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Thermal conductivity of ultra-wide bandgap thin layers – high Al-content AlGaN and $\beta$-Ga$_2$O$_3$

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Abstract

Transient thermoreflectance (TTR) technique is employed to study the thermal conductivity of $\beta$-Ga$_2$O$_3$ and high Al-content Al$_x$Ga$_{1-x}$N semiconductors, which are very promising materials for high-power device applications. The experimental data are analyzed with the Callaway’s model taking into account all relevant phonon scattering processes. Our results show that out-of-plane thermal conductivity of high Al-content Al$_x$Ga$_{1-x}$N and (-201) $\beta$-Ga$_2$O$_3$ is of the same order of magnitude and approximately one order lower than that of GaN or AlN. The low thermal conductivity is attributed to the dominant phonon-alloy scattering in Al$_x$Ga$_{1-x}$N and to the strong Umklapp phonon-phonon scattering in $\beta$-Ga$_2$O$_3$. It is also found that the phonon-boundary scattering is essential in thin $\beta$-Ga$_2$O$_3$ and Al$_x$Ga$_{1-x}$N layers even at high temperatures and the thermal conductivity strongly deviates from the common 1/T temperature dependence.

Keywords: thermal conductivity, Ga$_2$O$_3$, AlGaN
1. Introduction

β-Ga$_2$O$_3$ and Al$_x$Ga$_{1-x}$N semiconductors are promising materials for next generation high-power electronic devices which is indicated by a higher Baliga’s figure of merit compared to that of GaN or SiC [1, 2]. There have been numerous reports on the breakdown voltage in devices based on Al$_x$Ga$_{1-x}$N and β-Ga$_2$O$_3$ with the highest recorded values of 1.7 kV [2, 3] and 1.6 kV [4], respectively. The wide-bandgap semiconductors used today for high-power electronic applications, such as GaN and SiC, exhibit a high thermal conductivity. For GaN substrates grown by Hydride Phase Vapor Epitaxy (HVPE) having threading dislocation density of 5×10$^6$ cm$^{-2}$, a room-temperature thermal conductivity of 265±10 W/mK have been measured by 3ω technique [5]. For semi-insulating 4H-SiC substrates a value of 471±24 W/mK have been measured by time-domain thermoreflectance (TDTR) technique [6]. The thermal conductivity of β-Ga$_2$O$_3$ and Al$_x$Ga$_{1-x}$N, however, is approximately one order of magnitude smaller than that of GaN and AlN as shown by the theoretical estimations [7, 8] and the experimental data [8-10]. The low thermal conductivity is expected to be a major obstacle for high-power devices based on these materials due to the self-heating issue, which seriously degrades the device performances such as lowering breakdown voltage due to the abrupt increase of the local temperature [11].

The available experimental data for the thermal conductivity of in Al$_x$Ga$_{1-x}$N are very limited [8, 12, 13], e. g. there is no data for the thermal conductivity in alloys with high-Al-content. A room temperature value of 29.5 W/mK has been measured by 3ω technique in a HVPE grown Al$_{0.4}$Ga$_{0.6}$N layer [13]. This value is almost 10 times smaller than that in binary compound GaN and AlN [5]. Such large reduction has been attributed to the strong phonon-alloy scattering, i. e. the phonon scattering due to the mass and size difference of the constituent atoms in the alloy [8]. Similar behavior of the thermal conductivity with the composition have been reported in other III-nitride alloys, In$_x$Ga$_{1-x}$N [14] and Al$_{1-x}$In$_x$N [15].
So far, the thermal conductivity of $\beta$-Ga$_2$O$_3$ has been measured only in bulk samples grown by the edge-defined fed growth [9, 10, 16] and the Czochralski method [17]. In all these studies, a high anisotropy of the thermal conductivity has been found which is not surprising having in mind the low crystal symmetry of $\beta$-Ga$_2$O$_3$. The largest thermal conductivity value at room temperatures was reported along the [010] crystallographic direction – 29 W/mK in a nominally undoped material [10]. Doping with Sn with concentration up to $5 \times 10^{18}$ cm$^{-3}$ was found to have a little effect on the thermal conductivity [9, 10]. Due to the low dislocation density in bulk samples the effect of the phonon-dislocation scattering on the thermal conductivity is negligible. In contrary, the thin layers growth on the foreign substrates exhibit a higher dislocation density due to the lattice mismatch. Also, in layers with a thickness smaller than the phonon mean free path, the phonon-boundary scattering significantly affects the thermal conductivity values.

