Towards AlN optical cladding layers for thermal management in hybrid lasers

Ian Mathews,¹ Shenghui Lei,¹ Kevin Nolan,¹ Guillaume Levaufre,² Alexandre Shen,² Guang-Hua Duan,² Brian Corbett,³ and Ryan Enright¹

¹Efficient Energy Transfer Department, Bell Labs, Alcatel-Lucent, Dublin, Ireland
²III-V Lab, a joint lab of 'Alcatel-Lucent Bell Labs France', Thales Research and Technology' and 'CEA Leti', Marcoussis 91460, France
³Tyndall National Institute, Lee Maltings, University College Cork, Cork, Ireland

ABSTRACT
Aluminium Nitride (AlN) is proposed as a dual function optical cladding and thermal spreading layer for hybrid ridge lasers, replacing current benzocyclobutene (BCB) encapsulation. A high thermal conductivity material placed in intimate contact with the Multi-Quantum Well active region of the laser allows rapid heat removal at source but places a number of constraints on material selection. AlN is considered the most suitable due to its high thermal conductivity when deposited at low deposition temperatures, similar co-efficient of thermal expansion to InP, its suitable refractive index and its dielectric nature. We have previously simulated the possible reduction in the thermal resistance of a hybrid ridge laser by replacing the BCB cladding material with a material of higher thermal conductivity of up to 319 W/mK. Towards this goal, we demonstrate AlN thin-films deposited by reactive DC magnetron sputtering on InP.

Keywords: Silicon photonics, hybrid laser, aluminium nitride, magnetron sputtering, thin-film, thermal management

1. INTRODUCTION
Silicon photonics promises higher data transmission rates in optical networks due to the close integration of the optical and electrical components.¹ A primary bottleneck to developing optical chips with silicon is its indirect bandgap that causes a significant challenge to the generation of light from the material.² The most advanced strategy to produce light from a silicon platform involves the integration of III-V gain material on silicon i.e. hybrid lasers.³ These devices combine the light generating III-V layers on silicon using a number of methods including direct epitaxial growth, wafer-bonding and die transfer.⁴ ⁵

Hybrid lasers generally have poorer thermal characteristics as compared to traditional monolithic III-V lasers.⁶ In principle, integrating the III-V source with silicon should lead to improved thermal performance due to the almost 100% greater thermal conductivity of the silicon substrate (k_Si = 149 W/mK) versus an InP substrate (k_InP = 68 W/mK)⁵. In practice, for wafer-bonded devices the higher thermal resistance is attributed to their integration on SOI wafers, where the buried SiO₂ layer has a low thermal conductivity (k_SiO₂ = 1.38 W/mK) and acts as a barrier to heat flow into the substrate (Fig. 1). The SiO₂ layer is provided to optically confine light in the Si waveguide. Additionally, a polymer or SiO₂ layer is typically used between the III-V material and the SOI substrate to enable the bonding process, creating another thermal blocking layer.

In hybrid ridge laser architectures fabricated using bonding processes, the MQW active region, that is the primary heat source in the device, sits above the level of the substrate. This places it in direct contact with the encapsulating material (Fig. 1: Spreader) used to provide mechanical support for the electrode contact pads and environmental protection for the III-V materials. The low thermal conductivity material BCB (k_BC = 0.29 W/mK⁻¹) is commonly used as the encapsulation material in the photonic device community.

These structural characteristics contribute to create significant barriers to heat removal from the active region of the device. The heat is both generated in the MQW and confined there leading to reduced performance. As compared to monolithic III-V lasers with a buried ridge structure, hybrid lasers have lower lasing efficiencies and reduced optical output power due to elevated temperatures in the active region, especially under high electrical power dissipation.
We propose to replace the BCB encapsulation currently used in hybrid laser designs with materials of higher thermal conductivity. The choice of cladding material is constrained by a number of technological features. The material must be dielectric in nature to prevent electrical shorting of any p-type or n-type layers in the device or the positive and negative electrodes that are typically located on the top surface of the device, adjacent to or on the ridge. Ideally a material will have a similar coefficient of thermal expansion as the InP based materials in the laser structure to prevent the creation of stress/strain in the device under operation. The refractive index of the material must be low enough to confine the optical mode in the ridge waveguide and the material must exhibit high thermal conductivity, despite the restriction of low processing temperatures inherent in work with wafer-bonded materials with different CTEs. The rest of this paper describes in detail our choice of Aluminium Nitride (AlN) thin-films for use as dual-function thermal spreading and optical cladding layers for hybrid ridge lasers. Its dielectric nature and similar CTE to InP (both 4-5 ppm/°C) satisfy two of the pre-defined conditions for optimum cladding materials. The following sections discuss its thermal conductivity when processed at low temperatures, presenting our own initial depositions on InP but firstly outline our modelling that illustrate its optical properties are suitable for mode confinement in hybrid laser waveguides.

