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Investigation of the thermal boundary resistance at the III-Nitride/substrate interface using optical methods

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Heat removal from III-Nitride-based devices into a substrate depends also on an acoustic coupling at III-Nitride/substrate interface. We investigate thermal boundary resistance (TBR) and its effects on temperature distribution for GaN layers on Si, SiC, or sapphire substrates. Micro-Raman method is used for the investigation of TBR at the GaN/Si interface while the transient interferometric mapping (TIM) method is used for investigation of GaN/SiC and GaN/sapphire systems. Thermal modeling is used to analyze the experimental data. We found TBR to be $\sim 7 \times 10^{-8} \text{ m}^2 \text{ K/W}$ for GaN/Si and $\sim 1.2 \times 10^{-7} \text{ m}^2 \text{ K/W}$ for GaN/SiC interfaces. The role of TBR at the GaN/sapphire interface in the poor heat transfer from GaN to substrate is found to be less important. It is suggested that the substrate cooling efficiency may be improved if fewer defects are present at the interface to the GaN epistructure. © 2007 American Institute of Physics. [DOI: [10.1063/1.2435799](https://doi.org/10.1063/1.2435799)]

I. INTRODUCTION

Fast developing of the high-power GaN-based high electron mobility transistors (HEMTs) requires optimization of the device thermal management. Therefore understanding of the mechanism of the heat removal from the device through the substrate is needed. A particular attention has recently been devoted to the investigation of the thermal coupling at the III-nitride/substrate interface.¹⁻⁵ It has been shown that a difference in acoustic impedance of the materials forming the interface gives the level of thermal coupling and determines the thermal boundary resistance (TBR).^{1,2} It has also been pointed out that dislocations at the interface may give rise to an additional increase of TBR and the effect from dislocations may become dominant.^{1,2} Although substantial device “overheating”² and performance degradation due to TBR has been reported,³ most of reports ignore the effect of TBR in thermal modeling.

Apart from a few reports^{1,4,5} there is a lack of experimental values of the TBR at the III-nitride/substrate interface. The value of $\text{TBR} = 7-8 \times 10^{-8} \text{ m}^2 \text{ K/W}$ at the AlN/Si interface of the sputtered AlN film on Si has been obtained by combining pulsed photothermal reflectance technique with thermal modeling.¹ In another study the TBR of $1 \times 10^{-4} \text{ m}^2 \text{ K/W}$ at GaN/sapphire at 4.2 K⁴ (representing $1-5 \times 10^{-7} \text{ m}^2 \text{ K/W}$ at 300 K)³ has been extracted using the

noise analysis. In our previous report GaN-based HEMTs were analyzed in the pulsed operation, giving the TBR value of $7-8 \times 10^{-8} \text{ m}^2 \text{ K/W}$ at the III-nitride/Si interface.⁵ We used a combination of the transient interferometric mapping (TIM) technique with the thermal modeling and the HEMT electrical characterization technique.⁵

In this work we study TBR and its effect on thermal management in transfer length method (TLM) GaN HEMT test structures grown alternatively on three kinds of commonly used substrates materials: Si, SiC, and sapphire. The temperature drop at the III-nitride/Si interface is investigated by using a Micro-Raman spectroscopy technique under the direct current (DC) conditions. The TBR at III-nitride/SiC and III-nitride/sapphire interfaces is characterized in transient mode by TIM. We show that the TBR plays an important role in the thermal management of GaN-based devices.

II. METHODS AND STRUCTURES

A. Methods

Micro-Raman measurements have been performed using a Labram micro-Raman system.⁶ The temperature dependence of the semiconductor phonon frequencies and Stokes/anti Stokes peak intensity⁷ is used for calibration in which an externally heated sample is probed by a laser beam of the Raman system. The temperature increase due to the self-heating effect in the AlGaIn/GaN/Si HEMT test structure is investigated afterwards by comparing the phonon frequen-

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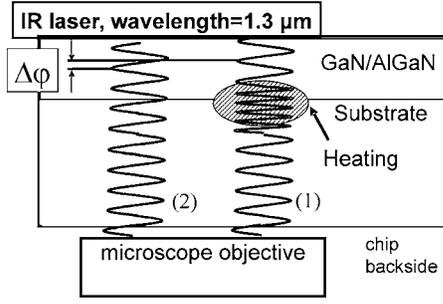


