On the preparation of AlN single crystals and substrates for AlGaN devices

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AlN single crystal substrates are employed in deep-UV device research to provide pseudomorphically strained $Al_xGa_{1-x}N$ layers with low defect density. Bulk AlN grown by physical vapor transport (PVT) at temperatures in the range of 2000-2100°C has a threading dislocation density (TDD) well below 10^5 cm^{-2} when grown in N-polar (000-1) direction on AlN seed wafers. However, the distribution especially at the border regions of the crystal has a decisive impact on macroscopic defect formation when seeds including such areas are used for subsequent growth runs. Dislocation distribution and evolution are particularly influenced by growth on prismatic facets during diameter increase. In a non-optimized growth technology these areas may contribute to lattice plane bending/curvature in subsequently grown crystals. In polished substrates, such curvature leads to a varying off-orientation on the substrate surface that may hamper homogeneous step flow in subsequent epitaxy.

Deep-UV transparency is desired for AlN substrates, at least for measuring EQE and light outcoupling simple by on-wafer testing. Crystals with $\alpha < 25$ cm^{-1} at 265 nm are regularly grown when the concentrations of oxygen, silicon, and carbon impurities [O], [Si], and [C] satisfy the inequalities $3[C] < ([O] + [Si])$ and $([O] + [Si] + [C]) < 10^{19}$ cm^{-3} [1]. These conditions can be reached using getter materials for carbon and oxygen, such as tungsten and TaC, respectively. Best values of $\alpha(265nm) = 14$ cm^{-1} are achieved at $[O] = 6.4x10^{18}$ cm^{-3}, $[C] = 1.8x10^{18}$ cm^{-3}, $[Si] < 5x10^{16}$ cm^{-3}. Furthermore, a remaining deep-UV absorption affects the optical properties under LED operation. We will present evidence of a Fermi level effect that renders the carbon-induced absorption bands inactive under the point defect regime achieved in our crystals. Recent improvements in substrate preparation are confirmed by further achievements in homo- and heteroepitaxy and properties of demonstrator devices on our AlN substrates.

Finally, we will present a novel approach to prepare substrates that are lattice matched to high Al-content AlGaN by alloying AlN with ScN [2]. AlN substrates with Sc concentrations of up to 1.0 at% have been prepared by a modified PVT growth technique. While lattice matching to e.g. $Al_{0.5}Ga_{0.5}N$ would require 3-5 at% of Sc in the crystals, the amount achieved would least contribute to increase the critical thickness for pseudomorphic growth. We will discuss the results obtained so far and provide perspectives and limitations.

[1] C. Hartmann, J. Wollweber, S. Sintonen et al., CrystEngComm 18 (2016) 3488-3497

[2] A. Dittmar et al. Patent Application WO 2017/050532 (30.03.2017)

