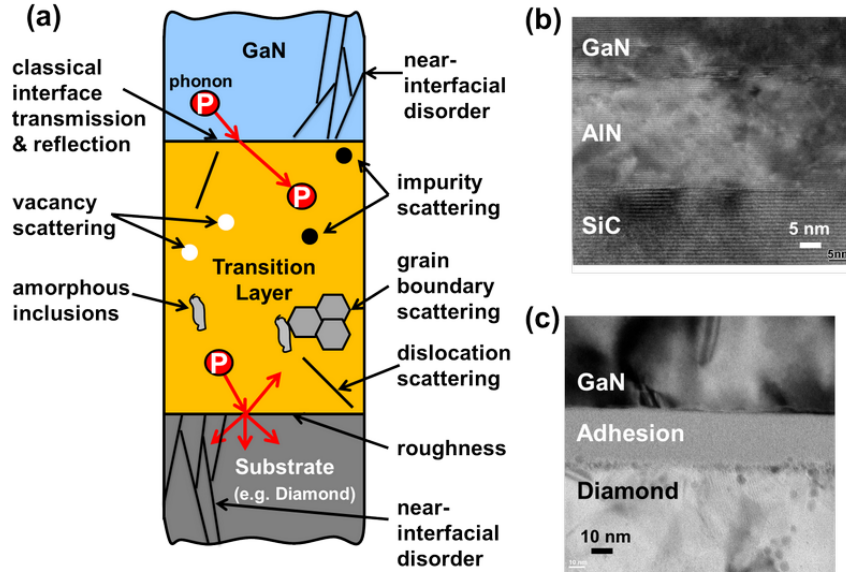


FIG. 6: (a) Physical mechanisms governing the interface thermal resistance in GaN composite substrates. At present, the resistance is still governed by thermal resistances associated with phonon scattering on crystal imperfections rather than discrete phonon scattering at interfaces. Heteroepitaxy of GaN on SiC is generally achieved with a strained AlN transition layer, while GaN heteroepitaxy on Si involves much thicker and more complex transition layers. For GaN on diamond, the best transition layer is a subject of vigorous research. (b,c) Representative cross-sectional transmission electron micrographs near the GaN-substrate interface of GaN on SiC and GaN on diamond, respectively.

responsible for the GaN-substrate thermal interface resistance: (i) phonon scattering at the transition layer boundaries with the GaN and substrate, (ii) phonon-phonon Umklapp scattering and phonon scattering on point defects, dislocations, and other defects within the volume of the transition layer, and (iii) phonon scattering by near-interfacial disorder in the GaN and substrate. These mechanisms are often not possible to separate experimentally and can also be coupled in quasi-ballistic phonon transport study.^{44,80–82} The three contributions are therefore lumped and represented as a single effective interface resistance, as described earlier.

A theoretical model based on an approximate solution to the phonon Boltzmann transport equation (BTE) can predict the GaN-substrate thermal interface resistance in composite substrates, accounting for potential sources of phonon scattering within the volume of the transition layer and acoustic mismatch at its two boundaries with the GaN and the substrate.⁴⁴ For phonon transport normal to a homogeneous and defective thin film, this model is given by

$$\frac{1}{R_{\text{GaN-Substrate}}} = \frac{v_s}{3} \int_0^{\theta_D/T} \frac{C_V(x, T)}{(d/v_s)\tau^{-1} + (4/3)[(1/\alpha_0) + (1/\alpha_1) - 1]} dx \quad (12)$$

where $R_{\text{GaN-Substrate}}$ is the GaN-substrate thermal interface resistance and d is the transition layer thickness.⁴⁴ Phonon scattering rates on point defects, dislocations, and/or other types of disorder within the transition layer volume are combined into the total phonon scattering τ^{-1} by Matthiessen's rule. The phonon specific heat function $C_V(x_\omega, T)$ can be found in Goodson et al.⁸³ The DMM [see Eq. (11)] predicts the possibility of phonon transmissions from within the transition layer into the GaN and the substrate, which are α_0 and α_1 , respectively. The definition of other variables can be found in Eq. (5) in Section 3.1.

Of greater interest is the temperature dependence of the GaN-substrate thermal interface resistance at temperatures relevant to the operation of power transistor devices. As the classical mismatch models predict, discrete thermal interface resistances generally decrease with increasing temperature due to the increasing phonon heat capacity.^{67,69,71} But phonon scattering on lattice imperfections could result in the opposite temperature trend, as reported by Klemens (1960),⁸⁴ due to the strong frequency dependence of phonon scattering by point defects. The theoretical study by Klemens⁸⁴ showed that the lattice thermal resistance increases with temperature—varies as $T^{1/2}$ —at high temperatures (e.g., $T > 80$ K for Ge-Si alloys) in the limit at which the point defect scattering is stronger than the Umklapp scattering. If the thermal interface resistance is governed by a disordered adhesion film between the GaN and the substrate, which corresponds to one of the fabrication approaches for GaN on diamond composites, then the interface resistance may decrease with temperature because the thermal conductivity of that disordered adhesion film will likely increase.^{85,86} Since all of the mechanisms above could be involved, the GaN-substrate thermal interface resistance could either increase or decrease with temperature, or could be steady with temperature, depending on which mechanisms dominate the interface resistance. Micro-Raman thermometry on GaN/AlN/SiC device structures has suggested that the interface resistance associated with the AlN transition layer increases dramatically with temperature.^{8–10} A recent study using time-domain thermoreflectance (TDTR) and phonon transport theory for both GaN/AlN/SiC and GaN/AlN/Si composites

indicates that the temperature dependence is much weaker than was found in these Raman measurements and that point defects within the AlN transition layer and near-interface defects could be the dominant scattering mechanisms responsible for the temperature trend of the interface resistance.⁴⁴ Considerable work remains to be done on understanding the temperature-dependent behavior and the governing physics of the GaN-substrate thermal interface resistance.