FIG. 1. Laser interferometer measuring principle. The substrate and III-Nitrides epilayer refractive indexes are changes due to the device self-heating. A probe beam (1) and a reference beam (2) are combined in an interferometer. The phase of the probe beam changes due to the self-heating effect (exaggerated for visibility).

cies. For the 514.5 nm line of an Argon-ion laser beam the GaN layer is transparent. However for the given wavelength the beam is strongly absorbed in the Si substrate (what is not a case for SiC and sapphire substrates) with an absorption coefficient of $0.76 \times 10^4 \text{ cm}^{-1}$.⁸ Consequently, by applying the probe beam from the device topside, we can investigate temperature discontinuity ΔT at the III-nitride/Si interface by getting the information both from GaN and from a part of the Si substrate 1–2 μm far from the interface. We notice that the temperature drop at the GaN/SiC and GaN/sapphire interfaces cannot be analyzed by the used Raman setup as in this case the excitation beam penetrates over the whole substrate and a no confocal arrangement was available.

The scanning TIM method is based on measuring of temperature-induced changes in a semiconductor refractive index from the device backside, using a probe laser beam ($\lambda=1.3 \mu\text{m}$). The beam reflected from the device topside undergoes an optical phase shift $\Delta\varphi(t)$, which is measured interferometrically by combining the probe beam (located in the heated area) with an unperturbed reference beam (other branch of the interferometer), see Fig. 1. The phase shift is a sum of two contributions $\Delta\varphi_{\text{GaN}}$ and $\Delta\varphi_{\text{sub}}$ that are proportional to the integral of temperature distribution $T(x, y, z)$ along the beam path (z -axis) in the GaN or substrate, respectively, weighted by dn/dT (Ref. 9):

$$\begin{aligned} \Delta\varphi(x, y, t) &= \Delta\varphi_{\text{GaN}}(x, y, t) + \Delta\varphi_{\text{sub}}(x, y, t) \\ &= \frac{4\pi}{\lambda} \frac{dn}{dT} \Big|_{\text{GaN}} \int_{\text{GaN}} \Delta T(x, y, z, t) dz \\ &\quad + \frac{4\pi}{\lambda} \frac{dn}{dT} \Big|_{\text{sub}} \int_{\text{sub}} \Delta T(x, y, z, t) dz. \end{aligned} \quad (1)$$

The TIM method operates in the transient (pulsed) regime of the self-heated device with a ns time and 1.5 μm space resolution. The TIM method allows also to extract the two-dimensional power density P_{2D} distribution according to Ref. 10:

TABLE I. Thermo-optical parameters used in the thermal modeling.

	dn/dT (K^{-1})	k (W/m K)	c_V (J/K m^3)
SiC	3×10^{-5} (Ref. 13)	490 (Ref. 15)	1.9×10^6 (Ref. 18)
Sapphire	1.3×10^{-5} (Ref. 17)	30 (Ref. 15)	3×10^6 (Ref. 19)
GaN on SiC	5.2×10^{-5} (Ref. 12)	130 (Ref. 15)	3×10^6 (Ref. 18)
GaN on sapphire	4×10^{-5} (Ref. 16)	130	3×10^6

$$\begin{aligned} P_{2D}(x, y, t) &= \frac{\lambda}{dn} \frac{c_V}{4\pi} \frac{\partial \Delta\varphi(x, y, t)}{\partial t} \\ &\quad - \frac{\lambda}{dn} \frac{\kappa}{4\pi} \left(\frac{\partial^2 \Delta\varphi(x, y, t)}{\partial x^2} + \frac{\partial^2 \Delta\varphi(x, y, t)}{\partial y^2} \right), \end{aligned} \quad (2)$$

where c_V and k are the volume specific heat and heat conductivity, respectively. This equation is derived for a homogeneous semiconductor system. Heat transfer to top metallization is neglected in (2) which is good approximation for the short time scale. For a heterogeneous system like GaN on substrate we define so-called *apparent* two-dimensional power density P_{2DA} which is obtained from Eq. (2) by putting for c_V and k only the parameters of GaN.⁵ The values of P_{2DA} can be compared with the “true” P_{2D} obtained as $I(t)V(t)/(\text{heat dissipation area})$ where $I(t)$ and $V(t)$ are current and voltage waveforms. Using this comparison we can *qualitatively* and *directly* trace the heat transfer across the interface.⁵ The higher is the heat transfer from GaN to substrate and the more is the difference between dn/dT , c_V , and k parameters of GaN and the substrate, the more P_{2DA} deviates from P_{2D} . On the other hand the coincidence of $P_{2DA}(t)$ with $P_{2D}(t)$ is obtained either for a homogeneous system or if the value of TBR is infinitive (i.e., no heat transfer to substrate).