In this work, we aim at unveiling the dominant phonon-scattering mechanism affecting the thermal conductivity in thin unintentionally doped and Sn-doped $\beta$-Ga$_2$O$_3$ layers and attempt to make a comparison of the thermal conductivity of $\beta$-Ga$_2$O$_3$ with that of the Al$_x$Ga$_{1-x}$N alloys with a similar bandgap. The experimental data are analyzed by numerical simulations based on the Callaway-Debye formalism considering the contribution of various phonon-scattering processes. The effects of Sn doping concentration of $\beta$-Ga$_2$O$_3$, as well as the phonon-alloy scattering in high Al-content Al$_x$Ga$_{1-x}$N are discussed, giving a quantitative estimation of the threshold Sn concentration, where Ga$_2$O$_3$ thermal conductivity starts to degrade, and the thermal conductivity of the Al$_x$Ga$_{1-x}$N saturates.

2. Experimental

$\beta$-Ga$_2$O$_3$ samples were grown on c-plane sapphire substrates using pulsed laser deposition (PLD) as described elsewhere [18]. Two (-201)-oriented layers were examined –
one unintentionally doped with a nominal thickness of 245 nm and one Sn-doped with a nominal thickness of 255 nm. The Sn concentration in unintentionally doped (< $5 \times 10^{17}$ cm$^{-3}$) and in doped ($2.6 \times 10^{20}$ cm$^{-3}$) $\beta$-Ga$_2$O$_3$ layers was measured by secondary ion mass spectroscopy (SIMS). The high-Al content Al$_x$Ga$_{1-x}$N samples were grown by hot-wall Metal-Organic Chemical Vapor Deposition (MOCVD) on 4H-SiC substrates. A 450-nm-thick AlN buffer layer and a 100-nm-thick graded Al$_x$Ga$_{1-x}$N are introduced before the growth of Al$_x$Ga$_{1-x}$N in order to avoid cracking. Nominally undoped Al$_{0.84}$Ga$_{0.16}$N, Al$_{0.89}$Ga$_{0.11}$N and AlN layers, all with a thickness of 450 nm, were examined. The thicknesses of the studied layers were measured by UV-VIS ellipsometry and confirmed by cross-section Scanning Electron Microscopy (SEM). The crystal quality of the samples was examined by X-ray diffraction (XRD). The analysis of FWHM of the XRD rocking curves reveals a screw-type dislocation density of $\approx 10^8$ cm$^{-2}$ in Al$_x$Ga$_{1-x}$N layers. The dislocation density in $\beta$-Ga$_2$O$_3$ using the same method is harder to access. We only can qualitatively estimate a dislocation density in the range of $\approx 10^9$ cm$^{-2}$ in $\beta$-Ga$_2$O$_3$ layers. The layer thicknesses, doping concentrations and dislocation densities of the studied samples are summarized in Table 1.

**Table 1.** Layers thickness (L), Sn doping concentration ($N_{Sn}$), screw-type dislocation density ($D_S$), measured room-temperature thermal conductivity ($k$), and the calculated relative contribution of the $k_2$ for all studied samples.

