PCSI
Room Keahou I - Session PCSI-SuE2
Wide Bandgap Materials I

Moderator: Scott Crooker, Los Alamos National Laboratory

8:30pm **PCSI-SuE2-13 "High Throughput" Exploration of Oxide MBE Growth Space through Cyclical in situ Growth and Etching**, *Stephen Schaefer, Davi Fébba, Michelle Smeaton, Kingsley Egbo, Glenn Teeter, Syed Hasan, William Callahan, Andriy Zakutayev, **Brooks Tellekamp**,* National Renewable Energy Laboratory

Beta phase gallium oxide (β-Ga_2O_3) is an emerging ultra-wide bandgap semiconductor that has attracted attention for its potential to outperform existing materials operating at high breakdown voltages and high temperature. Alloying of In and Al in β-Ga_2O_3 provides the ability to individually engineer the bandgap and lattice parameters of the material, providing a useful toolbox for heterostructure engineering. However, the tendency of $(Al,In,Ga)_2O_3$ alloys to form competing phases, along with the complex suboxide chemistry of Ga and In, results in a growth window that is difficult to map and an alloy which is difficult to control.

We report on a high-throughput molecular beam epitaxy (MBE) technique to screen the growth conditions for the ternary alloy $(In_yGa_{1-y})_2O_3$, and the application of these findings to the successful synthesis of monoclinic $(Al_xGa_{1-x-y}In_y)_2O_3$. By leveraging the sub-oxide chemistry of Ga_2O_3 and *in-situ* monitoring by reflection high-energy electron diffraction (RHEED), a cyclical growth and etch-back method is developed to rapidly characterize the $(In_yGa_{1-y})_2O_3$ growth space. This cyclical method provides approximately 10x increase in experimental throughput and 46x improvement in Ga_2O_3 substrate utilization. Growth conditions for monoclinic $(In_yGa_{1-y})_2O_3$ are identified and targeted growths are characterized *ex-situ* to confirm improved In incorporation. These conditions are then used to grow quaternary $(Al_xGa_{1-x-y}In_y)_2O_3$ with Al cation composition *x* ranging from 1% – 24% and In cation composition *y* ranging from 3% to 16%. The structural, chemical and optical properties of the alloys are investigated. An $(Al_{0.17}Ga_{0.76}In_{0.07})_2O_3$ alloy lattice-matched to Ga_2O_3 is examined by high resolution microscopy, highlighting the correlation between surface facets and composition. Such lattice-matched material can be grown arbitrarily thick without elastic strain and relaxation, making it suitable for high voltage diodes, transistor barriers, and epitaxial dielectrics.

8:35pm **PCSI-SuE2-14 Stability of Interface Morphology and Thermal Boundary Conductance of Direct Wafer Bonded GaN|Si Heterojunction Interfaces Annealed at Growth and Annealing Temperatures**, *Kenny Huynh, Michael Liao,* University of California Los Angeles; *Xingxu Yan,* University of California Irvine; *John Tomko, Thomas Pfeifer,* University of Virginia; *Viorel Dragoi, Nasser Razek,* EV Group, Austria; *Eric Guiot, Raphael Caulmilone,* Soitec, France; *Xiaoqing Pan,* University of Irvine; *Patrick Hopkins,* University of Virginia; ***Mark Goorsky***, University of California Los Angeles

Evolution of the structural and thermal interfacial properties of direct wafer bonded (0001) GaN to (001) Si during annealing is investigated. Direct wafer bonding provides a pathway to fabricate and engineer heterointerfaces free of lattice mismatch restrictions. Here, an EVG® ComBond® wafer bonder was used to bond the GaN and Si under high vacuum at room temperature by first removing native oxide with an Ar^+ beam prior to bonding. We have demonstrated as-bonded GaN on Si with high thermal boundary conductance of 143 MW/(m^2·K) prior to annealing. High resolution transmission electron microscopy of the as-bonded structure revealed abrupt bonded interfaces with a ~1.3 nm amorphous interface due to the Ar^+ surface treatment. After annealing at 450 °C up to 7 hours, a 1 nm Ga-rich layer is observed across the interface near the surface of the Si in addition to SiN_x formation at the original bonded interface. Further annealing at 700 °C up to 24 hours led to the formation of Ga-rich pyramidal features that form across the bonded interface in the Si along the (111) planes. While recrystallization was observed to have a beneficial impact in other bonded systems, the chemical and structural reconfiguration of these GaN-Si interfaces resulted in poorer interfacial thermal transport by a factor of two (71 MW/(m^2·K)). This reduction is attributed to the degradation of thermodynamically less stable phases as the GaN breaks down into SiNx and Ga in the presence of silicon.We show that high TBC can be achieved through wafer bonding of GaN and Si and that interfacial properties that are stable at typical device operating temperatures (250 °C), but higher temperature annealing processing steps are deleterious to thermal transport across GaN-Si interfaces.

