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Phonon conduction in GaN-diamond composite substrates

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The integration of strongly contrasting materials can enable performance benefits for semiconductor devices. One example is composite substrates of gallium nitride (GaN) and diamond, which promise dramatically improved conduction cooling of high-power GaN transistors. Here, we examine phonon conduction in GaN-diamond composite substrates fabricated using a GaN epilayer transfer process through transmission electron microscopy, measurements using time-domain thermoreflectance, and semiclassical transport theory for phonons interacting with interfaces and defects. Thermoreflectance amplitude and ratio signals are analyzed at multiple modulation frequencies to simultaneously extract the thermal conductivity of GaN layers and the thermal boundary resistance across GaN-diamond interfaces at room temperature. Uncertainties in the measurement of these two properties are estimated considering those of parameters, including the thickness of a topmost metal transducer layer, given as an input to a multilayer thermal model, as well as those associated with simultaneously fitting the two properties. The volume resistance of an intermediate, disordered SiN layer between the GaN and diamond, as well as a presence of near-interfacial defects in the GaN and diamond, dominates the measured GaN-diamond thermal boundary resistances as low as $17 \text{ m}^2 \text{ K GW}^{-1}$. The GaN thermal conductivity data are consistent with the semiclassical phonon thermal conductivity integral model that accounts for the size effect as well as phonon scattering on point defects at concentrations near $3 \times 10^{18} \text{ cm}^{-3}$. Published by AIP Publishing. [<http://dx.doi.org/10.1063/1.4975468>]

I. INTRODUCTION

Phonon conduction governs the heat removal and cooling of a variety of modern semiconductor electronic devices.^{1–3} Electrons traversing the device junction generate phonons, which transport heat to the underlying substrate.¹ In many transistors, defects and interfaces near the active junction impede phonon conduction through the near-junction materials,⁴ increasing junction temperatures and degrading device performance and reliability.^{5,6} The problem is arguably most severe in high-power GaN transistors, where local power densities can approach tens of kW cm^{-2} .⁷ Chemical-vapor-deposited (CVD) synthetic diamond attracts particular attention as a substrate material due to its superior heat spreading capability ($\sim 1500 \text{ W m}^{-1} \text{ K}^{-1}$) compared to silicon carbide (SiC) ($\sim 400 \text{ W m}^{-1} \text{ K}^{-1}$).⁴ But fabrication challenges associated with the large lattice mismatch of 11% between GaN and diamond (as compared to 3.5% between GaN and SiC) yield a high density of defects within the GaN layer and across the GaN-diamond interface, which scatter phonons in such a lattice-mismatched, hetero-integrated system. Heat dissipation in composite GaN-diamond substrates is therefore governed primarily by the spreading resistance of the GaN layer and the thermal boundary resistance at the GaN-diamond interface as well as the spreading resistance of the diamond substrate.

Much progress has been made recently in characterizing the thermal properties of composite GaN-diamond substrates.^{8–12} This includes measurements of the thermal boundary resistance at the GaN-diamond interface using micro-Raman thermometry⁸ and the nanosecond transient thermoreflectance technique.^{9–11} There has been some success on systematically determining the thermal conductivity of the GaN layer and GaN-diamond thermal boundary resistance,¹² although an experimental approach to simultaneously extract both properties from the same composite substrate remains to be established. In this paper, we use time-domain thermoreflectance (TDTR) to simultaneously measure the GaN thermal conductivity and GaN-diamond thermal boundary resistance for two sets of GaN-diamond composite substrates with GaN thicknesses of $0.58\text{--}0.85 \mu\text{m}$ at room temperature. Our approach involves the use of a combination of amplitude and ratio TDTR signals (of the in-phase and out-of-phase readings of a radio-frequency lock-in amplifier) and multiple modulation frequencies to extract these parameters. Transmission electron micrographs (TEMs) and the semiclassical phonon thermal conductivity integral model are employed to interpret the TDTR data and discern the impact of defects and interfaces on phonon conduction in a GaN-diamond composite substrate structure.

II. EXPERIMENTAL METHODS

Here, we describe sample preparation and the experimental approach. A major challenge in this experimental

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effort is managing the uncertainties associated with the unknown properties in the diamond, the GaN, and near the interface. We address this challenge by (i) using multiple components (i.e., amplitude and ratio) in the TDTR signal and multiple modulation frequencies in our data analysis, (ii) developing a detailed uncertainty model based on those propagated from input parameters (e.g., the thickness of a topmost metal transducer layer, etc.) to our multilayer thermal model, and (iii) considering errors associated with simultaneously fitting two unknown properties (i.e., the GaN thermal conductivity and GaN-diamond thermal boundary resistance). We combine the latter two to estimate the total uncertainties in the extracted properties.

A. Sample preparation

Current GaN-on-diamond fabrication technologies can be grouped broadly into two categories: (i) Direct GaN heteroepitaxy on single crystalline diamond^{13–15} and (ii) GaN epilayer transfer to polycrystalline CVD diamond.^{8–12,16} We use the latter method to fabricate two sets (A and B) of samples. An AlGaIn/GaN heterostructure is first grown on a Si substrate by metal-organic CVD. The Si substrate and highly resistive AlGaIn/AlN transition layers¹² are etched away. The next fabrication step involves depositing a thin disordered (amorphous) SiN layer (20–30 nm)—which acts as an

adhesion layer—onto the backside of the GaN layer and growing CVD diamond of approximately 100 μm on top of the SiN layer. More details of the fabrication process are documented in Ref. 16. Set A consists of one sample with a single GaN thickness (0.85 μm) on the 31 nm SiN interlayer on an $\sim 100\text{-}\mu\text{m}$ -thick hot-filament CVD diamond substrate. Set B consists of two samples with varying GaN thicknesses (0.58 and 0.74 μm) on the 22 nm SiN interlayer on an $\sim 100\text{-}\mu\text{m}$ -thick microwave plasma CVD diamond substrate.