<table>
<thead>
<tr>
<th>Samples</th>
<th>L (nm)</th>
<th>$N_{Sn}$ (cm$^{-3}$)</th>
<th>$D_S$ (cm$^2$)</th>
<th>$k$ (W/mK)</th>
<th>$k_2/k$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\beta$-Ga$_2$O$_3$ (unintentionally doped)</td>
<td>245</td>
<td>$&lt; 5 \times 10^{17}$</td>
<td>$\approx 10^9$</td>
<td>5.35±0.55</td>
<td>0.315</td>
</tr>
<tr>
<td>$\beta$-Ga$_2$O$_3$ (Sn doped)</td>
<td>255</td>
<td>$2.6 \times 10^{20}$</td>
<td>$\approx 10^9$</td>
<td>2.53±0.26</td>
<td>0.222</td>
</tr>
<tr>
<td>Al$<em>{0.84}$Ga$</em>{0.16}$N</td>
<td>450</td>
<td>-</td>
<td>$4.6 \times 10^7$</td>
<td>12.5±1.38</td>
<td>0.034</td>
</tr>
<tr>
<td>Al$<em>{0.89}$Ga$</em>{0.11}$N</td>
<td>450</td>
<td>-</td>
<td>$2.2 \times 10^8$</td>
<td>12.0±1.32</td>
<td>0.040</td>
</tr>
<tr>
<td>AlN</td>
<td>450</td>
<td>-</td>
<td>$3.8 \times 10^8$</td>
<td>84±9.24</td>
<td>0.405</td>
</tr>
</tbody>
</table>
The thermal conductivity of the $\beta$-Ga$_2$O$_3$ and Al$_x$Ga$_{1-x}$N layers was measured by TTR technique. The system we have used (Transometer D8, TMX Scientific) includes a pump and a probe laser beam as schematically shown Fig. 1 (a). The pulse pump laser (532 nm Nd:YAG with a pulse duration of 8 ns and a repetition rate of 50 Hz) heats the sample through an absorbing Au transducer. The decay in the sample temperature after every pump laser pulse is monitored by measuring the transients of the reflectance of the probe laser (continuous-wave Ar laser emitting at 488 nm) (see Fig. 1 (b)). The power of the pump laser is much larger than that of the probe laser resulting in a negligible influence of heating effect due to probe laser. The spot size of the pump and probe laser beams is 200 $\mu$m and 15 $\mu$m, respectively. Thus, the heat transport can be regarded as one-dimensional propagation along vertical direction, and therefore our measurement always gives the out-of-plane thermal conductivity. Since we are interested in the thermal conductivity above room temperature the measurements are done in a temperature range of 280-355 K.

**Figure 1** (a) Schematic setup for TTR measurements of the thermal conductivity. (b) Normalized thermoreflectance transients measured for unintentionally doped and Sn-doped $\beta$-Ga$_2$O$_3$ layers.
3. Callaway-Debye formalism for the thermal conductivity in solids

The common treatment of the lattice thermal conductivity in solids is based on Callaway’s phenomenological formalism [19], where a Debye-like phonon spectrum is assumed and the various phonon scattering processes are accounted for by introducing frequency- and temperature-dependent relaxation times. Here, the thermal conductivity in \( \beta\)-Ga\(_2\)O\(_3\) and Al\(_x\)Ga\(_{1-x}\)N is analyzed using the modified Callaway’s model where the contributions of longitudinal and transverse acoustic (LA and TA) phonons are treated separately [20, 21]. In this approach, the thermal conductivity is given by

\[
k_1 = k_1 + k_2,
\]

where

\[
k_1 = \sum_s \frac{k_B^4}{6\pi^2\hbar^3v_s} T^3 \int_0^{\theta_D/T} \tau_C^s \frac{x^4 \exp(x)}{[\exp(x) - 1]^2} dx \tag{2}
\]

\[
k_2 = \sum_s \frac{k_B^4}{6\pi^2\hbar^3v_s} T^3 \left[ \int_0^{\theta_D/T} \frac{\tau_C^s}{\tau_N^s}[\exp(x) - 1]^2 dx \right]^2 \left[ \int_0^{\theta_D/T} \frac{\tau_C^s}{\tau_N^s \tau_R^s}[\exp(x) - 1]^2 dx \right] \tag{3}
\]

Here, \( k_B \) is the Boltzmann constant, \( T \) is the temperature, \( \hbar \) is the reduced Planck constant, \( v_s \) is the acoustic phonon velocity, and \( \theta_D \) is the Debye temperature (determined from the maximum phonon frequency at the zone boundary). The variable of integration \( x \) is related to the phonon frequency \( \omega \) and is defined by \( x = \hbar \omega / k_B T \). The summation is over all three acoustic phonon modes – one longitudinal and two transverse, i. e. \( s = \text{LA}, \text{TA1}, \text{TA2} \). In Eqs. (2-3) \( \tau_N^s \) denotes the relaxation time for normal (N) phonon-phonon scattering, \( \tau_R^s \) is the relaxation time for all resistive (R) scattering processes, which are taken to be additive, and \( \tau_C^s \) is the combined relaxation time given by \( (\tau_C^s)^{-1} = (\tau_N^s)^{-1} + (\tau_R^s)^{-1} \). The resistive scattering processes are the Umklapp (U) phonon-phonon scattering, the phonon-isotope (I) scattering, the phonon-point-defect (PD) scattering, the phonon-dislocation (D) scattering, the phonon-boundary (B)
scattering, and the phonon-alloy scattering \((A)\). Then, the resistive scattering rate is expressed as \((\tau_R^s)^{-1} = (\tau_U^s)^{-1} + (\tau_P^s)^{-1} + (\tau_D^s)^{-1} + (\tau_P^s)^{-1} + (\tau_B^s)^{-1} + (\tau_A^s)^{-1}\). Note that the phonon-alloy scattering takes place only in semiconductor alloys, i.e. in \(Al_xGa_{1-x}N\) considered here.