8:40pm **PCSI-SuE2-15 Plasma Deposition of GaN Thin Films on Silicon Substrates at Low Temperature**, *Lakshman Hussey, Jean-Luc Maurice, Pere Roca I. Cabarrocas, **Karim Ouaras**,* Ecole Polytechnique, France

Gallium nitride is attracting increasing attention in the semiconductor industry, especially for high-power and high frequency electronic applications, owing to its unique features, i.e. direct band gap of 3.4 eV, high electron mobility, good thermal stability, and elevated mechanical hardness. MOCVD and MBE are the most employed methods to produce high quality GaN layers, yet they have their own drawbacks. On the one hand, MOCVD uses toxic gases as precursors and operates at very high temperatures (~1000 °C) to enable the pyrolysis of precursors. On the other hand, MBE faces issues of (i) high cost associated with the use of ultra-high vacuum pumping, and (ii) scalability. Additionally, it also operates at high temperature. This latter point induces thermal mismatch strain due to large thermal expansion coefficient difference between GaN and Si that may produce interface defects, film cracking and wafer bowing upon cooling. A potential solution to avoid those issues is to resort to a lower temperature method such as low-pressure plasma deposition. In this work, we demonstrate the direct growth of GaN thin films on silicon substrate using reactive sputtering of a liquid Ga target by an Ar/N_2 plasma at room temperature [1]. The morphology, microstructure, and composition profile of the GaN thin films have been analyzed using a set of ex-situ solid-state characterization techniques while the plasma has been investigated using in-situ technics, including OES, MW interferometry and TALIF to measure electron density, gas temperature and N-atoms density, respectively. In the presentation, we will discuss the resulting properties of the films as a function of plasma characteristics.

[1] L. Srinivasan et al. J. Vac. Sci. Technol. A. Vol.41, Issue 5 (2023)

8:45pm **PCSI-SuE2-16 Si-Integrated Ferroelectric Films for Optical Computing**, ***Alex A. Demkov**, A.B. Posadas, A. Raju, D. Wasserman,* The University of Texas at Austin **INVITED**

The integration of optical components with traditional silicon technology, known as integrated silicon photonics (SiPh), is experiencing explosive growth. It offers many advantages such as lower power consumption, higher speed, and higher bandwidth when compared to the traditional CMOS-based information technology [1,2]. Electro-optic (EO) modulators are among the key active photonic components of SiPh, they can modulate either the amplitude or the phase of light. The operation of some of the most promising high frequency EO modulators is based on the linear EO effect, commonly referred to as the Pockels effect [2]. The linear EO effect constitutes the change in the refractive index of a material in response to an external electric field. Silicon is transparent below 1.1 eV and demonstrates extremely low optical loss, around 0.1 dB/m that is ideal for integrated photonic devices with applications in optical communications, optical neuromorphic and quantum computing, however, Si doesn't exhibit linear EO effect [3]. Barium titanate BaTiO3 (BTO) is an emerging material in SiPh with one of the largest known linear electro-optic coefficients. However, in BTO-based devices, high optical losses are consistently observed, typically an order of magnitude larger than those observed in lithium niobate. I will show that the origin of optical loss in BTO waveguides is non�absorptive and is caused by internal interfaces, aka planar defects such as e.g., ferroelectric domain walls. I will then discuss monolithic barium titanate photonic structures fabricated from BTO grown epitaxially by RF-sputtering on silicon-on-insulator substrates. Three types of test structures will be discussed: simple cut-back structures, high-Q ring resonators, and high-Q racetrack resonators. The record low loss of our monolithic barium titanate waveguide structures enables the demonstration of high-Q resonators with quality factors of Q > 100, 000. The low loss of the barium titanate photonic structures, coupled with barium titanate's large non-linear optical response offers a path to compact and high efficiency barium titanate photonic devices and structures for high-speed modulation, optical computing, and non-linear applications. This research is supported by a Multidisciplinary University Research Initiative from the Air Force Office of Scientific Research (AFOSR MURI Award No. FA9550-22-1-0307).

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