B. Simulation

The MATLAB toolbox was used for 2D numerical thermo-optical simulation.⁵ Due to numerical reasons and meshing TBR at the III-Nitride/substrate interface in the model is represented by a virtual 100 nm thick thermally insulation layer having a thermal conductivity k_{ISO} (i.e., $\text{TBR}=100 \text{ nm}/k_{\text{ISO}}$).⁵ Adiabatic boundary conditions were assumed for calculations in the transient state however for a steady-state simulation we considered 300 μm thick substrate with isothermal (300 K) condition at the backside.

Quantitative evaluation of TBR value is based on the comparison of measured $P_{2DA}(t)$ or $\Delta\varphi(t)$ dependencies with the corresponding quantities calculated using the thermal simulation and Eqs. (1) and (2). TBR and dn/dT are taken as fitting parameters. The dn/dT values of the substrate material as well as the heat conductivity and specific heat used in the simulation are given in Table I.

C. Devices

AlGaIn/GaN heterostructures were grown by metal organic chemical vapor deposition systems on different

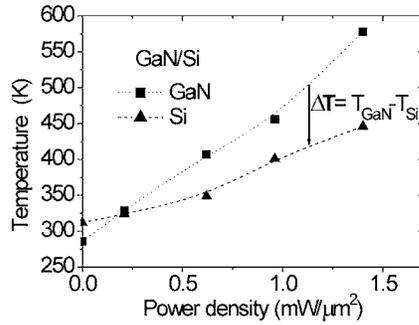


FIG. 2. Micro-Raman measurements of the temperature discontinuity at the GaN/Si interface in the steady state in AlGaN/GaN/Si TLM structure.

$\sim 300 \mu\text{m}$ thick substrates (undoped Si, 2 in. semi-insulating 4H-SiC or sapphire).^{5,11,12} They differ in the used growth sequence. AlN nucleation layer, a $3 \mu\text{m}$ thick GaN buffer and 20 nm AlGaN capped with a 10 nm GaN was used on the sapphire, while for the case of SiC the thickness of the GaN buffer was only $1 \mu\text{m}$. The sequence on Si was more complex having (from the bottom) AlN seed, 450 nm GaN, 12 AlN interlayer, 800 nm GaN and 25 nm AlGaN.⁵

TLM structures consist of annealed Ti/Al/Ni/Au ohmic contacts with 10 and $16 \mu\text{m}$ spacing. The structure width of $100 \mu\text{m}$ is defined by RIE-etched mesa insulation. Conventional optical lithography was used for the device processing, more technological details are given elsewhere.^{5,11,12} Substrates have been polished from the backside to achieve an optical quality for TIM experiments. The use of large area TLM structures is advantageous in respect to short-channel HEMT structures since the uncertainty in the heat dissipation area for TBR calculation can be minimized. As well the space derivative term in (2) plays a minor role for the P_{2DA} evaluation in the middle of the structure where the data are taken, so the P_{2DA} extraction is not affected by the error related to the numerical differentiation.

The transient measurements were performed using an Agilent 8114A pulser.

III. RESULTS AND DISCUSSIONS

A. TBR at GaN/silicon interface

Figure 2 shows a steady-state dependence of temperature T on dissipated power density P_{2D} ($=V \times I$)/area at the GaN/Si interface extracted by the Micro-Raman measurements. One can observe a linear increase of $\Delta T = T_{\text{GaN}} - T_{\text{Si}}$ with P_{2D} , where T_{GaN} and T_{Si} are the temperatures at the GaN and Si side of the interface. We estimate TBR as $\Delta T/P_{2D}$ giving a value of $\sim 7 \times 10^{-8} \text{ m}^2 \text{ K/W}$. This value is in a very good agreement with our previous study ($\text{TBR}_{\text{GaN on Si}} \sim 7-8 \times 10^{-8} \text{ m}^2 \text{ K/W}$) using TIM.⁵ Considering this agreement and the accuracy of the Raman method of $\pm 10 \text{ K}$ (Ref. 6) we assume that the margin of our $\text{TBR}_{\text{GaN on Si}}$ extraction is $\pm 20\%$.