The explicit expressions for different phonon scattering rates are available from the numerous theoretical works and their validity have been shown by comparison with the experimental thermal conductivity data in various materials [20-25]. Generally, the strength of the phonon scattering rates depends on physical parameters of the particular material, which are usually well known. The only unknown parameters that influence the thermal conductivity but are unknown are the Grüneisen parameters, which account for the anharmonicity of the atomic interactions in the crystal structure. Then, the standard way to analyze the thermal conductivity in semiconductor materials is to fit the experimental data with Eqs. (1-3) using the Grüneisen parameters as adjustable parameters [21, 26].

To find the Grüneisen parameters in \(Al_xGa_{1-x}N\) and \(\beta\)-Ga\(_2\)O\(_3\) we fit the experimental temperature-dependent thermal conductivity data in temperature range of 290-420 K for nominally undoped bulk GaN and AlN [5] and 220-480 K for bulk (-201) \(\beta\)-Ga\(_2\)O\(_3\) [9]. In this analysis only the normal and Umklapp phonon-phonon scattering and the phonon-isotope scattering are taken into account. For simplicity only two Grüneisen parameters for both materials, \(\gamma_L\) for the LA phonon mode and \(\gamma_T\) for the two TA phonon modes, are used. The Debye temperatures, which are different for different phonon modes, are determined from the zone-boundary acoustic phonon frequencies as calculated in the three materials [9, 27, 28]. The acoustic phonon velocities in GaN and AlN are calculated from the stiffness constants using the standard formulas for the hexagonal crystals [29, 30]. We note that the two TA modes in GaN and AlN (respectively, in \(Al_xGa_{1-x}N\)) are degenerated along (0001) crystallographic direction (this is the out-of-plane direction for the layers studied here). For \(\beta\)-Ga\(_2\)O\(_3\) we use the velocities obtained from first-principles calculation [9]. In fact, the two TA modes in (-201) \(\beta\)-
Ga$_2$O$_3$ are not degenerated but they have a very similar dispersion and the same frequencies at the zone-boundary [9], so we regard them as degenerated. The calculated strengths of the phonon-isotope scattering in Ga$_2$O$_3$, GaN, and AlN are $2.76 \times 10^{-4}$, $2.74 \times 10^{-4}$, and $4.39 \times 10^{-6}$, respectively. The analysis procedure yields $\gamma_L^{Ga_2O_3} = 1$, $\gamma_T^{Ga_2O_3} = 2$, $\gamma_L^{AlN} = 1.2$, $\gamma_T^{AlN} = 0.3$, $\gamma_L^{GaN} = 0.6$, and $\gamma_T^{GaN} = 0.3$.

The above values of the Grüneisen parameters are used for the analysis of our experimental data for the thermal conductivity in $\beta$-Ga$_2$O$_3$ and Al$_x$Ga$_{1-x}$N layers. In this analysis all resistive phonon scattering processes are considered. For Al$_x$Ga$_{1-x}$N, we use the virtual crystal approximation, in which the disordered alloy is replaced by an ordered virtual crystal with the virtual atomic weight, atomic volume and lattice constants [8, 25]. Then, the acoustic phonons are scattered by the perturbations of the virtual crystal. The atomic mass, the atomic volume, and the lattice constants, as well as the stiffness constants, the Debye temperatures, the Grüneisen parameters, and the strengths of the phonon-isotope scattering are linearly interpolated between the values for the binary GaN and AlN compounds. Such approach is justified by the experimental findings of a linear composition dependence of the lattice constants [31] and the sound velocities [32] in Al$_x$Ga$_{1-x}$N.