3.4 Atomistic Simulation Techniques

The discussion of the thermal property modeling in this section has so far focused on the semiclassical phonon conductivity integral models, which use solutions to the phonon Boltzmann transport equation under the relaxation time approximation. Beyond the semiclassical models, atomistic simulations, such as molecular dynamics and first principles density functional theory calculations, can improve understanding of thermal conduction in GaN composite substrates. Recent molecular dynamics simulations have studied the size effect as well as the impact of different types of microstructural defects (e.g., dislocations, stacking faults, voids, etc.) on the lattice thermal conductivity of wurtzite GaN.^{87–89} Another molecular dynamics study investigated the effects of interfacial morphology and interfacial defects on thermal boundary resistance between Al and GaN.⁹⁰ Hu et al.⁹¹ also used molecular dynamics simulations to predict the spectral distribution of the vibrational density of states for different GaN-SiC interfacial structures and their propagation into temperature profiles as well as thermal resistance across the GaN-SiC interface. A first principles approach was employed to examine the lattice thermal conductivity of wurtzite GaN and its dependence on isotopes.⁶⁴ The same approach was used to calculate the lattice thermal conductivities of diamond, wurtzite AlN, cubic SiC (3C-SiC), and cubic aluminum-V and gallium-V compounds.^{65,92,93} Although these types of atomistic simulations have been successful for simple bulk crystals or very small systems, they incur high computational cost and are often difficult to extend to large and complex structures. The challenge still exists to extend these atomistic simulations to complex nanostructures such as a multilayer structure containing defects (which is the case of GaN composite substrates).

4. THERMAL PROPERTY MEASUREMENTS

Many techniques are available to measure thermal properties—thin film thermal conductivity and thermal boundary resistance (TBR)—at nanometer length scales.^{76,94} All of these techniques rely on probing the thermal response of a material to heat input. The intricate sample geometries of GaN composite substrates necessitate the use of thermal measurement techniques capable of confining their thermal penetration depths to regions of interest. Depending on the method used for controlling thermal penetration depth, measurement techniques can be grouped broadly into two categories: temporal and spatial confinement techniques. Temporal confinement techniques use brief optical heating pulses or a high-frequency electrical heating signal to confine the thermal penetration depth to the region of interest; examples of these techniques include time-domain thermoreflectance (TDTR)^{95–97} and the 3ω technique.⁹⁸ The temporal thermal penetration depth is defined

by the relation $d_{\text{char}} = \sqrt{Dt}$, where d_{char} is the characteristic thermal penetration depth, D is the thermal diffusivity of the heated material, and t is the characteristic time scale of the heating event. The modulation frequency and/or the pulse width of the heating event can affect this time scale. On the other hand, spatial confinement of the heating event often involves the use of varying widths of heater structures to spatially confine the heat to a certain depth into the material stack interrogated. One example is DC Joule heating thermometry with nanopatterned metal bridges of widths from 100 μm (Ref. 99) down to 50 nm,¹⁰⁰ where different heater widths provide different sensitivities to in-plane and out-of-plane film thermal conductivities. This allows us to determine the in-plane thermal conductivity and isolate the conductivity anisotropy for the material of interest without the use of a suspended structure.^{99,100}

Temporal and spatial confinement techniques have been actively used to measure thermal conduction properties of GaN composites; TDTR and DC Joule heating thermometry using patterned nanoheaters are of special interest.^{22,37,101} In addition to both techniques, micro-Raman thermometry^{8,102,103} has found its utility in temperature distribution measurements of AlGaIn/GaN device structures. It is based on measuring the shift of material phonon frequencies with temperature. This section reviews TDTR, DC Joule heating thermometry, and micro-Raman thermometry, as well as their application to the thermal property investigation of GaN composite substrates.

4.1 DC Joule Heating Thermometry Using Variable Width Heaters

The electrical Joule-heating and thermometry technique yields data on both in-plane and out-of-plane thermal conductivities of individual layers by optimizing the width of the heater bridge.^{37,99,100,104} The metal heater bridges of widths from 100 μm (Ref. 99) down to 50 nm (Ref. 100) are fabricated on top of the sample stack with a four-probe configuration. The fabrication process is comprised of two major steps: (i) optical photolithography patterns the larger components in the periphery including contact pads and contacting paths, and (ii) electron beam (e-beam) lithography patterns the fine nanoheaters in the center, as shown in Fig. 7(b). The high resolution of e-beam lithography achieves narrow heater widths in the sub-micrometer domain, which enables a successful fabrication of electrically stable 50 nm wide metal heaters.¹⁰⁰ A passivation layer—often one of Si_3N_4 , Al_2O_3 , and SiO_2 —is placed between the metal heaters and the top surface of the sample stack to provide electrical insulation. Either platinum or gold is used as a material for the nanoheaters (~ 50 nm thick); in the case of gold nanoheaters, a few nanometer-thick titanium layer is used for adhesion between the gold and the passivation layer. The electrical Joule-heating and thermometry technique captures the temperature by measuring the electrical resistance change in the metallic nanoheaters. The temperature coefficient of resistivity (TCR) of the metal film is dependent on its thickness partly due to the electron scattering at the film boundaries. Since the heater width affects the actual film thickness in the e-beam lithography process, it is necessary to calibrate the TCR of each heater width.

Figure 7(a) illustrates the application of this technique to a typical GaN composite structure and the concept of the spatial confinement using varying width heaters from 50

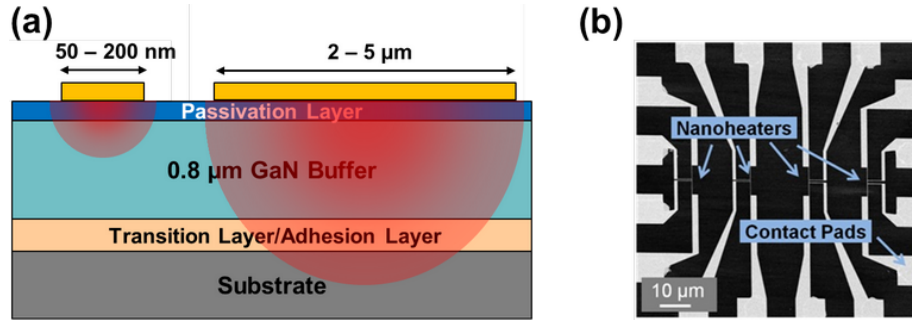


FIG. 7: (a) Spatial confinement by varying heater widths: electrical Joule heating and thermometry using patterned nanoheaters limits the heated region to the depth roughly scaled by the width of the bridge. This allows extraction of the thermal properties of the layers that are located within the volume of the heated region. Sub-micrometer narrow heaters (50–200 nm) confine the heat within a very shallow region on the top and are therefore more sensitive to the lateral heat spreading within the GaN buffer layer, whereas wider heaters (2–5 μm) are less sensitive to the in-plane thermal conductivity of the GaN. (b) Top-view scanning electron microscope (SEM) image of the patterned heater bridges fabricated using e-beam lithography. Heater width varies from 50 nm to 5 μm (not all widths are shown in this micrograph).

nm to 5 μm . The sub-micrometer narrow heaters (50–200 nm) make it possible to confine the heat within a very shallow region with DC Joule heating. For a heater width of 50 nm, most of the temperature drop occurs within a shallow region of approximately 50–100 nm where the heat dissipates both vertically and laterally. This 2D heat conduction is sensitive to the lateral heat spreading within the GaN buffer layer. On the other hand, wide heaters such as a 5 μm one provide large spatial confinement and induce nearly 1D heat conduction across the GaN layer. Therefore, the widest heater (5 μm) provides high sensitivity to the GaN-substrate thermal interface resistance and low sensitivity to the in-plane GaN thermal conductivity. The temperature rise of the heater bridge is captured by measuring the voltage drop across, and the temperature data is fitted using the multilayer heat diffusion code described in Section 2.1 to determine the thermal properties of the underlying material.