High-resolution TEMs of the GaN-diamond interface, shown in Fig. 1, reveal microstructural differences in the near-interfacial volume of the GaN layer between the two sets of samples and also indicate the reduced thickness (~ 22 nm) of the SiN interlayer of the two samples in set B. For the sample in set A, the GaN layer contains near-interfacial disorders, including line defects (i.e., dislocations), and its interface with the disordered SiN layer is not abrupt (see Figs. 1(a) and 1(b)). In contrast, the GaN-SiN interface of the two samples in set B is relatively abrupt with no apparent near-interfacial defect structures (see Figs. 1(c) and 1(d)). It is of note that the current fabrication approach involves initial, nanocrystalline nucleation/coalescence regions of diamond—with a lower thermal conductivity than bulk diamond due to a smaller grain size and a presence of near-interfacial defects^{17–21}—in close proximity to the SiN interlayer and the backside of the GaN layer. The diamond nucleation region extends up to ~ 30 nm

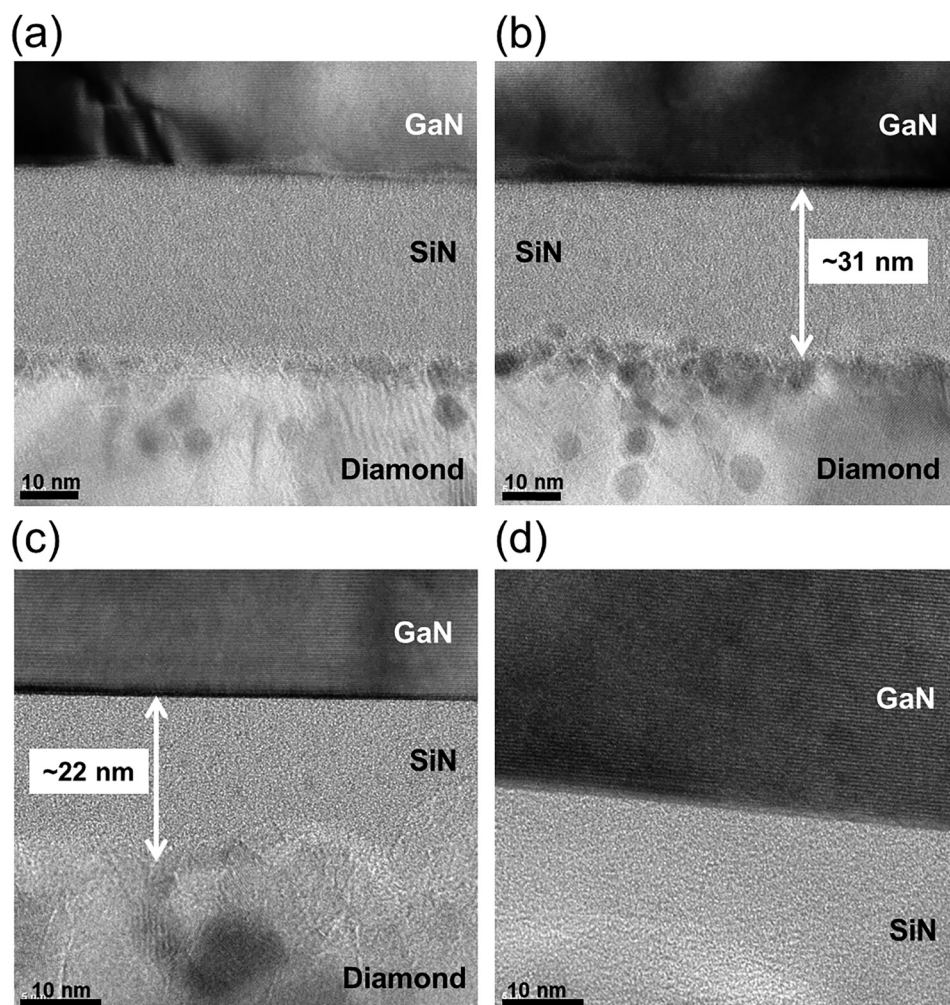


FIG. 1. Representative cross-sectional TEMs near the GaN-diamond interface of ((a) and (b)) the 0.85 μm GaN sample in set A and of the (c) 0.58 μm and (d) 0.74 μm GaN samples in set B. For the sample in set A, near-interfacial disorder, including dislocations, can be observed in the GaN layer close to the interface with the disordered (amorphous) SiN layer ((a) and (b)), whereas for the two samples in set B, the GaN-SiN interface is relatively abrupt with no apparent near-interfacial defects ((c) and (d)). The thickness of the SiN interlayer between the GaN and diamond is ~ 31 nm for the sample in set A, while that is ~ 22 nm for the two samples in set B.

from the growth interface with initial nanocrystal grains of ~ 6 nm for the sample in set A, whereas for the samples in set B this region is estimated to be slightly thinner (~ 23 nm) with an initial grain size of ~ 21 nm. We electron-beam evaporate a thin Al film of ~ 47 nm—which acts as the temperature transducer for TDTR measurements—on the two sets of samples.

