Faceting in AlN Bulk Crystal Growth and its Impact on Crystal Properties

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The Al-polar (0001) forms the chemically most stable facet in AlN. But in typical high-temperature PVT conditions used for growth of bulk single crystals, rhombohedral {01$\underline{1}$*n*} and prismatic {01$\underline{1}$0} facets are growing slower and eventually dominate the crystal habit. As the incorporation of impurities (or formation of vacancies) varies greatly on different crystallographic facets, the formation of these structures leads to inhomogeneous properties, such as electrical behaviour and deep-UV optical absorption, across single the crystal volume [1]. Depending on growth conditions, the crystals may also show complex zonar and defect structures [2].

Crystals grown under relatively high radial gradients on (0001) seeds will eventually develop into a single six-fold prism ending with a pyramid with rhombohedral facets, see Fig. 1. As all facets are symmetrical to the thermal field, crystals with homogeneous properties and low defect density can be obtained. However, extended structural defects originating in the seed or at the seed interface may lead to an 'unfinished habit' featuring pyramidal depressions. As a result, growth takes place on alternating (0001) and {01$\underline{1}$*n*} facets, resulting in complex zonar and defect structures, see Fig. 2. If crystals are grown on seeds with appropriate off-orientation, a single rhombohedral facet will form in the main crystal area, leading to homogeneous impurity incorporation in the whole single-crystal area. But due to its low symmetry and position in the thermal field, the facet tends to bend and break up into domains and low-angle grain boundaries. Finally, possible routes to enlarge the (0001) facet will be discussed, potentially leading to AlN bulk crystals with clearly different impurity content and optical properties.

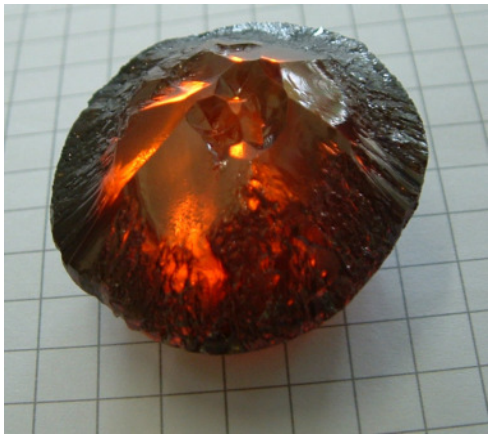

Fig. 1: AlN crystal with rhombohedral facets as well as pyramidal depressions in the center area (on 5 mm grid).

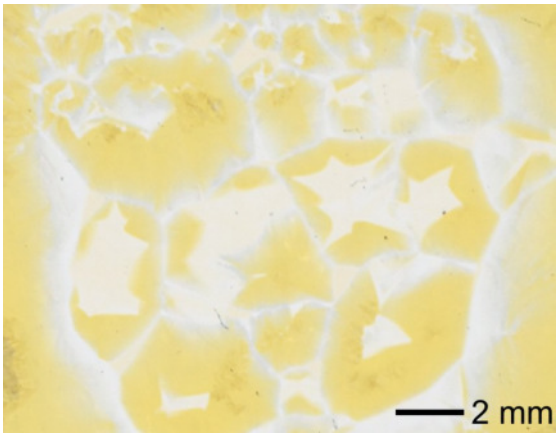

Fig. 2: Wafer from an AlN bulk single crystal with several pyramidal depressions on the surface. The wafer shows a pronounced zonar structure.

[1] M. Bickermann, B. M. Epelbaum, O. Filip, P. Heimann, S. Nagata, A. Winnacker, Phys. Status Solidi C **7** (2010) 21-24.

[2] M. Bickermann, S. Schimmel, B. M. Epelbaum, O. Filip, P. Heimann, S. Nagata, A. Winnacker, *Structural Defects in Aluminum Nitride Bulk Crystals Visualized by Cathodoluminescence Maps*, Proc. of the IWN 2010, held Sep 19-24, 2010 in Tampa (FL), USA; accepted for publication in Phys. Status Solidi C.