4.2 Time-Domain Thermoreflectance

In recent years, time-domain thermoreflectance (TDTR) has become a mature technique for measuring the thermal boundary resistance and properties of thin films for a wide range of temperatures.^{71,75,95–97,105–108} It uses a mode-locked laser that produces ultrafast laser pulses with picosecond pulse width at high repetition rates (from tens up to a few hundreds of megahertz), which temporally confine the heat to the near-surface region. Although many implementations of TDTR exist, the basic operating principle is the same. Typically, TDTR experiments involve the use of a single laser output, which is split into a pump beam (as a heat source) and a probe beam (as a thermometer), and the use of a top metal film,

which serves as both the pump absorber and probe transducer. The pump beam deposits heat in the metal transducer film, and the temporal evolution of the surface temperature of the metal film is then measured by the time-delayed probe beam via the temperature dependence of the optical reflectivity of metal, i.e., the thermorefectance. The pump beam is modulated at frequencies from 100 kHz (Ref. 108) up to 12 MHz (Ref. 107) by an electro-optic modulator (EOM) or an acousto-optic modulator (AOM) for lock-in detection, and it is then directed onto the sample through an objective lens at normal incidence. In some implementations of TDTR, the pump beam is frequency-doubled for a spectral separation of the pump and the probe.^{106,109} The probe beam is temporally delayed relative to the pump optical heating by a mechanical delay stage and is directed onto the sample through the same objective (i.e., the probe beam is coaxial with the pump beam). The changes in intensity of the reflected probe beam caused by the pump heating appear at the pump modulation frequency and are detected with an RF lock-in amplifier that has an in-phase $V_{in}(t)$ and out-of-phase $V_{out}(t)$ component. A 3D radial symmetric solution of the heat diffusion equation for the multilayer stack⁹⁷ is compared to the measured TDTR data to extract the thermal properties of interest beneath the metal transducer. Figure 8 illustrates one implementation of TDTR used in Panzer,¹⁰⁶ Reifenberg,¹¹⁰ Cho et al.,²² and others, which is based on the principle described above.

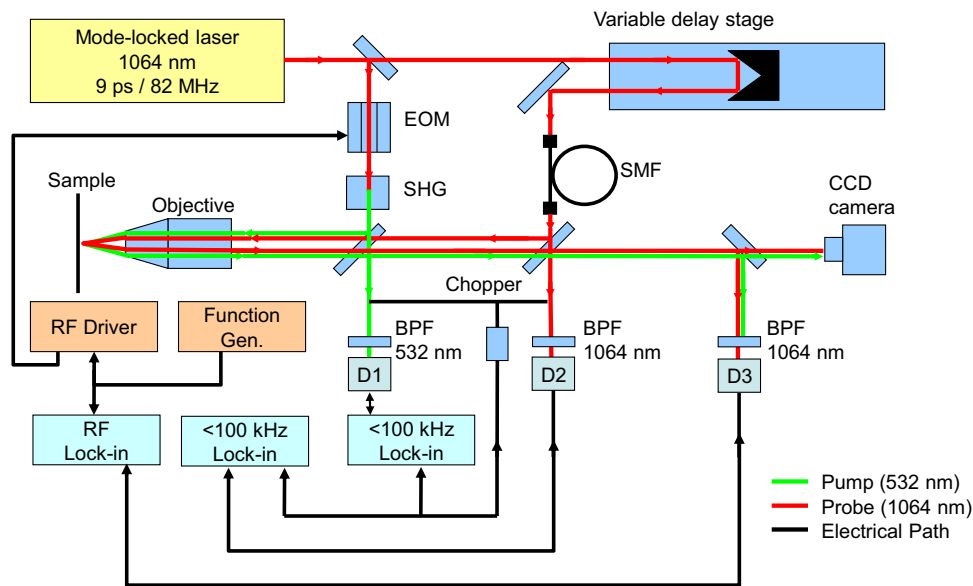


FIG. 8: One implementation of a two-color TDTR setup.^{22,106,110} In this setup, a mode-locked Nd:YVO₄ laser generates 9.2 ps optical pulses at 1064 nm wavelength and with 82 MHz repetition rate, which are divided into pump and probe beams. The pump beam passes through an electro-optic modulator (EOM) for lock-in detection, and a second harmonic generation (SHG) crystal for frequency-doubling to 532 nm, and it is then directed onto the sample through an objective lens. The time-delayed probe beam passes through a single-mode fiber (SMF) after the delay stage to minimize errors associated with beam divergence and beam overlap, and it is then directed onto the sample through the same objective lens.

Many efforts have been made over the past decades to achieve experimental improvements in implementation of TDTR^{96,109,111} and advance the data interpretation.^{44,71,78,97,105} Capinski and Maris⁹⁶ first used a single-mode fiber (SMF) after the delay stage to solve the problems caused by changes in the probe spot size (due to beam divergence) and the overlap of the pump and probe beams (due to beam steering) as the delay stage moves. Schmidt et al.¹⁰⁹ incorporated a beam expander before the delay stage and a beam compressor after the stage to reduce errors associated with the probe beam divergence at long delay times. They also used a double-pass delay stage to provide longer delay times (up to 7 ns). Cahill⁹⁷ described the frequency-domain solution for the surface temperature of a layered structure in cylindrical coordinates considering Gaussian-shaped laser beams (for the pump and probe) and applying the iterative algorithm of Feldman.⁴² Costescu et al.⁷¹ and Cahill⁹⁷ were the first to analyze the ratio of the in-phase to out-of-phase signal of the RF lock-in—equivalently the phase $\tan^{-1}[V_{\text{out}}(t)/V_{\text{in}}(t)]$ of the thermoreflected probe signal—to provide a simple way of minimizing errors caused by changes in the beam spot size and the beam overlap as a function of delay time and to utilize the additional information in the out-of-phase signal. Schmidt et al.¹⁰⁵ varied the modulation frequency and the pump spot size to measure both out-of-plane and in-plane thermal conductivities of an anisotropic thin film, while Feser and Cahill¹¹¹ recently suggested the pump-probe offset method to probe in-plane conduction. Reifenberg et al.⁷⁸ and Cho et al.⁴⁴ exploited a careful sample design to simultaneously determine film thermal conductivities and interface resistances.