B. Time-domain thermoreflectance

The thermal conductivity of the GaN layer and the thermal boundary resistance at the interface between the GaN and diamond are measured with TDTR,^{2,21–24} an ultrafast, pump-probe, optical measurement technique. In our implementation of TDTR, we use a mode-locked Nd:YVO₄ laser that generates ~ 9 ps wide pulses at a repetition rate of 82 MHz and a wavelength of 1064 nm. These pulses are split into two components: pump (heater) and probe (thermometer). An electro-optic modulator amplitude-modulates the pump pulses at frequencies between 2 and 8 MHz and a periodically poled LiNbO₃ crystal frequency-doubles the pump pulses to 532 nm. The modulated, frequency-doubled pump pulses heat the sample and a transient temperature field is created within the sample. The probe pulses are time-delayed up to 3.6 ns using the delay stage with respect to the heating of the pump pulses and measure the temporal variations in the surface temperature of the Al transducer via a proportional change in the reflectivity of Al at the pump modulation frequency. The laser spot sizes ($1/e^2$ diameters) are ~ 10.2 and ~ 6.2 μm for the pump and probe, respectively.²¹

A single-mode fiber is employed after the delay stage to minimize variations in the probe spot size and the overlap and alignment of the pump and probe with delay time.^{22,25} We independently monitor the amplitudes of the pump and the delay-time-dependent probe from the thermoreflectance signal and correct for laser intensity fluctuations and the dependence of the probe beam intensity on the delay time.²⁵ This enables us to utilize both the amplitude ($\sqrt{V_{in}^2 + V_{out}^2}$) and the ratio ($-V_{in}/V_{out}$) of the in-phase (V_{in}) and out-of-phase (V_{out}) readings of the lock-in amplifier as a function of pump-probe delay time in our data analysis. An analytical solution of the three-dimensional heat diffusion equation in cylindrical coordinates is compared to the TDTR data to extract the thermal parameters of interest.²³ We have validated the accuracy of our system with SiO₂ and single crystalline Si reference samples and found values ($1.33 \pm 0.1 \text{ W m}^{-1} \text{ K}^{-1}$ for SiO₂ and $145 \pm 15 \text{ W m}^{-1} \text{ K}^{-1}$ for Si) that are within 2% of literature values for both materials. Further details of the TDTR system used herein can be found in Refs. 21, 25, and 26. For more general and detailed descriptions of the TDTR methodology and data analysis, see Refs. 2, 23, and 24.

Both the amplitude and ratio data are compared with a three-dimensional, multilayer solution²³ to the heat diffusion equation to extract the three parameters: (i) the thermal boundary resistance at the interface between the Al and GaN layers (TBR_{Al-GaN}), (ii) the thermal conductivity of the GaN layer (k_{GaN}), and (iii) the thermal boundary resistance at the interface between the GaN layer and the diamond substrate ($TBR_{GaN-Diam}$). The GaN-diamond thermal boundary resistance is not the discrete boundary resistance but rather

involves multiple resistance contributions: (i) the thermal resistance of the near-interfacial, low-quality GaN region (i.e., the GaN region with localized defects near the interface with the SiN interlayer as observed in Figs. 1(a) and 1(b)), (ii) the two discrete boundary resistances at the SiN layer interfaces with the GaN and the diamond, (iii) the volumetric thermal resistance of the SiN layer, and (iv) the thermal resistance of the near-interfacial diamond (i.e., the resistance of the initial, nanocrystalline nucleation/coalescence regions adjacent to the growth interface). These resistance contributions are lumped and represented as a single effective boundary resistance, $TBR_{GaN-Diam}$.⁴

All other input parameters except these three fitting parameters in our multilayer thermal model are either determined from a separate measurement or assumed from literature values. We estimate the thermal conductivity of the topmost Al transducer layer (k_{Al}) by measuring the electrical conductivity with the four-probe technique and calculating the thermal conductivity using the Wiedemann-Franz law.² We measure the Al, GaN, and SiN layer thicknesses (d_{Al} , d_{GaN} , and d_{SiN} , respectively) via the cross-sectional TEM. The uncertainty in the thickness measurement is estimated to be less than 2%. A 2% error in d_{GaN} propagates to 2%–3% errors in k_{GaN} and $TBR_{GaN-Diam}$ for all measured three samples. The volumetric heat capacities of the Al, GaN, and diamond (C_{Al} , C_{GaN} , and C_{Diam} , respectively) are taken from literature values^{27–30} and assigned 2% uncertainty.³⁰ A 2% variation in C_{GaN} leads to an $\sim 4\%$ variation in k_{GaN} and an $\sim 4\%$ variation in $TBR_{GaN-Diam}$ for the $0.85 \mu\text{m}$ GaN sample in set A. For the $0.58 \mu\text{m}$ GaN sample in set B, the corresponding variations in k_{GaN} and $TBR_{GaN-Diam}$ are $\sim 4\%$ and $\sim 3\%$, respectively. The diamond thermal conductivity (k_{Diam}) is assumed to have a range of values from 400 to 700 $\text{W m}^{-1} \text{ K}^{-1}$, which represents the values for low-quality CVD diamond (i.e., within several micrometers of the growth interface).^{20,21,31} As discussed in Section II C, sensitivity analysis shows that variations in k_{Diam} have a minimal impact on the fitted parameters; for example, a 40% change in k_{Diam} results in an $\sim 2\%$ change in k_{GaN} and an $\sim 5\%$ change in $TBR_{GaN-Diam}$ for the sample in set A. All these procedures reduce the problem of transient heat conduction through the GaN-diamond multilayer structure to the $TBRs/k_{GaN}$ coupled problem. To uniquely separate these properties, we utilize multiple components in the TDTR signal and multiple modulation frequencies in our data analysis.

Note that we treat the GaN/SiN/diamond interfaces as a single interface in our data analysis. We extract a total $TBR_{GaN-Diam}$ value and ignore the heat capacitance of the SiN layer. This is a valid approach because in our measured samples the GaN layers are approximately 30 times thicker than the SiN layers and thus, the heat capacitance of the SiN layers is very small compared to that of the GaN layers. To further support our approach, we refit the data with considering the heat capacitance of the SiN layer between the GaN and diamond. In this case, we fit for the effective thermal resistance of the SiN layer, which combines the volumetric SiN resistance and the GaN-SiN and SiN-diamond boundary resistances. This yields an effective SiN resistance value of $17.3 \text{ m}^2 \text{ K GW}^{-1}$ for the thinnest GaN sample ($0.58 \mu\text{m}$ GaN sample), which is less than 1% different from the extracted

$TBR_{\text{GaN-Diam}}$ value of $17.4 \text{ m}^2 \text{ K GW}^{-1}$. Variations in the SiN heat capacity have a negligible impact on the fitted effective SiN resistance values; for example, a 50% change in the SiN heat capacity results in a less than 1% change in the fitted effective SiN resistance for the thinnest GaN sample.