2. OPTICAL MODE CONFINEMENT

Firstly we investigated the range of refractive index values that are allowed for the optical cladding material in our hybrid laser design before mode confinement is lost where the expected values for AlN are 1.8-2.2 depending on its crystal structure. The confinement factor of an optical mode within a given layer corresponds to the ratio of the power carried by the portion of the optical mode overlapping the considered layer, over the total power carried by the optical mode. In our case, the optical mode can be guided by both the III-V waveguide and the silicon waveguide, depending on the position in the longitudinal structure of the hybrid laser. The width of these waveguides affects the vertical position and repartition of this mode, and thus the proportion of the optical mode which is actually overlapping with the MQW layer or the silicon layer. In order to obtain modal gain, the confinement factor within this MQW layer must not be null, and the confinement factor in absorbing layers must be minimized. In all cases, the active ridge is encapsulated with a cladding material, which is used to passivate the active ridge and to decrease the optical propagation loss due to ridge wall roughness. Light is tightly confined in higher index contrast structures. As we increase the encapsulation layer
refractive index, e.g. as we decrease the optical index contrast of the guiding structure, the mode will become less confined and can be characterised by the confinement factor of the optical mode within the encapsulation layer.

Figures 2 & 3 show the simulation results obtained for a guiding structure including a 2 μm wide III-V active ridge buried in an encapsulating layer and a slab of silicon layer underneath. This configuration corresponds to the “worst” case in which the optical mode is the most sensitive to any change in the encapsulation layer, as it is guided in the III-V ridge and thus, located closer to the encapsulation layer. Variation in the refractive index of the encapsulation layer has a more significant impact on the mode effective index here (see inset Fig. 2) than the case where the Si slab is replaced with a Si ridge (as in Fig. 1). We varied the numerical value of the encapsulant refractive index, simulated the corresponding optical mode, and computed the above defined optical confinement factor in the encapsulating layer.

Figure 2 is a plot of the confinement factor in the encapsulation layer as a function of its refractive index. One can see that changing the encapsulation refractive index has only small effects on the confinement factor inside the encapsulating layer, when BCB is replaced by AlN. Changing the encapsulation from BCB to AlN will, in the worst case, change the optical power confined in the encapsulation from 0.07% to 0.14%, which is doubled, but remains negligible. When the mode effective index reaches the value of the encapsulation refractive index, the mode will be unconfined and will tend to spread out into the encapsulation layer (deconfinement limit).

Figure 3 outlines our computation of the normalized optical index, \( b \), of the waveguide as a function of its normalized frequency, \( V \). Both normalized parameters are conventionally used for a 1-D guiding structure, such as a slab waveguide. We transformed the 2-D hybrid waveguide structure into a 1-D model, by computing the effective index in the central III-V ridge, \( n_{\text{eff,III-V}} \), and the effective index in the cladding areas, \( n_{\text{clad}} \), on both sides of the core ridge. The cladding areas contain the encapsulation material. Once the 2-D structure is emulated by the 1-D structure, we computed the normalized optical index as a function of the normalized frequency. The normalized frequency \( V \) and the normalized waveguide index are defined by the following Equation 1 where, \( \lambda \) is the wavelength, \( w \), the width of the III-V ridge and, \( n_{\text{eff,tot}} \), the effective index of the optical mode.

\[
V = \frac{2\pi}{\lambda} \sqrt{n_{\text{eff,III-V}}^2 - n_{\text{clad}}^2} \quad \text{and} \quad b = \frac{n_{\text{eff,tot}}^2 - n_{\text{clad}}^2}{n_{\text{eff,III-V}}^2 - n_{\text{clad}}^2} \quad (1)
\]
One can see that when AlN replaces BCB material as the encapsulant, the normalized optical index does not vary significantly and its value is far from the de-confinement value. This simulation results confirm that AlN can replace BCB without significant change in the optical wave-guiding properties.