Since the picosecond time resolution of TDTR offers the possibility of nanometer-scale depth resolution,^{76,94} TDTR provides the potential to isolate the thermal boundary resistance from the thermal conductivity of a thin layer, often by utilizing the different sensitivities of the measurement to the different thermal properties at different modulation frequencies, delay times, and thicknesses. This is advantageous for accurate measurement of the GaN-substrate thermal interface resistance as well as the GaN thermal conductivity in GaN composites. Recent TDTR studies by Cho et al.^{22,44,101} simultaneously determined both properties using multiple samples with varying GaN thicknesses from the same fabrication process—i.e., using different thickness samples that share the same microstructure. This approach essentially uses the fact that the measurement sensitivities to these two properties vary with GaN thickness; the thickest GaN sample is most sensitive to the GaN thermal conductivity whereas the thinnest GaN sample is most sensitive to the GaN-substrate thermal interface resistance. In this approach, the measured TDTR data from three GaN thicknesses at the same modulation frequency are fit simultaneously under the assumption that these two properties do not vary strongly among the three samples.

4.3 Micro-Raman Thermometry

Confocal micro-Raman thermometry has been actively used in the measurement of the temperature distribution of GaN device structures in both two and three dimensions.^{8–10,102,103,112–115} The application of this approach to transistor thermometry dates back at least two decades to Abstreiter,¹¹⁶ Ostermeir et al.,¹¹⁷ etc. Raman thermometry is based on the inelastic scattering of light by phonons in solids, which includes

both Stokes (phonon creation) and anti-Stokes (phonon annihilation) Raman scattering processes.¹¹⁸ In experiments, the Stokes Raman scattering process is mostly used. Device temperatures can be determined by measuring the temperature-dependent phonon-frequency shift induced by device self-heating.¹¹³ The phonon-frequency shift with temperature is a result of anharmonic effects such as thermal expansion and phonon coupling.¹¹⁹ Typically, frequency shifts of the GaN E_2 (high) and/or A_1 (LO) phonon mode with temperature are used to determine the temperature of the GaN layer. Since the E_2 (high) mode is an order of magnitude stronger than the A_1 (LO) phonon mode in a Raman spectrum of GaN, many Raman measurements have used temperature information obtained only from the E_2 (high) mode.^{102,103,112,113} But the A_1 (LO) phonon mode alone has also been used in some Raman measurements.^{9,10,38} Alternatively, both the E_2 (high) and A_1 (LO) phonon modes can be used to account for the thermal-stress-induced contribution to the phonon frequency shift separately from the temperature-induced contribution, which improves the accuracy of the temperature measurement.^{8,115,120} Because the intensity ratio of the Stokes to the anti-Stokes scattering processes depends only on temperature, the ratio can also be used to determine the temperature.^{8,113,114} The substrate temperature is typically probed using the 778 cm^{-1} mode of SiC and the 520 cm^{-1} mode of Si.⁸

A continuous wave (CW) laser of either 488 or 532 nm wavelength is often employed as an excitation source for the implementation of Raman thermometry on GaN devices, which can measure time-averaged temperatures in DC-operated devices.^{8,102,112–115,120} The energies of the 488 and 532 nm optical excitations are below the GaN bandgap (3.4 eV); hence the GaN buffer layer is transparent to these optical excitations. This ensures that negligible laser-induced heating or photocurrent generation occurs in devices, and enables noninvasive temperature measurement during device operation.¹⁰² The SiC substrate is also transparent to these two optical excitations whereas the Si substrate is nontransparent.⁸ Therefore, Raman temperature measurements on GaN on SiC devices can be implemented from both the top side and the back side of the devices, whereas in GaN on Si devices only top-side measurements can be performed. Time-resolved Raman thermometry has been implemented using brief laser pulses of duration from 200 ns (Ref. 103) down to 30 ns (Ref. 9)—generated mostly by the modulation of the CW lasers—in devices operated with square electrical pulses. In this case, temporal resolution is determined by the laser-pulse duration used in the measurements.

Lateral spatial resolution is mainly limited by the laser spot size, which is $\sim 1\text{ }\mu\text{m}$ in most implementations of Raman measurements.^{8–10,102,103,112,113,115,120} Depth resolution is limited either by the depth of field (DoF) of confocal microscopy or by the thickness of the layer.^{8,112,113} The theoretical diffraction limit for the depth of field is about $2\text{ }\mu\text{m}$ when the laser is focused on the device top surface,¹¹² but the actual depth of field is greater ($\sim 4.5\text{ }\mu\text{m}$) than the theoretical limit due to imperfect confocality.⁸ At greater probing depths inside the substrate (when the substrate is transparent to the optical excitation used), the depth of field is dominated by light refraction through the substrate and increases to tens of micrometers at a depth of $\sim 300\text{ }\mu\text{m}$ below the surface.^{8,112} Therefore, in the Raman measurement of GaN composites, the GaN temperature is averaged over the GaN layer thickness ($1\text{--}2\text{ }\mu\text{m}$) while the substrate temperature is averaged over the depth of field.

Three-dimensional finite difference thermal simulations are compared to the DC and/or time-resolved temperature data to extract thermal properties. Of increasing interest is the determination of the GaN-substrate thermal interface resistance.^{8–10,38} Two methodologies have been developed to extract the GaN-substrate interface resistance.^{8,9} In the first approach, the GaN-substrate interface resistance is determined from the temperature discontinuity at the GaN-substrate interface in a temperature-depth scan through the substrate.⁸ This approach requires that the measured temperature discontinuity be corrected for the averaging of the substrate temperature near the interface with the aid of the finite difference thermal simulation. In the second approach, the GaN-substrate interface resistance is determined from the transient GaN temperature within the first 300 ns after the device is turned on.⁹ This approach is beneficial in that the averaging effect of the substrate temperature near the interface needs not to be considered. Both approaches use the GaN-substrate interface resistance as the only adjustable parameter in the data fitting procedure. Other input parameters in GaN composites must therefore be assumed from the literature or measured independently. The substrate thermal conductivity is determined by fitting the simulation to the measured temperature distribution as a function of depth inside the substrate.⁸ The presence of the thin AlGaIn layer (~ 30 nm) on top of GaN is often neglected because its impact on the GaN temperature is not significant.⁸ The GaN thermal conductivity and its temperature dependence are taken from the literature: typically, 150 or 160 W m⁻¹ K⁻¹ as room temperature thermal conductivity and $T^{-1.4}$ as temperature dependence.⁸