C. Sensitivity analysis

We define the TDTR sensitivity coefficient as

$$S_\beta = \frac{\partial \ln(R)}{\partial \ln(\beta)}, \quad (1)$$

where R is the amplitude or ratio thermoreflectance signal and β is the parameter of interest in the multilayer thermal model.^{2,21,24,26} Figure 2 illustrates representative sensitivity plots of the $0.85 \mu\text{m}$ GaN sample in set A. As shown in Fig. 2(a), the amplitude signal at a high modulation frequency

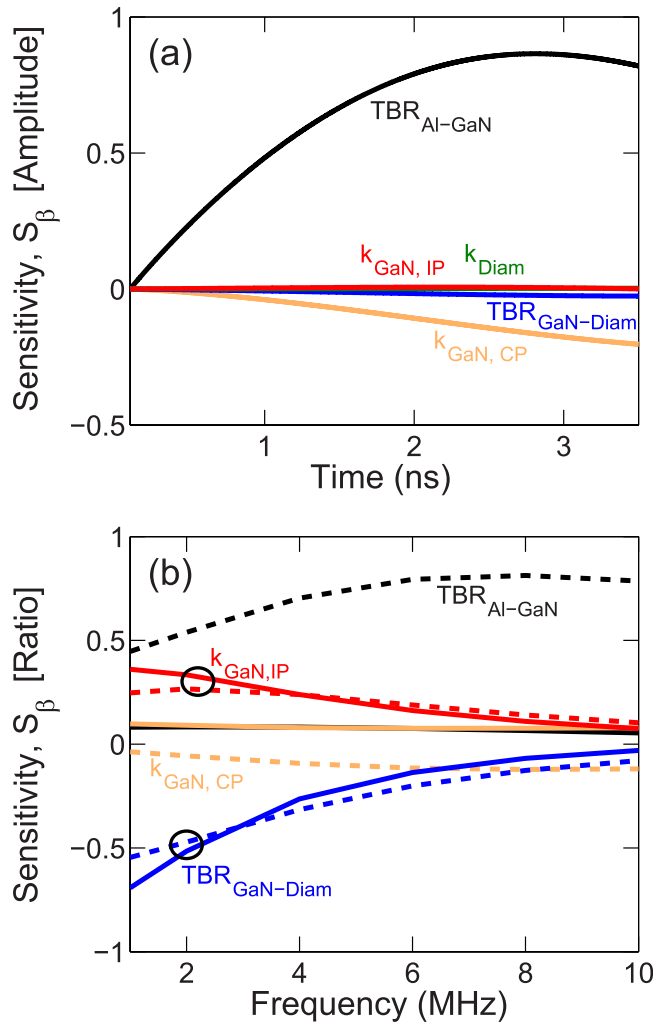


FIG. 2. Sensitivity, S_β , to major variable parameters, β , in the multilayer thermal model for the $0.85 \mu\text{m}$ GaN sample in set A. We plot the measurement sensitivities to the thermal boundary resistances at the Al-GaN and GaN-diamond interfaces ($TBR_{\text{Al-GaN}}$ and $TBR_{\text{GaN-Diam}}$, respectively), the cross-plane and in-plane thermal conductivities of the GaN layer ($k_{\text{GaN,CP}}$ and $k_{\text{GaN,IP}}$, respectively), and the diamond thermal conductivity (k_{Diam}) (a) as a function of pump-probe delay time at a modulation frequency of 8 MHz and (b) as a function of modulation frequency at fixed delay times of 200 ps (solid lines) and 3.5 ns (dashed lines). The sensitivities to k_{Diam} are now shown in (b) for brevity (~ 0.08 at both delay times).

(8 MHz) is mostly governed by $TBR_{\text{Al-GaN}}$ and minimally affected by the other parameters over the entire delay time. The use of the high-frequency amplitude data therefore enables us to separate $TBR_{\text{Al-GaN}}$ from the other parameters. We determine $TBR_{\text{Al-GaN}}$ mainly from the 8 MHz amplitude data, but the extracted $TBR_{\text{Al-GaN}}$ values from the amplitude data across the frequencies from 2 to 8 MHz are fairly independent of the modulation frequency; variations in $TBR_{\text{Al-GaN}}$ are less than 2%. This suggests that the Al-GaN boundary resistance extracted here is nearly independent of the other parameters.

Utilizing the values of $TBR_{\text{Al-GaN}}$ obtained by fitting the amplitude signal at 8 MHz, we fit the ratio signal at a low modulation frequency (2 MHz) to simultaneously extract k_{GaN} and $TBR_{\text{GaN-Diam}}$. When extracting these two parameters, the GaN layer is assumed to be isotropic, thus, the extracted k_{GaN} is the (isotropic) effective thermal conductivity that averages in-plane and cross-plane thermal conductivities. Due to relatively high values of $TBR_{\text{GaN-Diam}}$ ($17\text{--}32 \text{ m}^2 \text{ K GW}^{-1}$, as shown later in Section III) and the associated enhanced lateral spreading of heat within the GaN layer, the ratio signal is highly sensitive to the in-plane thermal conductivity of the GaN layer ($k_{\text{GaN,IP}}$) as well as $TBR_{\text{GaN-Diam}}$, while less sensitive to the cross-plane thermal conductivity of the GaN layer ($k_{\text{GaN,CP}}$). This is more significant at lower modulation frequencies (see Fig. 2(b)). At 2 MHz, the absolute values of the ratio of the sensitivities to $k_{\text{GaN,IP}}$ and $k_{\text{GaN,CP}}$ (i.e., $|S_{k_{\text{GaN,IP}}}/S_{k_{\text{GaN,CP}}}|$) are ~ 4 and ~ 5 at delay times of 200 ps and 3.5 ns, respectively, in Fig. 2(b). The sensitivity to k_{Diam} is ~ 0.08 at both delay times for the 2 MHz ratio signal (not shown in Fig. 2(b) for the sake of clarity).