Fig. 3: Normalized optical index of the waveguide as a function of its normalized frequency.

### 3. LOW TEMPERATURE PROCESSING OF AlN

The high thermal conductivity of AlN is well established where it is commonly used, in ceramic form, for sub-mounts in electronics and photonics packaging. The thermal conductivity of AlN depends, however, on its crystal morphology. The highest measured value for a high purity single crystal is 319 W/mK\(^9\) while values as high as 250 W/mK have recently been measured for thin-films comprising polycrystalline material \(^10\). Therefore, even polycrystalline films have expected values three orders of magnitude greater than BCB \((k_{BCB} = 0.29\ \text{W/mK})\). The thermal conductivity of AlN thin-films is intrinsically linked to the crystal grain size within the film and therefore the processing conditions.

A substantial challenge lies in embedding polycrystalline AlN with large crystal sizes in wafer-bonded hybrid laser architectures. Two key constraints will likely reduce the grain size in the deposited films, and thus the film thermal conductivity. Firstly a thermal budget exists for the deposition process, above which critical mechanical failure can be expected in the hybrid laser structure. As the III-V layers are grown in an inverted configuration on an InP substrate and transferred to Si (with subsequent InP substrate removal) before processing of the laser structures, it is not possible to deposit AlN around the ridge before the III-V/Si bonding process. Failure is likely to occur through delamination of the III-V layer from the Si substrate when exposed to large temperatures that will introduce stress/strain between the materials which have significantly different CTEs. We consider the limit to the acceptable processing temperature to be 350°C. Depositing films at these low temperatures will reduce \(k_{AlN}\) as smaller grains will be formed. Secondly there is a significant difference in the lattice constant of InP (5.87 Å) and the a-axis of AlN (3.11 Å). It is expected the difference will result in thicker amorphous AlN region at the interface between InP and AlN than previously seen on Si (5.43 Å) substrates and discussed below.

There has been significant progress in the development of AlN thin-films at low processing temperatures using pulsed laser deposition and reactive sputtering. Figure 4 outlines data from the literature for the measured thermal
conductivities of AlN thin-films where we have restricted the data shown to films where the substrate temperature during processing was $< 350 \, ^\circ\text{C}$. It should be noted all these films were deposited on Si (100) substrates and the thermal conductivity of AlN films on InP has, to our knowledge, never been presented. All the data shown, except Jacquot et al., is for reactively sputtered thin-films. Jacquot et al. used pulsed laser ablation of an Al source in a reactive nitrogen atmosphere to achieve effective thermal conductivity values $< 1 \, \text{W/mK}$\textsuperscript{11}. Zhao et al.\textsuperscript{12} and Pan et al.\textsuperscript{13} used balanced reactive sputtering to produce films with thermal conductivities of less than 10 W/mK. Duquenne et al. completed considerable work investigating the different regions within sputtered AlN thin-films deposited on Si substrates and their effect on the thermal conductivity values measured\textsuperscript{14, 15}. They showed the layers are characterised by a number of distinct crystal morphology regions. At the interface between the Si and AlN materials a 1-2 nm amorphous region is formed due to the strain between the lattice mismatched materials. From this region polycrystalline growth of AlN begins and an initial transition region develops where the grain size is lower than the bulk of the film. The bulk of the film, i.e. beyond the initial $\sim 100$ nm, is characterised by polycrystalline material with larger grain sizes with the deposition parameters now having a significant effect on this grain size and thus effective thermal conductivity of the film. They used balanced DC reactive magnetron sputtering to achieve grain sizes on the order of 20-30 nm with $k_{\text{AlN}}$ values between 2 and 40 W/mK, increasing as a function of thickness and improvements to their deposition parameters. In the same paper they proposed and demonstrated unbalanced reactive DC magnetron sputtering, where the increased ion intensity improves the density of the films with larger grain sizes produced. The AlN grain sizes grown in the bulk film were on the order of 100-150 nm with a measured conductivity in the bulk of these films of 170 W/mK. The measured effective thermal conductivities in 3500 nm thick AlN films produced by unbalanced reactive DC magnetron sputtering were 130 W/mK\textsuperscript{14} owing to the effect of the amorphous region on the cross-plane measurement. The amorphous layer between the bulk AlN film and substrate was now the main obstacle to achieving effective thermal conductivities close to single-crystals. Ait Aissa et al.\textsuperscript{10} were able to deposit AlN thin-films with no obvious sign of this amorphous region by switching from DC magnetron sputtering to a high power impulse magnetron sputtering (HiPIMS). The increased metal ion density in the high power density plasma leads to the increased smoothness and grain size of these films. Impressive effective thermal conductivities values of 250 W/mK were measured for 3400 nm films deposited on Si substrates representing the state of the art for high thermal conductivity AlN thin-films produced with low level or no intentional substrate heating.