5. THERMAL PROPERTIES IN GALLIUM NITRIDE COMPOSITE SUBSTRATES

5.1 GaN Thermal Conductivity

There have been many experimental studies on the thermal conductivity of bulk GaN and GaN films,^{55,57,121–124} but few studies have provided data for the thermal conductivity of GaN buffer layer directly extracted from GaN composite substrates.^{22,37,101,125} Figure 9 shows the available experimental data for the GaN thermal conductivity k_{GaN} as a function of temperature from 80 to 550 K, including the bulk GaN data as well as the data extracted from GaN composites. All the GaN data included here are the cross-plane thermal conductivity data except for the in-plane thermal conductivity data reported by Hodges et al.¹²⁵ and the effective thermal conductivity data reported by Cho et al.³⁷ Overall, the thermal conductivity of GaN decreases with increasing temperature, which is characteristic of semiconducting materials in this temperature range due to the increasing impact of phonon-phonon scattering. The temperature-dependent thermal conductivity data of AlGaIn alloy films^{55,121} and a polycrystalline GaN film¹²¹ are also included for comparison.

A common crystal structure for GaN is the wurtzite structure, which has hexagonal symmetry. All the GaN studies reviewed here used the wurtzite phase. Cubic GaN of the zinc-blend or rock salt structure can be achieved depending on growth conditions as well as the substrate material and orientation, but GaN in either of these two phases is metastable and its thermal properties have not been much investigated.^{126,127} Because of its noncubic symmetry, wurtzite GaN may have an anisotropic thermal conductivity. Slack et al.¹²²

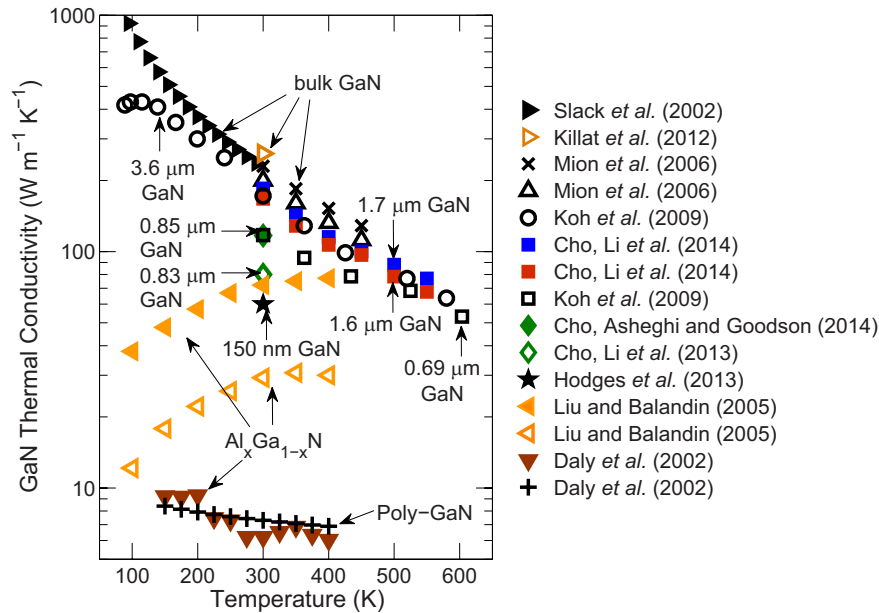


FIG. 9: Temperature-dependent thermal conductivity data for bulk GaN and GaN films. The data from Slack *et al.*¹²² (right-facing solid triangles) and Mion *et al.*¹²³ (crosses and up-facing open triangles) are for GaN samples grown by hydride vapor phase epitaxy (HVPE) to different thicknesses; 200 μm (right-facing solid triangles), 2000 μm (crosses), and 370 μm (up-facing open triangles). The data from Killat *et al.*¹²⁴ (right-facing open triangle) is for a 2 μm thick GaN film grown by MOCVD on a 500 μm thick bulk GaN substrate. The data from Koh *et al.*⁵⁷ are for a MBE-grown 0.69 μm GaN film (open squares) and a MOCVD-grown 3.6 μm GaN film (open circles). The data from Cho *et al.*^{37,44,101} (solid squares, a solid diamond, and an open diamond) are for different types of GaN composite substrates: MBE-grown 1.7 μm GaN on Si (upper solid squares), MOCVD-grown 1.6 μm GaN on SiC (lower solid squares), and 0.85 μm GaN (a solid diamond) and 0.83 μm GaN (an open diamond) on diamond fabricated using epitaxial transfer. The data for the 0.83 μm GaN on diamond are the effective thermal conductivity (a direction-averaged value lying between in-plane and cross-plane conductivity values). The in-plane thermal conductivity of a 150 nm thick GaN film measured by Hodges *et al.*¹²⁵ is also included (a solid pentagram). Thermal conductivity values for a polycrystalline GaN film (grown by MBE on a GaAs substrate) from Daly *et al.*¹²¹ (pluses) are an order of magnitude lower than the bulk GaN values, which shows the impact of grain boundary scattering on the thermal conductivity reduction. The data for the thermal conductivity of $\text{Al}_x\text{Ga}_{1-x}\text{N}$ alloy films from Liu and Balandin⁵⁵ ($x = 0.09$ for left-facing solid triangles and $x = 0.4$ for left-facing open triangles) and Daly *et al.*¹²¹ ($x = 0.44$, down-facing solid triangles) are included to show the impact of phonon scattering by alloy defects.

argued that the thermal conductivity anisotropy in wurtzite GaN at room temperature is 1% or less because (i) the sound velocities perpendicular to and parallel to the c -axis,

calculated by Polian et al.,¹²⁸ differ by 1% and (ii) the Grüneisen parameters along the two directions, determined by Iwanaga et al.,¹²⁹ are almost the same at room temperature. An atomistic first principles calculation by Lindsay et al.⁶⁴ also suggested that the thermal conductivity anisotropy in wurtzite GaN is not significant over the temperature range of 100–500 K; for example, the difference between the thermal conductivities perpendicular to and parallel to the *c*-axis is $\sim 1\%$ at room temperature.