D. Uncertainty analysis

The uncertainties in k_{GaN} and $TBR_{\text{GaN-Diam}}$ are evaluated via the standard error propagation analysis, which has been commonly used in thermal property measurements employing TDTR.^{2,21,26,32,33} The uncertainty of the measurement of errors of the input parameters β_i in the multilayer thermal model, as defined by the following equation:

$$\Delta k_{\text{GaN}} = \sqrt{\sum_i \left(\frac{\partial k_{\text{GaN}}}{\partial \beta_i} \Delta \beta_i \right)^2},$$

$$\Delta TBR_{\text{GaN-Diam}} = \sqrt{\sum_i \left(\frac{\partial TBR_{\text{GaN-Diam}}}{\partial \beta_i} \Delta \beta_i \right)^2},$$

$$\beta_i = d_{\text{Al}}, k_{\text{Al}}, d_{\text{GaN}}, C_{\text{GaN}}, k_{\text{Diam}}, TBR_{\text{Al-GaN}}. \quad (2)$$

In Eq. (2), we consider the errors propagated from uncertainties in the Al thickness and thermal conductivity (d_{Al} and k_{Al}), the GaN thickness and heat capacity (d_{GaN} and C_{GaN}), and the diamond thermal conductivity (k_{Diam}), as well as that in the Al-GaN boundary resistance ($TBR_{\text{Al-GaN}}$, determined from the 8 MHz amplitude data). The extent of the error bars for $TBR_{\text{Al-GaN}}$ is predominantly governed by the uncertainty in d_{Al} .

In addition, we consider the sum of the deviation between the TDTR data and the model prediction in a manner similar to those of Refs. 32 and 33,

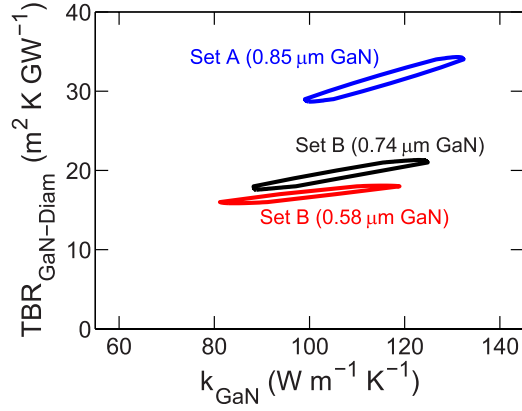


FIG. 3. Contour of the sum of the deviation between the TDTR data and the model prediction in the two-dimensional parameter space of k_{GaN} and $TBR_{\text{GaN-Diam}}$ for all three samples measured in this work. Each contour line represents the set of solution pairs of the two parameters with the deviation sum set as the twice of the minimum deviation (i.e., $\sigma = 2\sigma_{\min}$).

$$\sigma = \frac{\sum_{i=1}^n \left(\frac{R_{m,i}(k_{\text{GaN}}, TBR_{\text{GaN-Diam}}) - R_{d,i}}{R_{d,i}} \right)^2}{n}, \quad (3)$$

where R_m and R_d are the thermoreflectance ratios from the model calculation and the data, respectively, at each delay time and at the 2 MHz modulation frequency, and the summation is over delay times from 0.1 ns to 3.5 ns (n is the total number of delay times). For the best-fit values of k_{GaN} and $TBR_{\text{GaN-Diam}}$, σ reaches its minimum ($\sigma_{\min}$ is ~ 0.0002 for all three samples measured here). Figure 3 plots contours of the deviation sum in the two-dimensional parameter space of k_{GaN} and $TBR_{\text{GaN-Diam}}$, where σ is set to $2\sigma_{\min}$.^{32,33} Each contour line is centered at the best-fit values of k_{GaN} and $TBR_{\text{GaN-Diam}}$, and represents the set of possible solution pairs that fit the TDTR data reasonably well. The uncertainties of k_{GaN} and $TBR_{\text{GaN-Diam}}$, determined from the contour plot, are $\sim 14\%$ and $\sim 9\%$, respectively, for the thickest GaN sample (the 0.85 μm GaN sample in set A) and are $\sim 17\%$ and $\sim 6\%$, respectively, for the thinnest GaN sample (the 0.58 μm GaN sample in set B). This reflects the decreased (increased) measurement sensitivity to k_{GaN} and the increased (decreased) measurement sensitivity to $TBR_{\text{GaN-Diam}}$ with decreasing (increasing) GaN thickness. The uncertainties estimated from the contour plot are associated with the ability of the current data extraction method to uniquely resolve k_{GaN} and $TBR_{\text{GaN-Diam}}$, as well as with the quality of the model fit.³²⁻³⁴ The total uncertainties of k_{GaN} and $TBR_{\text{GaN-Diam}}$ are evaluated by adding the uncertainties from the contour plot in quadrature together with the uncertainties propagated from the errors in estimating the input parameters in the multilayer thermal model (as discussed above). Table I reports the final

TABLE II. Percentage errors in k_{GaN} and $TBR_{\text{GaN-Diam}}$ from various sources of uncertainty for the 0.85 μm GaN sample in set A.

	d_{Al}	k_{Al}	d_{GaN}	C_{GaN}	k_{Diam}	$TBR_{\text{Al-GaN}}$	Contour plot	Total uncertainty
% Δk_{GaN}	15.1	0.6	2.6	3.8	2.2	8.6	14.2	23.0
% $\Delta TBR_{\text{GaN-Diam}}$	9.4	0.4	1.9	3.9	5.1	7.9	8.8	16.6

uncertainties of all the fitted parameters along with the best-fit values. Uncertainties associated with spot-to-spot variability in the measurements are relatively small and lie within the error bars reported in Table I. A representative error propagation analysis is provided in Table II, which shows the percentage errors contributed towards the extraction of k_{GaN} and $TBR_{\text{GaN-Diam}}$ from the various sources of uncertainty for the 0.85 μm GaN sample in set A.