B. TBR on GaN/SiC interface

Initially we have performed measurements in long times were the heat fully propagates into the SiC substrate and the signal from SiC dominates while the signal from GaN is

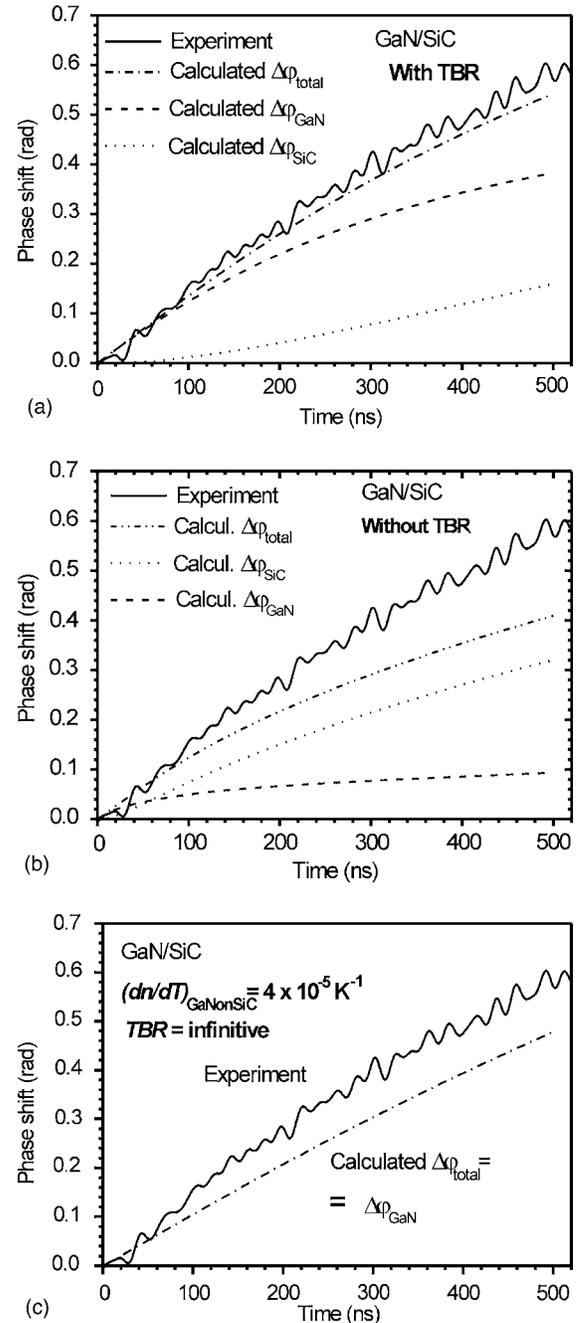


FIG. 3. Comparison of calculated $\Delta\varphi_{\text{total}}(t)$ with experimental TIM $\Delta\varphi(t)$ for $P_{2D} \sim 8.25 \text{ mW}/\mu\text{m}^2$ in AlGaN/GaN/SiC TLM structure for (a) $(\text{TBR})_{\text{GaN/SiC}} = 1.2 \times 10^{-7} \text{ W/m}^2 \text{ K}$, $(dn/dT)_{\text{GaN on SiC}} = 5.2 \times 10^{-5} \text{ K}^{-1}$ (b) $(\text{TBR})_{\text{GaN/SiC}} = 0$, $(dn/dT)_{\text{GaN on SiC}} = 5.2 \times 10^{-5} \text{ K}^{-1}$, and (c) $(\text{TBR})_{\text{GaN/SiC}} = \text{infinity}$, $(dn/dT)_{\text{GaN on SiC}} = 4 \times 10^{-5} \text{ K}^{-1}$. $\Delta\varphi(t)$ are calculated also for SiC and GaN.

negligible. Our measured phase shift values agrees well with the simulated phase shift (not shown) taking into account the $(dn/dT)_{\text{SiC}}$ value of SiC from Table I, calibrating thus $(dn/dT)_{\text{SiC}}$.

