HL 33: Nitrides I – Growth and fabrication

Time: Wednesday 16:30–17:45 Location: POT/0006

HL 33.1 Wed 16:30 POT/0006

Homoepitaxial growth of AlN by plasma-assisted molecular beam epitaxy — •Xin Du, Hossein Yazdani, and Yongjin Cho — Paul-Drude-Institut für Festkörperelektronik (PDI), Leibniz-Institut im Forschungsverbund Berlin e.V., Hausvogteiplatz 5–7, 10117 Berlin, Germany

Wurtzite AlN can be considered an electrical insulator because of its ultrawide bandgap of 6.2 eV. However, it can become electrically active as either n-type or p-type through direct chemical doping or polarization doping when alloyed with the other group-III cations. This broad tunability in electrical conductivity, combined with its high thermal conductivity of about 340 W/m·K, makes AlN highly attractive for power electronics and deep-UV optoelectronic devices. Interest in AlN has considerably increased with the recent development of high-quality AlN bulk substrates with dislocation densities below 10^4 cm^{-2}. To fully leverage the high structural quality of these substrates in subsequent epitaxial layers, the native oxide must be removed before growth. Although Al-assisted deoxidation of AlN substrates has recently been shown to be effective for MBE growth, achieving consistently complete oxide removal and subsequently high-quality AlN homoepitaxy remains challenging. In this talk, we show how various cleaning methods and MBE growth conditions influence AlN homoepitaxy. This work serves as a seeding study at PDI for future investigations aimed at achieving reliable doping control in AlN with minimized compensating defects.

HL 33.2 Wed 16:45 POT/0006

Phase transition regions of epitaxially sputtered TiAlN layers on TiN and AlN buffer layers — •Emine Kaynar, Florian Hörich, Jürgen Bläsing, Fabian Grossmann, Usha Velpuri, Armin Dadgar, André Strittmatter, and Arne Busse — Institut für Physik, Otto-von-Guericke Universität Magdeburg, Magdeburg, Germany

For manufacturing vertical GaN-based power devices on Si substrates, it is advantageous to replace insulating AlN/AlGaN layers at the Si interface. AlN/AlGaN layers are currently required to ensure high-quality GaN on Si. TiAlN alloys offer a tunable bandgap from metallic conduction up to 6 eV and thermal robustness, making them promising alternatives to insulating Al(Ga)N buffers when epitaxial growth on Si is feasible. In this work, TiAlN layers were epitaxially grown on n-type Si (111) using TiN and AlN buffers prepared by a two-step sputtering process at growth temperatures below 900 °C. Highly crystalline cubic TiN (ω-FWHM ~ 0.3°, RMS $<$ 1 nm) served as a conductive template. By tuning the power ratio between Ti and Al targets, Al content was systematically controlled, enabling direct mapping of the cubic-wurtzite transition. On TiN buffers, cubic TiAlN remained stable up to x ~ 0.4. On wurtzite AlN buffers, the opposite transition from wurtzite to cubic occurred as Ti incorporation increased. For all AlN-buffered samples, ω-FWHM stayed below 1° and RMS roughness remained $<$ 5 nm. These results demonstrate precise phase control and high crystalline quality, positioning TiAlN as a strong candidate for conductive buffer layers in vertical GaN-on-Si device architectures.

HL 33.3 Wed 17:00 POT/0006

Epitaxial Growth of ZrN on Si(111) — •Muthukani Kathiresan, Usha Velpuri, Arne Busse, Florian Hörich, Jürgen Bläsing, Armin Dadgar, and André Strittmatter — Institut für Physik, Otto-von-Guericke Universität Magdeburg, Magdeburg, Germany