III. RESULTS AND DISCUSSION

Table I summarizes the extracted room-temperature thermal properties with the error bars for all three samples measured in this work. The results indicate a factor of ~ 2 reduction in the GaN-diamond thermal boundary resistance between the two sets of samples and a slight reduction in the GaN thermal conductivity with a decrease in the GaN thickness. It is worth noting that the GaN thermal conductivity determined here is the effective thermal conductivity, i.e., a weighted average value between in-plane and cross-plane thermal conductivities. But more weight is on the in-plane thermal conductivity due to much higher measurement sensitivity to the in-plane conductivity than the cross-plane conductivity at the low modulation frequency used here (i.e., 2 MHz); see Fig. 2(b). The extracted GaN thermal conductivities here therefore well approximate the in-plane conductivities of the GaN layers.

We calculate the in-plane thermal conductivity versus GaN layer thickness utilizing the semiclassical phonon thermal conductivity integral model,³⁵⁻³⁸ which is based on an approximate analytical solution of the phonon Boltzmann transport equation. We use an isotropic sinusoidal dispersion^{39,40} for GaN with the three acoustic phonon branches lumped into a single, triply degenerate branch: $\omega = \omega_0 \sin(\pi q/2q_0)$, where ω and q are the phonon frequency and wavevector, respectively. Here, $q_0 = (6\pi^2\eta)^{1/3}$ is the Debye cut-off wavevector, η is the number density of primitive unit cells, $\omega_0 = 2v_s q_0/\pi$ is the highest phonon frequency at the boundary of the first Brillouin zone, and v_s is the average sound velocity.³⁹ The optical phonon modes are neglected in this calculation because they are insignificant for heat transport. All material parameters of wurtzite GaN are taken from Ref. 41. The Umklapp scattering ($\tau_U^{-1} = BT\omega^2 \exp(-C/T)$) and isotope scattering

TABLE I. Extracted room-temperature thermal properties.

Sample	$TBR_{\text{Al-GaN}}$ ($\text{m}^2 \text{ K GW}^{-1}$)	k_{GaN} ($\text{W m}^{-1} \text{ K}^{-1}$)	$TBR_{\text{GaN-Diam}}$ ($\text{m}^2 \text{ K GW}^{-1}$)
0.85 μm GaN/31 nm SiN/Diamond (set A)	11.3 ± 0.3	117 ± 27	31.8 ± 5.3
0.74 μm GaN/22 nm SiN/Diamond (set B)	15.6 ± 0.4	105 ± 32	19.8 ± 4.1
0.58 μm GaN/22 nm SiN/Diamond (set B)	10.5 ± 0.3	101 ± 28	17.4 ± 3.0

processes are considered to fit the thermal conductivity integral model to the temperature-dependent conductivity data of bulk GaN,⁴² yielding $B = 7.6 \times 10^{-20} \text{ s K}^{-1}$ and $C = 89 \text{ K}$. To account for the size effect due to phonon boundary scattering, we employed a conductivity reduction function, F , for thin films derived by Sondheimer⁴³

$$F(\delta) = 1 - \frac{3}{8\delta} + \frac{3}{2\delta} \int_1^\infty \left(\frac{1}{t^3} - \frac{1}{t^5} \right) \exp(-\delta \times t) dt, \quad (4)$$

where $\delta = d/\Lambda_{\text{bulk}}$, d is the layer thickness, Λ_{bulk} is the bulk phonon mean free path, t is a variable of integration, and phonon boundary scattering is assumed to be completely diffuse.^{44,45} In this approach, the bulk phonon scattering time, τ_{bulk} , is reduced by the conductivity reduction function through $\tau(\omega, T) = F(\delta)\tau_{\text{bulk}}(\omega, T)$, where $\tau_{\text{bulk}}(\omega, T)^{-1} = \tau_U(\omega, T)^{-1} + \tau_P(\omega)^{-1}$ and $\tau_P(\omega)^{-1}$ is the phonon scattering rate due to point defects. We model the point defect scattering rate with the Rayleigh theory (i.e., $\tau_P^{-1} \sim \Gamma\omega^4$, where Γ represents the strength of the point defect scattering) and consider the mass-difference-induced scattering, as well as the scattering owing to an elastic strain field of a point defect.^{46,47} A more refined modeling approach could consider phonon scattering on dislocation, stacking faults, and other imperfections, although the ambiguity could be created by introducing additional adjustable parameters.

In Fig. 4, we plot the room-temperature thermal conductivity of GaN layers versus layer thickness, including our data as well as other data in the literature. Filled markers represent the in-plane thermal conductivity, including our data (red filled circles) as well as the data by Hodges *et al.*⁴⁸ (blue filled square), where $60 \text{ W m}^{-1} \text{ K}^{-1}$ was measured for a $0.15 \mu\text{m}$ thick GaN film using micro-Raman thermometry on