In thin layers, the phonon-boundary scattering becomes very important as the layer thickness is much smaller than the phonon mean free path. The phonon-boundary scattering has been studied in detail in bulk samples at low temperature and the scattering rate is commonly expressed as [20]

$$\left(\frac{1}{\tau_B^s}\right)^{-1} = \frac{v_s}{L_E} = v_s \left(\frac{1}{L_C} + \frac{1}{L}\right).$$  \hspace{1cm} (4)

Here $L_E$ is the effective phonon mean free path, $L_C$ is the “so-called” Casimir length, and $L$ is the sample length in the direction of the heat transport. For thin films, where $L \ll L_C$, $L_E$ can be approximate as $L_E = a \times L$, where $a$ is non-dimensional parameter, which is usually extracted by fitting the Eq. 4 to the experimental data [33-35]. The analysis of our data for the thickness
dependence of the thermal conductivity in GaN epitaxial layers (not shown here) yielded \( a = 2.5 \). This value is very close to the previously reported, \( a = 2.38 \), for GaN layers [34, 35]. In the case of \((-201)\) \( \beta\)-Ga\(_2\)O\(_3\), we have found \( a = 1.87 \) as shown below.

Although the normal phonon-phonon scattering is a non-resistive process its contribution in the total thermal conductivity cannot be omitted as it has an essential role in the phonon distribution, thus influencing all resistivity scattering processes. Generally, it is assumed that the thermal conductivity is mainly determined by \( k_1 \) term in Eq. 1, but in many cases, one needs to add the second term, \( k_2 \), for the sake of the correctness. The contribution of \( k_2 \) strongly depends on the sample purity, thus it is very large for isotopically enriched or low-dislocation materials and small for highly doped or high-dislocation materials [20]. The trend of \( k_2 \) on the total thermal conductivity in the layers studied in this work is presented in Table 1, showing a significant contribution for the AlN (40.5%) and the unintentionally doped \( \beta\)-Ga\(_2\)O\(_3\) layer (31.5%).

**Figure 2** Calculated room temperature phonon scattering times as a function of Sn doping concentration in (a) bulk \((-201)\) \( \beta\)-Ga\(_2\)O\(_3\) and (b) \((-201)\) \( \beta\)-Ga\(_2\)O\(_3\) 250 nm thick layer.
As an example of our thermal conductivity model, in Fig. 2 are shown the calculated phonon scattering times as a function of Sn doping concentration in bulk and thin layer (-201) $\beta$-Ga$_2$O$_3$ samples at 300 K. In these calculations, the phonon-point-defect scattering is treated within the Callaway’s model [19, 25] and accounts for the disturbance of the lattice periodicity due to the mass and size difference between Sn impurity, which substitutes Ga, and the host atom. The contribution of the phonon-boundary scattering is extremely small in the bulk sample and thus it is omitted in the plot. It is seen that the Umklapp phonon-phonon scattering process dominates at low doping concentration and it is the major factors limiting the thermal conductivity of bulk $\beta$-Ga$_2$O$_3$. Our results are in line with the previous predictions for a dominance of the Umklapp phonon-phonon scattering in $\beta$-Ga$_2$O$_3$ [7, 9, 10]. The total scattering time is determined by the interplay between the phonon-point-defect scattering and the Umklapp phonon-phonon scattering in the bulk material. In thin layers, the total scattering time is determined by the phonon-point-defect scattering, the Umklapp phonon-phonon scattering and the phonon-boundary scattering. The phonon-point-defect scattering time is proportional to the doping concentration and it is seen that the threshold of the Sn doping concentration, where the total scattering time starts to degrade (i.e. becomes shorter), is about $6 \times 10^{18}$ cm$^{-3}$ for both the bulk and the thin layer $\beta$-Ga$_2$O$_3$.