Slack et al.¹²² used the steady-state heat flow technique to measure the thermal conductivity of a 200 μm thick bulk GaN sample grown by hydride vapor phase epitaxy (HVPE) on a sapphire substrate. They reported the room temperature value of $227 \text{ W m}^{-1} \text{ K}^{-1}$, and the temperature dependence of $T^{-1.22}$ from 80 to 300 K, which is characteristic of pure adamantane crystals in this temperature range.¹²² Two HVPE-grown bulk GaN samples with thicknesses of 370 and 2000 μm were measured by Mion et al.¹²³ using the 3ω technique from 300 to 450 K. Their reported room temperature thermal conductivity values are approximately $200 \text{ W m}^{-1} \text{ K}^{-1}$ for the 370 μm sample and $230 \text{ W m}^{-1} \text{ K}^{-1}$ for the 2000 μm sample, and their measured temperature dependence is $T^{-1.43}$ for both samples. Micro-Raman thermometry was used to determine the bulk GaN room temperature thermal conductivity of $260 \text{ W m}^{-1} \text{ K}^{-1}$ from the temperature depth profile in a GaN-on-GaN device.¹²⁴ Their device structure consisted of a 20 nm thick GaN/AlGaIn device layer, a 2 μm thick GaN buffer layer, and a 500 μm thick bulk GaN substrate from the top, and their data fitting procedure assumed zero resistance at the GaN-GaN interface and a homogeneous GaN thermal conductivity. Koh et al.⁵⁷ measured the thermal conductivity of a 3.6 μm thick GaN film grown by MOCVD on a sapphire substrate over the temperature range 90–580 K using TDTR. They also measured the thermal conductivity of a MBE-grown GaN film (0.69 μm) on 4 nm AlN on that 3.6 μm thick GaN film at temperatures between 300 and 600 K using TDTR. Their room temperature thermal conductivities are approximately $170 \text{ W m}^{-1} \text{ K}^{-1}$ for the 3.6 μm GaN film and $120 \text{ W m}^{-1} \text{ K}^{-1}$ for the 0.69 μm GaN film.

Cho et al.⁴⁴ used TDTR to simultaneously extract the GaN thermal conductivity and the GaN-substrate thermal interface resistance from MOCVD-grown GaN/AlN/SiC composites and MBE-grown GaN/AlN/Si composites. For each type of GaN composite, three different GaN thicknesses were used on the same AlN/substrate structure; the GaN thicknesses used were 0.6, 0.9, and 1.6 μm for SiC-based composites and 0.5, 1.3, and 1.7 μm for Si-based composites. The three different thickness samples were simultaneously fitted to determine both properties under the assumption that they do not vary strongly among the three samples. Because of the different measurement sensitivities to these two properties at different GaN thicknesses, the GaN thermal conductivity is mostly determined by the thickest GaN sample whereas the GaN-substrate interface resistance is primarily governed by the thinnest GaN sample. Their measured room temperature thermal conductivity values are 185 and $167 \text{ W m}^{-1} \text{ K}^{-1}$ for the MBE-grown GaN/AlN/Si and MOCVD-grown GaN/AlN/SiC composites, respectively. Their observed temperature dependence from 300 to 550 K is $T^{-1.44}$ for the GaN/AlN/SiC composites and $T^{-1.42}$ for the GaN/AlN/Si composites, in reasonable agreement with the dependence obtained in Mion et al.¹²³ Cho et al.³⁷ also performed DC Joule heating measurements with narrow heater widths (from 200 nm to 1 μm) to measure the effective thermal conductivity (a

direction-averaged value lying between in-plane and cross-plane conductivity values) of a 0.83 μm GaN buffer layer in a GaN-AlGaIn-diamond composite fabricated using the epitaxial transfer technique. Their measured room temperature thermal conductivity of $80 \text{ W m}^{-1} \text{ K}^{-1}$ is lower than that of other GaN composites, which can be attributed in part to the contribution from the resistive GaN/AlGaIn device layer ($\sim 20 \text{ nm}$) on top of their GaN buffer layer. A very recent TDTR measurement on similar GaN-diamond composites used two GaN thicknesses (0.85 and 0.37 μm) and determined the room temperature GaN thermal conductivity of $117 \text{ W m}^{-1} \text{ K}^{-1}$ by simultaneously fitting the two samples.¹⁰¹ Hodges et al.¹²⁵ used micro-Raman thermometry to estimate the in-plane thermal conductivity of a 150 nm thick GaN layer from the lateral temperature profiles in an AlGaIn/GaN/AlGaIn/Si device structure. Their estimated room temperature value is $60 \text{ W m}^{-1} \text{ K}^{-1}$, which is somewhat lower than the effective conductivity value of $80 \text{ W m}^{-1} \text{ K}^{-1}$ reported by Cho et al.³⁷

Overall, the thermal conductivities of GaN buffer layers directly measured from GaN composite substrates are lower than the bulk GaN values, as indicated in Fig. 9. Variations in the measured conductivities of GaN buffer layers are relatively large, e.g., from 60 to $185 \text{ W m}^{-1} \text{ K}^{-1}$ at room temperature. This can be attributed to the effects of material defects, including point defects, and also to the size effect, as depicted in Fig. 10. Figure 10 shows the measured room temperature thermal conductivities of GaN buffer layers in composite substrate structures from the sources illustrated in Fig. 9. For the data by Cho et al.,⁴⁴ the largest film thicknesses are considered for both GaN/AlN/SiC and GaN/AlN/Si composites because the GaN thermal conductivity is mostly determined by the thickest

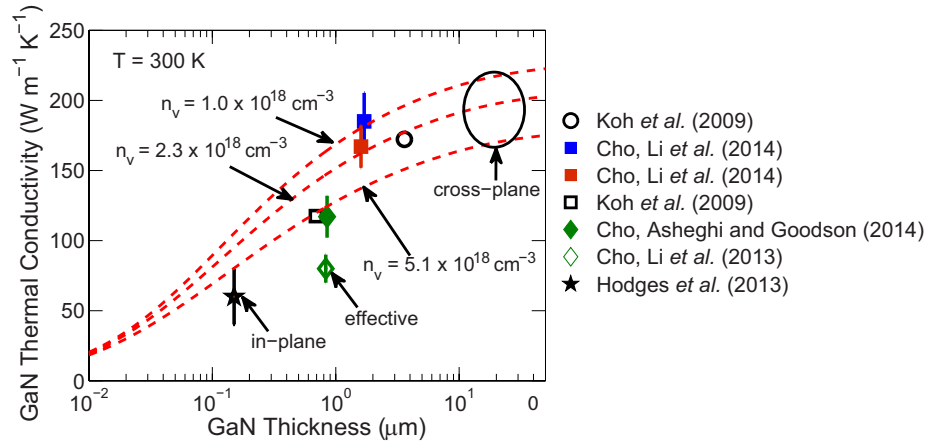


FIG. 10: Room temperature thermal conductivity of GaN films as a function of film thickness. The data by Hodges et al.¹²⁵ is the in-plane GaN thermal conductivity, and the data by Cho et al.³⁷ is the effective GaN thermal conductivity that averages in-plane and cross-plane conductivity values. The data by others are the cross-plane GaN thermal conductivities. Modeled cross-plane GaN thermal conductivities (red dashed lines) using the thermal conductivity integral model (see Section 3.1) are shown at different vacancy concentrations (n_v). The model accounts for phonon-phonon Umklapp scattering, phonon-vacancy Rayleigh scattering, and phonon-boundary scattering in the Casimir limit.