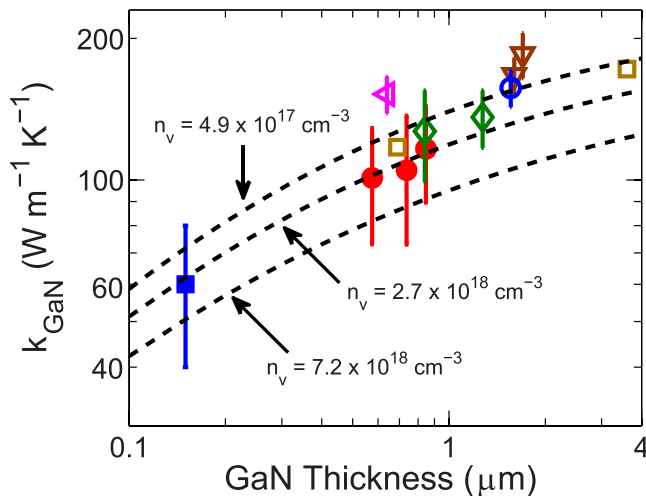


FIG. 4. Thermal conductivity of GaN layers as a function of layer thickness at room temperature, showing how our data (red filled circles) compare with literature and model predictions. Filled markers, including our data and the data by Hodges *et al.*⁴⁸ (blue filled square), correspond to in-plane thermal conductivity, while open markers correspond to cross-plane thermal conductivity. The results of the thermal conductivity integral model for the in-plane GaN thermal conductivity are shown at different vacancy concentrations, n_v (black dashed lines). Legend: light brown open squares,⁴⁹ green open diamonds,⁵⁰ magenta open left-facing triangle,⁵¹ blue open circle,⁵² and brown open down-facing triangles.²⁶

GaN device structures. Open markers represent the cross-plane thermal conductivity. These cross-plane conductivity data are from Ref. 49, where 117 and $172 \text{ W m}^{-1} \text{ K}^{-1}$ were measured for 0.69 and $3.6 \mu\text{m}$ thick GaN films, respectively, Bougher *et al.*⁵⁰ where 127 and $136 \text{ W m}^{-1} \text{ K}^{-1}$ were measured for 0.84 and $1.3 \mu\text{m}$ thick GaN films, respectively, Ziade *et al.*⁵¹ where $\sim 150 \text{ W m}^{-1} \text{ K}^{-1}$ was measured for a $0.64 \mu\text{m}$ thick GaN film, and Cho *et al.*^{26,52} where 157 , 167 , and $185 \text{ W m}^{-1} \text{ K}^{-1}$ were measured for 1.5 , 1.6 , and $1.7 \mu\text{m}$ thick GaN films, respectively. These cross-plane thermal conductivity values appear to be slightly higher than the in-plane conductivity values measured in this work. This could be a result of a higher density of defects in the current set of samples. Another possibility is due to a potential role played by anisotropy in thermal conductivity in GaN thin films, although a recent study⁵³ using first principles calculations has reported the insignificance of thermal conductivity anisotropy in bulk wurtzite GaN over the range of temperatures from 100 to 500 K . It has been previously suggested that the orientation of defects, relative to the direction of heat flow, influences thermal conductivity of defective thin films,^{54,55} which may lead to anisotropic heat conduction in such films.

Figure 4 also shows the predictions of the thermal conductivity integral model for the in-plane GaN thermal conductivity, which considers a vacancy as a type of point defect for simplicity (since a vacancy is the strongest scatterer due to the largest mass difference).²⁶ The in-plane thermal conductivity data (filled markers) are consistent with the model using a vacancy concentration near $3 \times 10^{18} \text{ cm}^{-3}$, suggesting that phonon scattering by material defects and interfaces governs the thermal conductivity (hence the thermal spreading resistance) of the GaN layer. Note that our model considers the reduction in thermal conductivity due to phonon scattering processes but does not consider phonon confinement effects (e.g., modification of the phonon dispersion relation and the associated reduction of the phonon group velocity),^{56,57} which are expected to be negligible at our GaN film thicknesses and measurement temperature.^{45,57}

As shown in Table I, we observe a factor of 2 reduction in the GaN-diamond thermal boundary resistance between the $0.85 \mu\text{m}$ GaN on 31 nm SiN on the diamond sample in set A and the $0.58 \mu\text{m}$ GaN on 22 nm SiN on the diamond sample in set B. The reduction observed in the GaN-diamond boundary resistance can be attributed to the relatively abrupt GaN/SiN interface and the reduced SiN thickness of the two samples in set B (see Figs. 1(c) and 1(d)), as compared to the sample in set A. Different near-interfacial diamond quality—which depends on near-interfacial imperfection, grain size, and nucleation region thickness—could also play a role in the observed reduction in the boundary resistance.^{10,11,17–21} Previous works have shown that near-interfacial defects such as dislocations and planar defects can be responsible for a factor of 2–18 increase in thermal boundary resistance for GaSb/GaAs and AlN/SiC interfaces.^{58,59} The lowest of the GaN-diamond boundary resistances measured in this work, $\sim 17 \text{ m}^2 \text{ K GW}^{-1}$, is close to the lower end of the range of reported literature values at room temperature, from 12 to

$50 \text{ m}^2 \text{ K GW}^{-1}$, measured by micro-Raman thermometry⁸ and the nanosecond transient thermoreflectance technique.^{9–11}

We make a further effort to assess the relative contributions from the different components of the GaN-diamond thermal boundary resistance. We predict the discrete boundary resistances at the two SiN boundaries (with the GaN and the diamond) using the diffuse mismatch model (DMM), and then compare the sum of the two discrete boundary resistances with the measured (total) GaN-diamond boundary resistance to separate interface and volumetric contributions. Here, we use the variant of the DMM described by Bellis *et al.* (Ref. 60). This modification of the model considers the actual phonon density of states in materials—the original model, proposed by Schwartz and Pohl (Ref. 61), assumes the Debye density of states in both contacting materials—by using the measured volumetric heat capacity data. While many variations of the DMM exist, the DMM using measured heat capacity data has been used to model thermal boundary resistances at room temperature and above for a number of interfaces,^{4,51,52,62–64} and is given by

$$TBR = \left(\frac{\alpha_{1 \rightarrow 2}}{12} c_{1D}^3 \sum_j c_{1j}^{-2} \right)^{-1} C_1(T)^{-1}, \quad (5)$$

where $C_1(T)$ is the measured heat capacity of material 1 at temperature T , c_{ij} 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. The transmission coefficient $\alpha_{1 \rightarrow 2}$ quantifies the percentage of phonons that transmit from material 1 to 2 and hence transfer thermal energy, and is given by a ratio of the phonon speeds in each material

$$\alpha_{1 \rightarrow 2} = \frac{\sum_j c_{2j}^{-2}}{\sum_j c_{1j}^{-2} + \sum_j c_{2j}^{-2}}. \quad (6)$$

