

# Favorable Growth Conditions and Diameter Enlargement of Bulk AlN Single Crystals Grown by Physical Vapor Transport

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Single-crystalline bulk AlN substrates with high structural quality are considered mandatory to exploit the full potential of AlGaN-based devices for applications in deep ultraviolet (UV) photonics<sup>1,2</sup> and high-power electronics<sup>3</sup>. Recently developments show that both the substrate quality and epitaxial technology are decisive to harvest this potential. But still, further development and commercialization is hampered by the continued lack of high-quality substrates in terms of size and quantity, as well as in uniformity and homogeneity of optical and structural properties.

In this contribution, we report on the growth and characterization of bulk AlN single crystals in respect to the control of impurities, dislocations, growth rate, and diameter enlargement. We show how optical properties depend on growth conditions in our set-up. Deep-UV absorption is reduced in crystals growth at higher temperatures. We attribute this to a lower oxygen incorporation due to enhanced chemical reaction with the crucible parts. Also, the structural quality of the crystals increases significantly with temperature: Dislocation densities in the order of  $10^3$ – $10^4$  cm<sup>-2</sup> are typically achieved for seed temperatures above 2220°C. On the other hand, growth rate depends on both seed temperature and temperature gradient. When using a higher seed temperature, a lower axial (source-to-seed) gradient still yields reasonable growth rates of about 200 µm/h at excellent crystal quality<sup>4</sup>.

Even more, we recently tailored the hot-zone geometry to allow for a significantly increased lateral temperature gradient. In such a setting, the lateral growth rate and thus the diameter increase can be substantial. This results in crystals with fully faceted prismatic sides where the final diameter spans over the full crystal length, providing maximum yield. We have grown AlN crystals up to one inch in diameter. X-ray diffraction rocking curves obtained across different positions on the crystal shows excellent quality with FWHM values lower than 12 arcsec for both the 0002 and 10-13 reflections. Such scalable and reproducible expansion of small AlN seeds has not been published so far.

[1] A. Yoshikawa, R. Hasegawa, T. Morishita, K. Nagase, S. Yamada, J. Grandusky, J. Mann, A. Miller, L.J. Schowalter, *Applied Physics Express*, **2020**, 13, 022001.

[2] Z. Zhang, M. Kushimoto, A. Yoshikawa, K. Aoto, L.J. Schowalter, C. Sasaoka and H. Amano, *Applied Physics Express*, **2022**, 15, 041007.

[3] S. Ozaki, J. Yaita, A. Yamada, Y. Kumazaki, Y. Minoura, T. Ohki, N. Okamoto, N. Nakamura, J. Kotani, *Applied Physics Express*, **2021**, 14, 041004.

[4] C. Hartmann, L. Matiwe, J. Wollweber, I. Gamov, K. Irscher, M. Bickermann, T. Straubinger, CrystEngComm, **2020**, 22, 1762-1768.

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