HL 58: Nitrides: Preparation and Characterization II

Time: Friday 9:30–10:30 Location: H14

HL 58.1 Fri 9:30 H14

Random Alloy and Ordered Phases of Cubic Indium Gallium Nitride From a First-Principle Perspective — •Jan M. Waack[1,2], Markus Kremer[1,2], Nils Andre Schäfer[1,2], Michael Czerner[1,2], and Christian Heiliger[1,2] — [1]Institut für theoretische Physik, Justus-Liebig-Universität Gießen, Germany — [2]Center for Materials Research (LaMa), Justus-Liebig-Universität Gießen, Germany

Although the miscibility gap in cubic zincblende indium gallium nitride ($In_xGa_{1-x}N$) has been overcome, the specific role of ordered phases in this process remains unclear. First-principle density functional theory calculations provide a reference point for addressing this question. Ordered phases, such as CuPt-type and chalcopyrite-type structures, exhibit unique structural and electronic properties that differentiate them significantly from the random alloy. An understanding of these distinctive features of ordered phases provides a basis for their experimental identification.

We present a comprehensive data set on key structural parameters, including lattice constants and bond lengths, as well as elastic properties such as elastic constants and phonon modes. Furthermore, we explore electronic properties including the band gap and Bloch spectral function using *ab-initio* approaches such as LDA-1/2 and the mBJ functional. The presented insights into the physical properties of ordered phases and the random alloy offer a robust foundation for their experimental detection and further exploration.

HL 58.2 Fri 9:45 H14

Characterization of structural and optical properties of a red InGaN/GaN MQW LED — •Niklas Dreyer[1], F. Bertram[1], G. Schmidt[1], H. Eisele[1], S. Petzold[1], O. August[1], A. Dempewolf[1], K. Wein[1], J. Christen[1], B. Sheng[2], and X. Wang[2] — [1]Otto-von-Guericke-Universität Magdeburg, 39106 Magdeburg, Germany — [2]Peking University, Beijing 100871, China

An InGaN/GaN LED with an intended red emission (> 600 nm) was grown by MOVPE on a sapphire substrate. On an undoped GaN buffer followed by a doped n-GaN layer, the active region consists of a stack of three identical sequences, each with three quantum wells (QWs). The first two QWs nominally contain 15 % In (blue) and the third 40 % In (red). Each sequence is confined by an $Al_{0.32}Ga_{0.68}N$ layer. Finally, a p-doped $Al_{0.17}Ga_{0.83}N$ EBL is positioned, which is further capped by a dielectric DBR and processed, including metal contacts.

The LED is comprehensively characterized by cross-sectional cathodoluminescence performed in scanning transmission electron microscopy (STEM-CL) and by electroluminescence (EL). The luminescence along the growth direction is directly visualized in CL linescans: in particular, each QW can be spectrally and spatially resolved and shows a distinct emission. A wavelength shift for all QWs is observed. Furthermore, the n-GaN exhibits near-band-edge (NBE) luminescence at 356.7 nm at $T = 16$ K corresponding with a high free carrier concentration due to Burstein-Moss Shift.

The EL spectrum shows intense, broad emission around 650 nm, with a weak shift to shorter wavelengths for higher injection current.

HL 58.3 Fri 10:00 H14

Advanced nano-characterization of doped and undoped InGaN/GaN MQW-LED structures — •Luca Greczmiel, F. Bertram, G. Schmidt, P. Veit, H. Eisele, A. Dempewolf, S. Petzold, J. Christen, C. Berger, A. Dadgar, and A. Strittmatter — Otto-von-Guericke-Universität Magdeburg, 39106 Magdeburg, Germany

In this study, we comprehensively investigate structural and optical properties of InGaN/GaN MQW-LED-structures by cathodoluminescence (CL) directly performed in a scanning transmission electron microscope (STEM). The LEDs are grown by MOVPE on top of an optimized GaN/sapphire template. The first pn-junction is formed by an 1.6 μm thick GaN:Si layer and a 345 nm thick GaN:Mg layer, which are nominally doped with a concentration of $7 * 10^{18}$ cm^{-3} and $2 * 10^{19}$ cm^{-3}, respectively. In between the n- and p-layer a MQW is located, which is composed of a stack of five InGaN QWs being separated by GaN:Si barriers, with a thickness of 3 nm and 7 nm, respectively. The InGaN wells have a nominal In content of 12 %. In STEM-linescans of the active region along the sample cross-section, the first QW shows emission at shorter wavelengths with respect to the subsequent following QWs. For comparison, a second MQW structure was investigated, which was identically grown, but sandwiched between uGaN. In contrast to the first sample, the CL of the 1st QW shifts to longer wavelengths, with respect to the subsequently following QWs. Hence, this spectral shift of the 1st QW is supposed to depend on the electric field in the space charge region.

HL 58.4 Fri 10:15 H14

Physical properties and thermal stability of zirconium platinum nitride thin films — Rebecca Gallivan[1], Ana Michelini[1], Nensi Toncich[1], Nerea Abando Beldarrain[1], Julia Manser[1], Arnold Müller[2], Christof Vockenhuber[2], and •Henning Galinski[1] — [1]Laboratory for Nanometallurgy, Department of Materials, ETH Zurich,8093 Zurich, Zurich, Switzerland — [2]Laboratory of Ion Beam Physics, Department of Physics, ETH Zurich, 8093 Zurich, Zurich, Switzerland

By providing new functionality, ternary transition metal nitrides (TMNs) have the potential to greatly broaden the material design space. Nevertheless, the majority of systems have only been studied computationally, and translation to experimental synthesis is restricted by a lack of knowledge about their stabilizing mechanisms. In this talk, we discuss the fabrication of ternary Zr-Pt-N thin films and examine their physical properties [1]. We show that Pt replaces nitrogen on the nonmetallic sublattice, destabilizing the rock salt structure and forming a complicated cubic phase. Additionally, we observe the exsolution of Pt nano precipitates from the Zr-Pt-N films upon annealing as well as degradation in the nitridic film's thermal stability. Even at low concentrations, Pt facilitates a solid reaction with the Si substrate that is otherwise inaccessible in ZrN films.

References: [1] Appl. Phys. Lett. 125, 221901 (2024)