4. Results and discussion

The calculated Sn doping dependence of the out-of-plane thermal conductivity in (-201) $\beta$-Ga$_2$O$_3$ together with the room temperature data in the two studied samples is shown in Fig. 3(a). There is very good agreement between the experimental data and the model for a 250 nm thick layer. The calculations are done using the Grüneisen parameters extracted above for bulk (-201) $\beta$-Ga$_2$O$_3$ and without any adjustable parameters. For the phonon-boundary scattering in thin layers, the pre-factor in the $L_E$ ($a = 1.87$) is determined by fitting the temperature-dependent
data shown in Fig. 3(b). At low doping concentrations the thermal conductivity of the layer is less than half of that the bulk material, which is mainly due to the contribution of the phonon-boundary scattering. The effect of the phonon-dislocation scattering is less significant. The threshold Sn concentration, where the thermal conductivity starts to decrease with increasing doping, is found to be $\approx 2 \times 10^{18} \text{ cm}^{-3}$ in the bulk material and $\approx 1 \times 10^{19} \text{ cm}^{-3}$ in the thin layer. The difference is attributed to the fact that at low doping concentrations the phonon-boundary scattering dominates over the phonon-point-defect scattering (see Fig. 2(b)).

Figure 3 Thermal conductivity of bulk and thin layers (-201) $\beta$-Ga$_2$O$_3$ as a function of (a) Sn doping concentrations and (b) temperature. The solid lines represent the calculated thermal conductivity at room temperature (a) and the least square fitting of the temperature dependence (b). The thermal conductivity data of bulk (-201) $\beta$-Ga$_2$O$_3$ [9] are also shown.

The temperature dependence of the thermal conductivity of $\beta$-Ga$_2$O$_3$ layers are shown in Fig. 3(b). Our model using pre-factor $a$ in the $L_E$ as an only adjustable parameter fits very well the measured data and yields $a = 1.87$. At elevated temperatures (above the Debye
temperature determined from the maximum acoustic phonon frequency at the zone boundary) the lattice thermal conductivity of semiconductors is expected to follow $1/T^m$ dependence, where $m = 1$ for pure materials, meaning that the Umklapp phonon-phonon scattering is the dominant resistive process [36]. For bulk $\beta$-Ga$_2$O$_3$ values of $m = 1.1 \text{--} 1.3$ have been extracted in a temperature range 200-500 K depending on the direction of the heat transport [9, 16]. For Sn-doped $\beta$-Ga$_2$O$_3$, however, $m$ values below 1 have been reported in a narrower temperature range ($T = 300\text{--}400$ K) [10]. Here, for the data presented on Fig. 3 (b) we obtained $m = 0.6$ for the unintentionally doped and $m = 0.3$ for the Sn-doped layers. We note that a decrease of $m$ with increasing doping level have been observed in GaN:Si [26] as well as in $n$- and $p$-type SiC [37].

In Fig. 4 we show the measured thermal conductivity of the Al$_x$Ga$_{1-x}$N layers with three different Al compositions as specified in Table 1. The Callaway’s model, which in this case also includes the phonon-alloy scattering, gives a very good fit to the experimental data. The thermal conductivity in alloys is seen to quickly degrade from the value of AlN thin layer as Ga is introduced even with a very small fraction. The reduction is almost saturated for Al compositions of less than 90%. At very low Al compositions, it is likely to observe almost the same trend – a strong decrease of the thermal conductivity (comparing to that of GaN) with increasing Al content. In fact, such trend has been seen from published data for Al$_x$Ga$_{1-x}$N layers with $x < 0.4$ [8, 12]. We also calculated the thermal conductivity of bulk Al$_x$Ga$_{1-x}$N, assuming an undoped, low-dislocation material, so only the phonon-phonon, the phonon-isotope and the phonon-alloy scattering are included in the model (Fig. 4 (a)). Due to the strong phonon-alloy scattering a thermal conductivity value as low as of $\approx 25\text{--}30$ W/mK is found in the composition range $x = 0.5\text{--}0.9$. The temperature-dependent thermal conductivity of Al$_x$Ga$_{1-x}$N layers have been measured and calculated in the temperature range from 280 K to 355 K as shown in Fig. 4 (b). In the calculations, $L_E = 2.5L$ is used in the Eq. 4 for the phonon-boundary scattering. While for the AlN layer $m = 1.26$ is extracted, almost a constant thermal conductivity of the
Al_{0.85}Ga_{0.15}N and Al_{0.89}Ga_{0.11}N layers is observed in the temperature range being investigated. However, due to the limited temperature range we are unable to draw a definitive conclusion about the temperature dependence of the thermal conductivity of these high-Al-content samples.