GaN sample and not much affected by the thinnest GaN sample. Cross-plane GaN thermal conductivity calculations using the semiclassical thermal conductivity integral model, which accounts for phonon-phonon Umklapp scattering, phonon-vacancy Rayleigh scattering, and phonon-boundary scattering in the Casimir limit (see Section 3.1), are shown in comparison to the experimental data at different vacancy concentrations. The dependence of thermal conductivity on film thickness for relatively high thermal conductivity materials such as Si—whose thermal conductivity of ~ 148 W/mK is comparable to the GaN buffer film conductivities discussed here—is well described in the literature.⁶¹ In addition to the size effect, the effect of material defects is important, as illustrated by the red dashed lines in Fig. 10, which indicate different vacancy defect concentrations, since these GaN layers are heteroepitaxially grown on a foreign substrate and highly defective due to lattice mismatch stresses.

Alloying, which introduces mass and strain disorder at the atomic scale, can scatter phonons strongly. This phonon scattering by alloy defects can be treated using the Rayleigh model [$\tau^{-1} \sim \omega^4$, see Eq. (8) for the full form of the model]. As a result of the alloy scattering, the measured thermal conductivities of AlGaN films are much lower than those of GaN: a factor of ~ 37 reduction is observed between the bulk GaN conductivity by Slack et al.¹²² and the lowest AlGaN conductivity measured by Daly et al.¹²¹ As the Al mass fraction increases approximately up to 0.6, the AlGaN thermal conductivity decreases due to the increased addition of alien atoms (Al) in the host crystal lattice (GaN).⁵⁵ Grain boundaries in a polycrystalline GaN film can provide another strong phonon scattering mechanism, as indicated by the data from Daly et al.¹²¹ The average grain size of their polycrystalline film is 7 nm, and such small grains significantly reduce the phonon mean free path.

5.2 GaN-Substrate Thermal Interface Resistance

Table 2 summarizes the available experimental data for the thermal interface resistance $R_{\text{GaN-substrate}}$ between the GaN buffer layer and three different substrates (Si, SiC, and diamond). The DMM predictions for the GaN-substrate interface resistance set the theoretical lower limits for three types of GaN composites (see Section 3.2). As discussed earlier in this chapter, the GaN-substrate interface involves the use of a transition layer; this can be a thin AlN layer for MOCVD-grown GaN-SiC composites^{8–10,22,44} and for MBE-grown GaN-Si composites,⁴⁴ or can be a rather complicated and thick transition layer for MOCVD-grown GaN-Si composites.^{8,130} It can also be a disordered adhesion layer (thinner than 50 nm) for GaN-diamond composites fabricated by the epitaxial transfer technique.^{37,38,101,131}

Temperature fields measured with micro-Raman thermometry were used to extract MOCVD GaN-SiC and GaN-Si interface resistances^{8–10} and GaN-diamond interface resistances (for GaN-diamond composites fabricated by epitaxial transfer).^{38,131} Several Raman studies^{8–10} for MOCVD GaN-SiC interface resistances reported relatively large thermal resistances (i.e., from $8 \text{ m}^2 \text{ K GW}^{-1}$ up to $60 \text{ m}^2 \text{ K GW}^{-1}$) and a very strong temperature dependence—a rapidly increasing trend with increasing temperature—between 330 and 520 K. Another Raman study⁸ reported $33 \text{ m}^2 \text{ K GW}^{-1}$ at 573 K as a MOCVD

TABLE 2: GaN-Substrate thermal interface resistances summary

Refs.	Measurement technique	Configuration	Temp. range	Transition/adhesion layer thickness [nm]	$R_{\text{GaN-Substrate}}$ [$\text{m}^2\text{K/GW}$]	DMM prediction [$\text{m}^2\text{K/GW}$]
8	Micro-Raman thermometry	GaN-Si	573 K	N/A	33	0.8
44	Time-domain thermoreflectance	GaN-Si	300 K to 550 K	38	7–10	0.8
130	Transient interferometric mapping	GaN-SiC	N/A	N/A	120	1.1
10	Micro-Raman thermometry	GaN-SiC	330 K to 530 K	40–200	8–60	1.1
22,44	Time-domain thermoreflectance	GaN-SiC	300 K to 550 K	26–36	4–6	1.1
132	Transient interferometric mapping	GaN-diamond	N/A	N/A	<10	3.0
37	Time-domain thermoreflectance	GaN-diamond	Room temp.	145–324	36–47	3.0
101	Time-domain thermoreflectance	GaN-diamond	Room temp.	29–33	29	3.0
38	Micro-Raman thermometry	GaN-diamond	409 K	25	27	3.0
131	Micro-Raman thermometry	GaN-diamond	443 K	50	18	3.0

GaN-Si interface resistance, which is comparable to Raman-measured MOCVD GaN-SiC interface resistances. Recent Raman measurements on two similar GaN-diamond device structures—both of which were fabricated by epitaxial transfer—estimated interface resistances of $27 \text{ m}^2 \text{ K GW}^{-1}$ at 409 K for one³⁸ and $18 \text{ m}^2 \text{ K GW}^{-1}$ at 443 K for the other;¹³¹ these two measurement temperatures are GaN-diamond interface temperatures, which are estimated by taking the average of GaN and diamond temperature at the interface from their depth temperature profiles. None of the Raman measurements mentioned here extracted the GaN thermal conductivity independently; instead, they assumed some common value for this property as an input parameter to the thermal model. As discussed in Section 4.3, a room temperature thermal conductivity of 150 or $160 \text{ W m}^{-1} \text{ K}^{-1}$ and a temperature dependence of $T^{-1.4}$ are typically assumed.