Figures 3(a)–3(c) show the experimental and modeled $\Delta\varphi$ transients of studied GaN/SiC TLM device for different values of $(dn/dT)_{\text{GaN on SiC}}$ and $(\text{TBR})_{\text{GaN/SiC}}$. Constant power $P_{2D} \sim 8.2 \text{ mW}/\mu\text{m}^2$ is dissipated in TLM devices for 500 ns . The best fitting of the data is obtained for $(dn/dT)_{\text{GaN on SiC}} = 5.2 \times 10^{-5} \text{ K}^{-1}$ and $(\text{TBR})_{\text{GaN/SiC}} = 1.2$

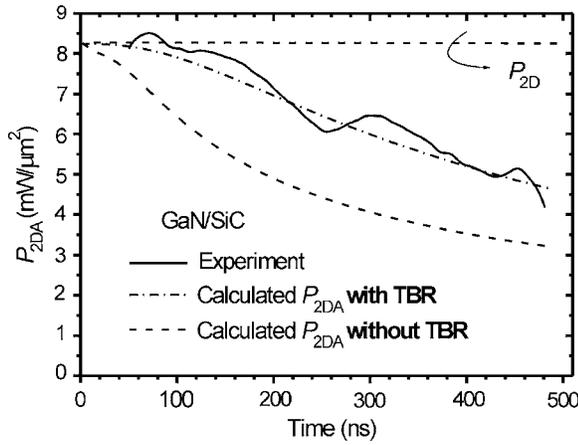


FIG. 4. Comparison of calculated P_{2DA} (with and without considering TBR) and experimental P_{2DA} in AlGaIn/GaN/SiC TLM structure. “True” P_{2DA} obtained from the electrical measurement is also shown.

$\times 10^{-7}$ W/m² K [Fig. 3(a)]. If no TBR is considered for the same $(dn/dT)_{\text{GaN on SiC}} = 5.2 \times 10^{-5}$ K⁻¹, the calculated and measured data differ by $\sim 30\%$, see Fig. 3(b). The contribution of phase shift coming from GaN and SiC are also given in the graphs. If TBR is included [Fig. 3(a)] the phase shift arises mostly from GaN where the heat is confined, and this is in contrary to the case of TBR=0 [Fig. 3(b)].

We have checked the uniqueness of the fitting parameters in our model. It could seem that if $(\text{TBR})_{\text{GaN/SiC}}$ increases, the value of $(dn/dT)_{\text{GaN on SiC}}$ can be reduced due to a resulting temperature rise in GaN [see Eq. (1)], giving rise to the same total phase signal. But our combined $\Delta\varphi$ and P_{2DA} analysis shows that a unique combination of $(dn/dT)_{\text{GaN on SiC}}$ and $(\text{TBR})_{\text{GaN/SiC}}$ exists to fit the experiments because the shape of $\Delta\varphi$ and P_{2DA} curves are specifically sensitive to the combination of dn/dT and TBR. In Fig. 3(c) we show the phase shift for $(dn/dT)_{\text{GaN on SiC}} = 4 \times 10^{-5}$ K⁻¹ and $(\text{TBR})_{\text{GaN/SiC}} = \text{infinity}$. Figure 3(c) represents the case where we took the $(dn/dT)_{\text{GaN on SiC}}$ value obtained for GaN on sapphire substrate (see Sec. III C). Even if we take TBR=infinity, i.e., there is no heat transfer to SiC and temperature in GaN is maximal, the simulated phase shift cannot fit the experiments with $(dn/dT)_{\text{GaN on SiC}} = 4 \times 10^{-4}$ K⁻¹.

The determined fitting parameters are further validated by comparing experimental P_{2DA} with the simulated one, see Fig. 4. The horizontal dashed line represents the “true” power density P_{2D} which is calculated from the device $I(t)$ and $V(t)$ wave forms (not shown). We note that the previously acquired value of $(dn/dT)_{\text{GaN on SiC}}$ can be also additionally independently checked and *calibrated* by experimental P_{2DA} as P_{2DA} should equal P_{2D} at the beginning of the pulse (i.e., at $t \sim 50$ ns). The P_{2DA} deviation from this line appears from $t \sim 100$ ns and that is the time instant when SiC cooling effect begins to affect $\Delta\varphi_{\text{total}}$. Again, the agreement between the model and the experiment is obtained for $(\text{TBR})_{\text{GaN/SiC}} = 1.2 \times 10^{-7}$ W/m² K, indicating that for our samples the thermal coupling between GaN and Si is better to that as between GaN and SiC.