Transition metal nitrides can add new functionalities to GaN devices. These range from conducting buffer layers for the growth of vertical GaN devices on Si, as template for the growth of N-polar GaN up to enhanced piezo- and ferroelectric properties when alloyed with AlN. Transition-metal nitrides (TMNs) such as ZrN, HfN, TiN and ScN crystallize in the rock-salt structure and exhibit metallic conductivity except for ScN which is semiconducting. For nitride growth, ZrN is particularly attractive due to its favorable lattice relationship, exhibiting an in-plane mismatch of only 1.35% between ZrN (111) and GaN (0001). Additionally, ZrN layers can be deposited by sputtering, whereas layer growth by MOVPE suffers from the low-vapor pressure of available precursors.In this work, we present recent progress in the sputter epitaxy of ZrN on Si (111). For 100-nm-thick films grown at 900 °C in N2/NH3, we achieved an ω-FWHM of 0.5°. Introducing NH3 promoted a transition from a columnar grain structure to a compact, two-dimensional morphology, with a surface roughness of 1.7 nm. The thermal stability of these layers was assessed through annealing at 1100 °C under NH3, which led to reduced film density by void formations, revealed by X-ray reflectivity (XRR) measurements and scanning electron microscopy (SEM).

HL 33.4 Wed 17:15 POT/0006

In-situ fabrication of $In_{0.3}Ga_{0.7}N$ pseudo-substrates on GaN (0001) templates via a three-step protocol in plasma-assisted molecular beam epitaxy — •Huaide Zhang, Aidan Campbell, Jingxuan Kang, Jonas Lähnemann, Oliver Brandt, and Lutz Geelhaar — Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Hausvogteiplatz 5-7, 10117, Berlin, Germany

The considerable lattice mismatch between GaN and InN introduces significant strain into (In,Ga)N epitaxial layers grown on GaN templates. This strain impedes the incorporation of In and induces a strong piezoelectric field in (In,Ga)N/GaN quantum wells, which diminishes the internal quantum efficiency. Furthermore, the accumulated strain can prompt plastic relaxation of the lattice, generating additional threading dislocations. The high In content required for (In,Ga)N-based light-emitting diodes (LEDs) operating in the amber/red spectral range necessitates, hence, a substrate with an adjusted lattice constant. In this work, we present a three-step growth method for fabricating a highly relaxed $In_{0.3}Ga_{0.7}N$ pseudo-substrate directly on GaN(0001) templates which is conducted entirely within a plasma-assisted molecular beam epitaxy system. In contrast to other approaches, our method does not require any ex-situ patterning, providing thus advantages in terms of scalability and cost. The resulting structure demonstrates superior characteristics in key properties, including In content, degree of strain relaxation, and surface smoothness compared to existing alternatives.

HL 33.5 Wed 17:30 POT/0006

Influence of A-Site Cations on Structure, Defect Density and Photoactivity of Tantalum-Based Perovskite Oxynitride Photoelectrodes — •Gabriel Grötzner[1,2], Aleksandr Kochergov[1,2], Oliver Brune[1,2], Laura I. Wagner[1,2], Saswati Santra[1,2], Verena Streibel[1,2], and Ian D. Sharp[1,2] — [1]Walter Schottky Institute, Technische Universität München, Germany — [2]Physics Department, TUM School of Natural Sciences, Technische Universität München, Germany

Perovskite oxynitrides are emerging materials for photoelectrochemical (PEC) water splitting, yet the influence of the A-site cation on their material properties remains poorly understood. Here, we investigate a series of $ATaON_2$ thin films (A = La, Ce, Pr, Nd, Gd, ordered by decreasing ionic radius) to elucidate the role of the A-site cation on structural, optoelectronic, and PEC properties. X-ray diffraction analysis reveals a systematic lattice contraction with decreasing ionic radius of the A-site cation. This structural change is accompanied by an increase in optical band gap from 1.8 eV to 2.2 eV and a reduction in sub-bandgap absorption, indicating lower defect densities for smaller A-site cations. Electrical measurements show reduced conductivity for $GdTaON_2$ compared to $LaTaON_2$, consistent with defect suppression. By changing the A-site cation from La to Gd, the photocurrent density in PEC measurements doubles, despite an increase in optical band gap, which indicates the beneficial impact of reduced defect-mediated recombination. These insights offer design principles for defect and band-structure engineering in perovskite oxynitride photoanodes.