Fig. 4: Measured thermal conductivity (at 300 K) of AlN thin-films as a function of film thickness. All data shown is for films produced with substrate processing temperatures of $< 350 \, ^\circ\text{C}$. All films were produced by sputtering except for Jacquot et al. (2002) who used pulsed laser deposition. [B] & [U] refer to balanced and unbalanced sputtering respectively while error bars have been shown where possible.
We have previously simulated the reduction in the thermal resistance of hybrid lasers possible by replacing the polymer encapsulant (BCB) surrounding the ridge, with a material of higher thermal conductivity such as AlN \textsuperscript{16}. Placing a high thermal conductivity material (> 50 W/mK) in intimate contact with the active region allows rapid heat removal at source reducing the overall thermal resistance of the device by 3x \textsuperscript{16}. Figure 5 is the simulated temperature profile of a hybrid-laser cross-section where on the left-hand-side of the diagram the profile for an optical cladding material with a thermal conductivity of 0.29 W/mK (BCB) is shown. The simulated temperature in the active region increases up to 35 K above the base temperature of 300 K for an applied current of 100 mA. The significant thermal barriers previously outlined confine the generated heat to the MQW and waveguide regions. The right-hand-side of the diagram represents the thermal performance for an optical cladding material with a thermal conductivity of 130 W/mK (the highest value measured for DC magnetron sputtering \textsuperscript{14}). Now the maximum temperature reached is 314 K in the Multiple Quantum Well (MQW) region while the InP waveguide temperature does not increase significantly as the increased thermal conductivity of the optical cladding material enables the heat generated in the MQW to dissipate in this material. This will result in reduced operating temperatures in the active region and improved laser performance by increasing optical power output and decreasing roll-off at higher applied current levels.

To demonstrate hybrid ridge lasers with AlN optical cladding layers and reduced thermal resistances, we are developing sputtered AlN thin-films for integration in these devices. The deposition of AlN thin-films was undertaken using CMOS compatible reactive DC magnetron sputtering, without intentional substrate heating. The AlN films were deposited on InP (100) substrates in an Oxford Plasmalab 400. The native oxide was removed from the InP substrates by chemical etching in a HF solution prior to film deposition. A pure Al target was supplied with a DC power of 2 kW. 100% N\textsubscript{2} was used as reactive gas at a gas flow rate of 6 sccm with the chamber pressure maintained at 6 mTorr. Film thicknesses of 450 nm were deposited at a growth rate of 18.7 nm/min.