Figure 4 Thermal conductivity of high Al-content Al_{x}Ga_{1-x}N layers: (a) the dependence on the Al composition, (b) the dependence on the temperature. The solid lines represent the calculated thermal conductivity at room temperature (a) and the least square fitting of the temperature dependence (b). The thermal conductivity data for bulk AlN are taken from Ref. 5.

Finally, we studied in more details the effect of the phonon-boundary scattering on the thermal conductivity in thin layers. The calculated thickness dependence of the thermal conductivity of (-201) β-Ga_{2}O_{3} and Al_{0.8}Ga_{0.2}N layers is shown in Fig. 5. The material quality in terms of the dislocation density was assumed to be the same as the layers we used in this work. In our model based on the Callaway-Debye formalism, the contribution of the phonon-boundary scattering solely depends on the parameter $a$ in the $L_{E}$, which in turn indicates how
fast the thermal conductivity increases with increasing thickness. The calculations are performed for thicknesses up to 5 µm, which guarantees almost saturated thermal conductivities. Our aim is to give a quantitative comparison between the (-201) $\beta$-Ga$_2$O$_3$ and Al$_{0.8}$Ga$_{0.2}$N layers. As shown in Fig. 5, both layers exhibit a comparable out-of-plane thermal conductivity for thicknesses of less than 1 µm. Above this thickness the thermal conductivity of (-201) $\beta$-Ga$_2$O$_3$ starts to saturate in accordance with the available experimental data [38]. A saturation of the thermal conductivity with increasing layer thickness has also been reported for GaN thin layers [35]. For Al$_{0.8}$Ga$_{0.2}$N layer, however, the increasing of the thermal conductivity is still observed up to a thickness of 5 µm. The effect is attributed to the fact that the thermal conductivity of bulk Al$_{0.8}$Ga$_{0.2}$N is more than twice larger than that of bulk (-201) $\beta$-Ga$_2$O$_3$.

**Figure 5** The calculated thickness-dependent thermal conductivity of (-201) $\beta$-Ga$_2$O$_3$ and Al$_{0.8}$Ga$_{0.2}$N layers. In the modeling, the same dislocation density ($2\times10^8$ cm$^{-2}$) was assumed for both materials.
5. Conclusion

The thermal conductivity of (-201) $\beta$-Ga$_2$O$_3$ and high-Al content Al$_x$Ga$_{1-x}$N layers was measured by TTR and analyzed in the frame of the Callaway-Debye formalism. The thermal conductivity in both types of layers was found to be lower than that in bulk materials due to the phonon-boundary scattering which plays an essential role even at room temperatures for layer with thicknesses below 1 $\mu$m. The very low thermal conductivity of (-201) $\beta$-Ga$_2$O$_3$ comparing to the other wide-bandgap semiconductors was attributed to the strong Umklapp phonon-phonon scattering. For the $n$-type (-201) $\beta$-Ga$_2$O$_3$ layers doped with Sn, it was shown that the doping effect has almost negligible influence on the thermal conductivity if the doping concentration is below $\approx 2\times 10^{18}$ cm$^{-3}$. Supported by a numerical analysis we found that the phonon-alloy scattering in Al$_x$Ga$_{1-x}$N degrades the thermal conductivity over a wide range of Al compositions by approximately one order of magnitude in comparison with that of the binary compounds. The temperature-dependent thermal conductivity of the investigated layers was found to follow $1/T^m$ dependence above the room temperature, but the power factor $m$ was much smaller than the value reported for the bulk materials. We conclude that this could be explained by the enhanced contribution of the phonon-boundary, the point-defect and the phonon-alloy scattering in the studied thin layers.

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References


Highlights

- New experimental data for thermal conductivity of (-201) $\beta$-Ga$_2$O$_3$ and high Al-content AlGaN layers measured by transient thermoreflectance (TTR) technique.
- Umklapp phonon-phonon scattering limited thermal conductivity in (-201) $\beta$-Ga$_2$O$_3$.
- Sn doping dependent thermal conductivity of (-201) $\beta$-Ga$_2$O$_3$.
- Phonon-alloy disorder determined thermal conductivity in high Al-content AlGaN.
- Effect of the phonon-boundary scattering on the thermal conductivity of (-201) $\beta$-Ga$_2$O$_3$ and AlGaN thin layers.