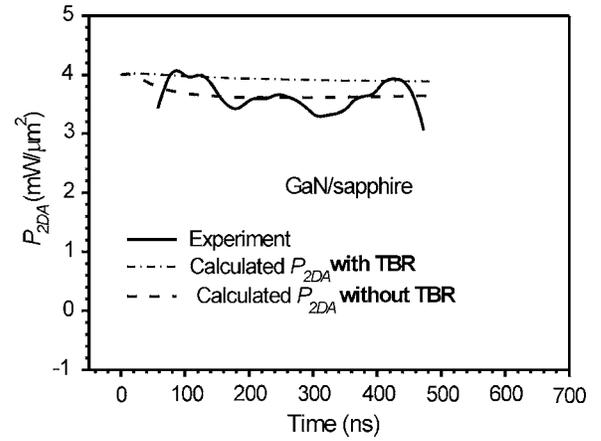


FIG. 5. Comparison of calculated P_{2DA} (with and without considering TBR) and experimental P_{2DA} in AlGaIn/GaN/sapphire TLM structure. The dissipated power was $P_{2DA} \sim 4$ mW/ μm^2 .

In comparison to TBR study of GaN/Si interface where both TIM (Ref. 5) and Micro-Raman were used, TBR at GaN/SiC is evaluated using the TIM method only and thus margins of this extraction is estimated to be $\pm 50\%$.

C. TBR at the GaN/sapphire interface

The simulation shows that for the GaN/sapphire system at $t < 500$ ns the heat penetration and the TIM optical signal coming from the sapphire are marginal. Thus the refractive index of GaN on sapphire $(dn/dT)_{\text{GaN on Sapphire}}$ can be obtained by fitting the $\Delta\varphi(t)$ at $t < 500$ ns (not shown). Another possibility is given by Eq. (1) as the space integration of $\Delta\varphi(x, y)$ at given time ($t < 500$ ns) is equivalent to the quantity of $I(t)V(t) \times t / (dn/dt \times 4\pi/\lambda)$.⁹ In agreement with the $\Delta\varphi(t)$ fitting this procedure also leads to $(dn/dT)_{\text{GaN on Sapphire}} = 4 \times 10^{-5}$ K⁻¹ on various samples.

Figure 5 shows that the simulated P_{2DA} with a chosen TBR as high as 1.2×10^{-7} m² K/W and TBR=0 differs less than 6%. For a comparison the difference in P_{2DA} in $(\text{TBR})_{\text{GaN/SiC}} = 1.2 \times 10^{-7}$ W/m² K and TBR=0 on GaN/SiC structure is $\sim 30\%$ (Fig. 4). As a result the estimation of TBR for the GaN/sapphire system is difficult. This is related to the low thermal conductivity of sapphire, which “screens” the effect of TBR.

D. Role of TBR in thermal management: Steady-state

In Fig. 6 we demonstrate the role of TBR values for different substrates by calculating the steady-state temperatures profiles in the cross-sections of TLM devices at $P_{2D} = 1$ mW/ μm^2 . The III-Nitride/substrate interface is located 1.2 μm from the surface for all structure types. For clarity the temperature profiles are shown only down to 5 μm from the surface. We assume $k_{\text{Si}} = 150$ W/m K.¹⁵ For the GaN/SiC interface we used the previously obtained TBR = 1.2×10^{-7} m² K/W, similarly for the GaN/Si we used the previously determined value of 7×10^{-8} m² K/W, and for the GaN/sapphire we tested TBR = 1.2×10^{-7} m² K/W. As expected, the highest surface temperature T_{surf} is obtained for the GaN grown on sapphire (~ 810 K), while the smallest value is obtained for the SiC substrate (~ 420 K). However,