Other studies used an optical transient interferometric mapping (TIM) technique to estimate interface resistances very approximately for GaN-SiC and GaN-diamond composites.^{130,132} They reported an interface resistance of $120 \text{ m}^2 \text{ K GW}^{-1}$ —with $\pm 50\%$ uncertainty—for a MOCVD-grown GaN-SiC composite¹³² and the upper bound of $10 \text{ m}^2 \text{ K GW}^{-1}$ for the interface resistance of MBE-grown GaN on single crystalline diamond.¹³⁰ However, these authors also did not assess the quality of their GaN layer and provided no explanation for the structural details of their GaN-diamond interface.

TDTR on multiple GaN thicknesses was used to extract both the GaN thermal conductivity and the GaN-substrate thermal interface resistance for MOCVD-grown GaN-SiC composites^{22,44} and MBE-grown GaN-Si composites.⁴⁴ These TDTR measurements extracted $4\text{--}6 \text{ m}^2 \text{ K GW}^{-1}$ for the MOCVD GaN-SiC interface resistance and $7\text{--}10 \text{ m}^2 \text{ K GW}^{-1}$ for the MBE GaN-Si interface resistance, both of which are over the temperature range of 300 to 550 K. These resistance values are much lower than those reported previously by micro-Raman thermometry,^{8–10} and the temperature dependence is considerably weaker than that of the past Raman data. Phonon transport arguments based on the Boltzmann transport equation [see Eq. (12)] suggest that a combination of point defects within the AlN transition layer and near-interface defects around the AlN interfaces may be responsible for the temperature trend of the interface resistance.⁴⁴ TDTR measurements on two GaN-AlGaN-diamond composites fabricated using epitaxial transfer reported room temperature interface resistances of $36\text{--}47 \text{ m}^2 \text{ K GW}^{-1}$ and suggested the possibility of achieving $\sim 30 \text{ m}^2 \text{ K GW}^{-1}$ at room temperature through the complete etching of the AlGa-N transition layer.³⁷ Cho et al.¹⁰¹ recently performed TDTR on two GaN thicknesses (0.85 and $0.37 \text{ }\mu\text{m}$)—with the AlGa-N transition layers completely etched away—and extracted the GaN-diamond interface resistance of $29 \text{ m}^2 \text{ K GW}^{-1}$ at room temperature.

The literature includes significant differences for interface resistances for GaN-SiC and GaN-Si taken using the TDTR and Raman techniques. This may arise from sample differences such as a different microstructural quality of the transition layers since the interface resistance scales with the density of defects in the AlN transition layer.⁴⁴ In other words, the lower interface resistances reported through the use of TDTR may be due to a lower density of defects in the AlN transition layer of the samples in those specific studies. A second possibility is that such differences may result from differences in the experimental methodologies. Micro-Raman thermometry measures lateral and/or vertical temperature distributions of operating devices induced by device self-heating. Owing to the depth of

focus of the optical beam path, the measured temperatures are depth-averaged within the GaN layer thickness (1–2 μm) and within the substrate over a dimension comparable with $\sim 5 \mu\text{m}$ (Ref. 9). Using temperature field data with this precision, micro-Raman thermometry can extract the interface resistance with the aid of a 3D finite difference thermal simulation. In order to extract the interface resistance, the authors have previously needed to make assumptions about the GaN thermal conductivity and the heat generation distribution within the active semiconducting region.^{8,9,38} Room temperature thermal conductivities of 150–160 $\text{W m}^{-1} \text{K}^{-1}$ were assumed for GaN buffer layers with thicknesses ranging from 1 μm (Ref. 38) to 2.35 μm (Ref. 9), and a uniform heat load was assumed in the active region between two standard ohmic contacts separated by from 5 (Ref. 9) to 20 μm (Refs. 8 and 38) in ungated transistor structures. These assumptions may contribute to the estimate of the uncertainty in the interface resistance measured using the Raman approach, which has been reported to be $\sim 10 \text{ m}^2 \text{K GW}^{-1}$.¹⁰ The TDTR technique provides temperature data only at the surface of the sample, but does so for a comparatively simple and well-characterized spatial and temporal distribution of heating. In other words, the primary benefit of TDTR is that the time dependence and spatial position of heating, as well as the position and time dependence of the resulting temperature, are both known with tremendous precision. This makes the technique particularly well suited for measurement of subsurface properties. The temporal response of the surface temperature is compared to a 3D model of transient multilayer heat diffusion to extract the interface and/or volumetric thermal properties.⁹⁷ Major sources of uncertainty for TDTR include the lack of precise knowledge of the metal transducer thickness and substrate thermal properties as well as the uncertainty associated with uniquely resolving the interface and volume thermal properties. The latter is the main challenge in applying TDTR to GaN composite substrates. The advantage of using TDTR on multiple GaN thicknesses is that it can determine both the GaN conductivity and the GaN-substrate interface resistance independently by utilizing the different measurement sensitivities to both properties with varying thicknesses.^{22,44} The overall uncertainty in the GaN-substrate interface resistance using TDTR with samples of different thicknesses is relatively low ($\sim 3 \text{ m}^2 \text{K GW}^{-1}$).⁴⁴

6. CONCLUDING REMARKS

This chapter presents a comprehensive review of thermal transport phenomena in GaN composite substrates containing Si, SiC, and diamond. The thermal conductivity of GaN buffer layers spans the range of 60–185 $\text{W m}^{-1} \text{K}^{-1}$, which can be attributed to the effects of material defects and film thicknesses. The data for the GaN-SiC and GaN-Si thermal interface resistances also show large variations and suggest the importance of the microstructural quality of the transition layer. Special attention has been paid to the GaN-diamond thermal interface resistance, and a simulation approach for the transistor temperature rise suggests that GaN HEMT on diamond with an interface resistance of $< 30 \text{ m}^2 \text{K GW}^{-1}$ can outperform GaN HEMT on SiC even with zero interface resistance. The current GaN on diamond technology seems to achieve this target interface resistance of $30 \text{ m}^2 \text{K GW}^{-1}$, as evidenced by several experimental observations, but there still remains a need for a detailed temperature-dependent study for GaN-diamond composite substrates that identifies

the temperature trend and the governing conduction physics of the interface resistance. With continued efforts, the GaN-diamond interface resistance is anticipated to be reduced to $<20 \text{ m}^2 \text{ K GW}^{-1}$ and eventually to the lower limit predicted by the diffuse mismatch model. With the anticipated advancements in reducing the GaN-diamond interface resistance and also in improving the quality of the near-interfacial diamond, GaN-diamond composites promise to significantly enhance the near-junction cooling of GaN HEMT devices.

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