Using the DMM (Eqs. (5) and (6)), we calculate the GaN/SiN thermal boundary resistance to be $\sim 1 \text{ m}^2 \text{ K GW}^{-1}$ and the SiN/diamond thermal boundary resistance to be $\sim 2 \text{ m}^2 \text{ K GW}^{-1}$. We subtract the sum of these two discrete boundary resistances from the measured GaN-diamond boundary resistance, and then estimate the volumetric resistance of the SiN layer. This procedure yields the SiN thermal resistances of $14\text{--}17 \text{ m}^2 \text{ K GW}^{-1}$ for the two samples with the 22 nm SiN layer in set B and $\sim 29 \text{ m}^2 \text{ K GW}^{-1}$ for the sample with the 31 nm SiN layer in set A, which account for 80%–90% of the measured GaN-diamond boundary resistance values. Although the DMM does not consider the contributions from near-interfacial defects within the GaN and the low thermal conductivity of near-interfacial diamond, this calculation implies that the measured GaN-diamond boundary resistance is predominantly associated with the low thermal conductivity of the amorphous SiN layer. The estimated SiN thermal resistances can be translated to the SiN thermal conductivity of $1.1\text{--}1.5 \text{ W m}^{-1} \text{ K}^{-1}$, consistent with previous reports^{65,66} in the literature of the thermal conductivity of amorphous SiN thin films. Phonon velocities of SiN and diamond for the DMM calculation are taken from Refs. 67 and 61, respectively.

Our findings, together with the past studies,^{4,8–12,26} suggest that the thermal resistance of GaN-SiN-diamond composite substrates is determined primarily by the strength of phonon scattering due to defects and interfaces. The minimum (maximum) possible thermal resistance (conductance) for composite GaN-diamond substrates can be therefore achieved when the GaN layer and interface approach near crystalline perfection. To estimate the maximum possible thermal conductivity of the GaN layers, we again use the thermal conductivity integral model with the Sondheimer-type reduction function but do not consider phonon scattering on external defects. We consider phonon scattering on isotopes; the isotope scattering strength Γ of 2.74×10^{-4} (Ref. 37)—which can be translated to a minimal defect concentration of $4.9 \times 10^{17} \text{ cm}^{-3}$ within the GaN layer (see the topmost black dashed line in Fig. 4)—yields $k_{\text{GaN}} = 120 \text{ W m}^{-1} \text{ K}^{-1}$ at $d_{\text{GaN}} = 0.58 \text{ }\mu\text{m}$ and $k_{\text{GaN}} = 134 \text{ W m}^{-1} \text{ K}^{-1}$ at $d_{\text{GaN}} = 0.85 \text{ }\mu\text{m}$, which are 15%–19% higher than our measured values at the same thicknesses. The GaN-diamond thermal boundary resistance can reach its lower bound when (i) the GaN and diamond directly form the interface without the SiN interlayer and (ii) phonon transport across the interface is dictated by the mismatch in the phonon density of states between GaN and diamond, not by scattering by any near-interfacial defects. Assuming direct contact between the GaN and diamond and using the DMM with the heat capacity correction to the phonon density of states (Eqs. (5) and (6)), we calculate the lower bound of the GaN-diamond boundary resistance to be $\sim 3 \text{ m}^2 \text{ K GW}^{-1}$.

Recent studies using molecular dynamics (MD) simulations^{68–71} have investigated the potential of reducing thermal boundary resistance below the limit set by the inherent mismatch in the phonon density of states between two materials forming an interface. These studies have shown that interfacial thermal transport between vibrationally mismatched materials may be enhanced by incorporating an interfacial film with mediating vibrational properties—which serves as a phonon bridge—between them.^{68,70,71} It was also suggested that surface nanostructuring (e.g., three-dimensional interlaced GaN and SiC nanopillars at GaN-SiC interfaces in Ref. 71) may benefit interfacial phonon transport primarily owing to the increased surface area and better phonon matching at the interface. For GaN-SiC interfaces, such interface nanoengineering may offer the possibility of reducing the thermal boundary resistance by up to 40%, compared to that of a bare GaN-SiC interface.⁷¹ This suggests that with further efforts in interface nanoengineering the GaN-diamond thermal boundary resistance may fall below the DMM limit, at which point the phonon conduction cooling of GaN-diamond electronics would be fundamentally enhanced.

IV. CONCLUSIONS

This work extracts the GaN thermal conductivity and the GaN-diamond thermal boundary resistance simultaneously for two sets of GaN-diamond composite substrates using TDTR. The GaN thermal conductivity values determined here ($101\text{--}117 \text{ W m}^{-1} \text{ K}^{-1}$) well approximate the in-plane thermal conductivity values due to enhanced lateral

spreading of heat within the GaN layer associated with relatively high values of the measured GaN-diamond thermal boundary resistances ($17\text{--}32\text{ m}^2\text{ K GW}^{-1}$). The data for the GaN thermal conductivity agree with the calculations of the semiclassical phonon thermal conductivity integral model for the in-plane thermal conductivity, which considers the size effect of increased phonon scattering at interfaces, as well as the scattering on point defects at concentrations near $3 \times 10^{18}\text{ cm}^{-3}$. The observations made in TEMs suggest that the SiN volume resistance and phonon scattering on near-interfacial defects in the GaN and diamond can be important for the thermal boundary resistance across the GaN-diamond interface. These findings highlight that the thermal resistance in lattice-mismatched, hetero-integrated systems, which are common for a variety of contemporary electronic device technologies, is dictated by phonon scattering due to material defects and interfaces.

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