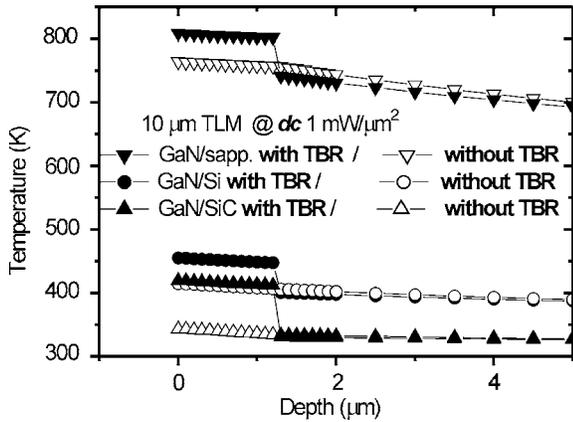


FIG. 6. Calculated steady-state temperature cross-section profiles in TLM structures on different substrates. Profiles are calculated for $P_{2D} \sim 1 \text{ mW}/\mu\text{m}^2$ with $(\text{TBR})_{\text{GaN/SiC}} = (\text{TBR})_{\text{GaN/sapphire}} = 1.2 \times 10^{-7} \text{ W}/\text{m}^2 \text{ K}$, $(\text{TBR})_{\text{GaN/Si}} = 7 \times 10^{-8} \text{ W}/\text{m}^2 \text{ K}$, and without considering TBR.

the influence of TBR on device thermal performance, well-represented by ratio $\Delta T/T_{\text{surf}}$, is the highest for the SiC ($\sim 65\%$), while it is the lowest for the sapphire ($\sim 10\%$).

IV. DISCUSSION

In this part the obtained values of $(dn/dT)_{\text{GaN}}$ and $(\text{TBR})_{\text{GaN/substrate}}$ and a comparison of the methods for TBR evaluation will be discussed.

The reason for observed different $(dn/dT)_{\text{GaN}}$ for different substrates is not clear. However various refractive index values n (from 1.8 to 2.2) for AlN in dependence of the sample preparation and microstructure were already reported.¹⁴ As dn/dT depends on n (Ref. 20) we may assume a similar structural dependence of $(dn/dT)_{\text{GaN}}$ in our case. On the other hand the experimental phase shift in a thin-film structure may slightly be influenced by multiple reflections, which can introduce some small nonlinearities in the phase-to-temperature dependence even if the reflection coefficients at the GaN/sapphire and GaN/SiC interfaces are low. However we believe that if the calibration is done for each particular sample the extracted TBR value will be not influenced significantly.

Our experimental indicate lower TBR values for GaN on Si in comparison to GaN on SiC substrate. We assume that also different thermal expansion coefficients,¹⁵ substrate roughness and defects related to particular growth techniques influence the TBR values. We have shown that if GaN is grown on the substrate with low k like the sapphire, the influence of TBR on the heat transport is less significant. On the other hand, from the point of view of possible benefits given by the high thermal conductivity of SiC, the TBR at GaN/SiC interface seems to be unacceptably high and a better thermal coupling with possible fewer defects at the interface are needed.

Finally, we comment on various techniques mentioned in previous^{1,4,5} and the present work. The optical TIM and photoreflectance¹ methods probe the device thermal behavior in the transient state with the resolution down to several ns. The advantage of TIM lies in its ability to probe all the heated layers, while the photoreflectance technique¹ probes

the thermal signal only from the surface. In addition TIM provides the information both on lateral and vertical heat spreading for times both before and after the heat front reaches the nitride/substrate interface. The electrical methods provide the averaged channel temperature and the spatial distribution cannot be obtained. For extraction of TBR, using both the above optical and electrical methods, a thermal modeling is necessary to analyze the TBR value. In contrast, the Raman method has a capability to extract the TBR *directly* from the measurements of the temperature drop at the interface (at least for GaN on silicon) and thus this method is the most accurate. However apart from a very last report where 200 ns time resolution was reported,²¹ the Raman method experiments were reported only under the steady-state conditions.

V. CONCLUSIONS

In conclusion we experimentally investigated TBR between GaN and Si, SiC, and sapphire. We found TBR to be $\sim 7 \times 10^{-8} \pm 20\% \text{ m}^2 \text{ K}/\text{W}$ at the GaN/Si interface and $\sim 1.2 \times 10^{-7} \pm 50\% \text{ m}^2 \text{ K}/\text{W}$ at the GaN/SiC. It is difficult to estimate TBR at the GaN/sapphire interface, however in this case the role of the TBR was shown to be less important. We suggest that the substrate cooling efficiency for SiC or Si substrates can be improved if the III-nitride/substrate interfaces contain less structural defects.

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