Supplementary information

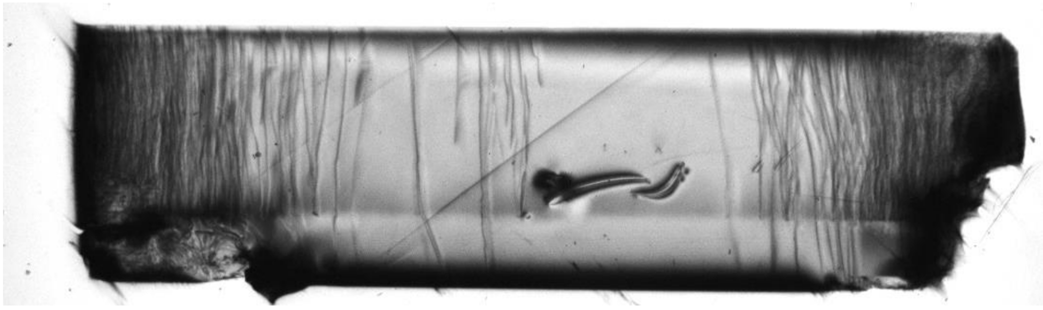
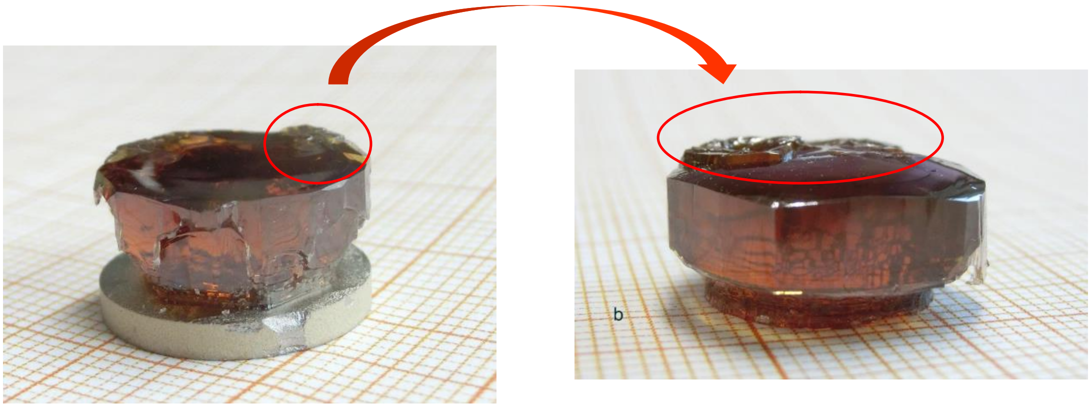


Fig. 1: 11-20 transmission X-ray topograph of an AlN wafer a-plane cross-section (the lower part is the seed; the width of the cross-section is about 10 mm)



Ø15 mm AlN bulk

Ø17.5 mm AlN bulk

Fig. 2: Evolution of a macro-defect during diameter increase in AlN bulk growth

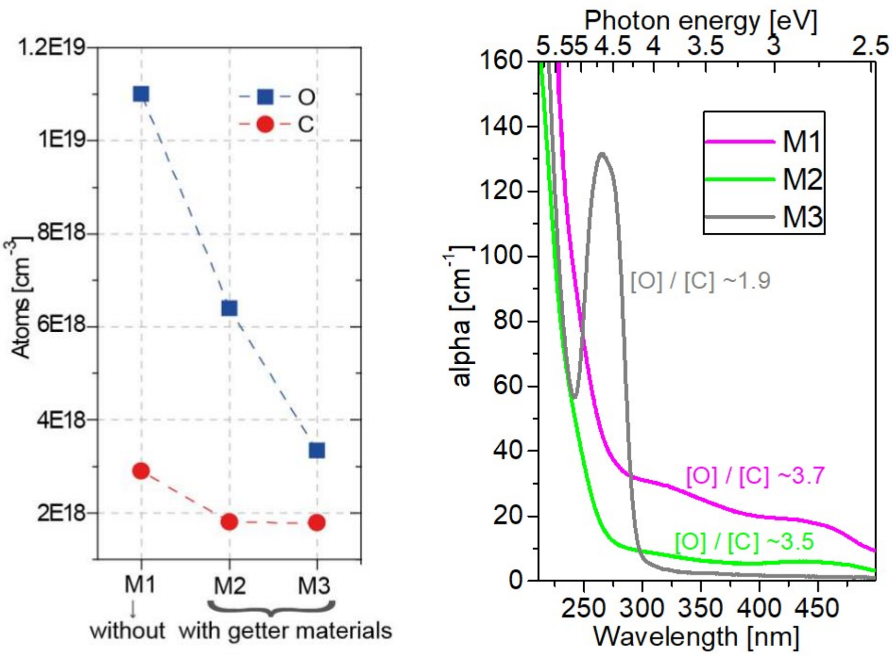


Fig. 3: Carbon and oxygen concentrations in AlN bulk crystals grown without and with getter materials (left) and corresponding optical absorption spectra in the UV range (right)