These films were used to investigate the structural morphology in the films and in particular the amorphous region thickness between the film and InP substrate that we expect to be larger than previously seen on silicon substrates. SEM and TEM images of the AlN films as grown on InP substrates are shown in Fig. 6 (a) and (b) respectively. The grain structure in the film is evident from the SEM image with columnar growth throughout the majority of the layer which is typical for films deposited by balanced magnetron sputtering. The columnar structure extends away from the...
substrate indicating preferential growth along the c-axis. The grain structure continues through the film and is evident on the top surface. The high-resolution cross-section TEM image reveals the nature of the interface between the deposited AlN film and InP substrates. The thickness of the amorphous interface between the AlN film and silicon substrate has previously been observed as 1-2 nm thick. Fig 6 (b) illustrates a 7 nm thick amorphous region at the AlN-InP interface in our samples. The larger thickness of this region as compared to AlN thin-films deposited on silicon is attributed to the larger lattice mismatch between AlN and InP than between AlN and Si.

Fig. 6: Electron microscope images of the magnetron sputtered AlN films. (a) SEM cross-sectional image of the complete 450 nm thick AlN films on an InP substrate (b) TEM image with the amorphous AlN region at the film-semiconductor interface highlighted.
In order to further investigate the nature of the amorphous region at the interface between the AlN thin-film and InP substrate we conducted selective area electron diffraction (SAED) and energy-dispersive x-ray spectroscopy (EDX) analysis of the region. The SAED data is not shown but did not indicate the presence of crystalline material in the 7 nm layer. To identify what material comprises this amorphous region, the EDX analysis (Figure 7) revealed a high concentration of Al, the N signal was not strong but this is typical in EDX analysis due the low bonding energy. This strong Al presence, and N content, indicates the region consists of amorphous AlN. Traces amounts of oxygen were also detected, most likely resulting from a small amount of native InO forming on the surface prior to the film deposition.

Our initial experiments reveal AlN thin-films deposited by reactive sputtering on InP exhibit thicker amorphous layers at the substrate interface than similar films deposited on silicon. Our application involves the deposition of these films around the ridge of a hybrid laser to rapidly remove heat from the MQW source. This amorphous layer will act as a barrier to heat transfer from the ridge and into the bulk AlN film where it would be dissipated. We estimate the thermal conductivity of amorphous-AlN is to be ~ 1.65 W/mK at 300 K using the method proposed by Slack. Therefore a 7 nm layers presents a significant thermal barrier. Ait Aissa et al. produced AlN thin-films using HiPIMS to effectively remove the amorphous-AlN layer at the interface between the Si substrate and film. In order to enable the benefits we expect by placing high thermal conductivity AlN optical cladding layers around the ridge of hybrid lasers, developing a process that removes the amorphous region, such as HiPIMS is critical.

5. CONCLUSIONS

We have proposed Aluminium Nitride (AlN) thin-films as dual function optical cladding and thermal spreading layers for hybrid ridge lasers, replacing current benzocyclobutene (BCB) encapsulation that has a thermal conductivity of 0.29 W/mK. A high thermal conductivity material placed in intimate contact with the Multi-Quantum Well active region of the laser allows rapid heat removal at source but places a number of constraints on material selection. The dielectric nature of AlN thin-films as well as their similar coefficient of thermal expansion to InP satisfy two of the primary criteria for thermal spreading cladding layers. The optical properties were deemed suitable for use as cladding material in hybrid
lasers as the mode confinement in the cladding layer remains below 0.14% for the expected refractive index values of 1.8–2.2 for AlN. We reviewed the state of the art in low temperature processing of AlN where values as high as 250 W/mK have been achieved using reactive sputtering. Towards our goal we presented AlN thin-films deposited by reactive DC magnetron sputtering on InP substrates. TEM imaging revealed a 7 nm amorphous region in the AlN film at the interface with the substrate. This layer is much thicker than previously revealed for AlN depositions on silicon substrates and could present a significant challenge in producing effective thermal conductivities on InP substrates comparable to the values achieved by others on silicon. Our future work requires the development of a sputter process that reduces or completely removes this amorphous region, to enable rapid heat transfer from a laser’s MQW to the bulk AlN film, and the measurement of the effective thermal conductivities of AlN thin-films as deposited on InP substrates, which has not previously been demonstrated.

ACKNOWLEDGEMENTS

The authors wish to acknowledge the financial assistance of the Irish Development Agency, the CTVR research centre (supported under SFI grant 10/CE/I1853 CTVR II), the French National Research Agency (grant VERSO - SILVER), and the European Union under the Horizon 2020 research programme (the TIPS project).

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