Faceting in AlN bulk crystal growth and its impact on crystal properties.

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Single-crystalline aluminium nitride (AlN) is a very promising substrate material for nitride-based optoelectronic devices performing in the deep UV spectral range. The feasibility of bulk AlN growth using sublimation-recondensation (PVT method) has been demonstrated. However, large AlN substrates of high crystalline quality are in fact not made available until now. In this presentation, we will show that faceting in AlN bulk crystal growth causes a complex zonar structure. This leads to inhomogeneous properties across the single crystal volume and also limits crystal size/habit by growth of slowest facets.

The Al-polar (0001) forms the chemically most stable facet in AlN. On the other hand, under typical high-temperature PVT growth conditions, rhombohedral $\{01\underline{1}n\}$ and prismatic $\{01\underline{1}0\}$ facets are growing slower and thus eventually dominate the crystal habit. Thus, increasing the single crystal diameter by subsequent re-growth on (0001) seeds requires growth conditions to avoid complete faceting. Still, the enlarged volume is often of very poor structural quality. This holds even for growth in off-oriented directions, e.g. by using the $(01\underline{1}2)$ or $(01\underline{1}3)$ plane as growth surface. Here, a single rhombohedral facet forms in the main crystal area. But due to its low symmetry and position in the thermal field, these facets tend to bend and break up into domains and low-angle grain boundaries. Enlargement of single crystal diameter is still hindered by prismatic facets as the crystal expands mainly along c-direction.

Crystal faceting is strongly enhanced as the presence of impurities such as silicon is lowered. Still, relatively flat crystals can be grown on (0001) seeds by tailoring growth temperature and thermal field in the recondensation area. However, extended structural defects, originating in the seed or at the seed interface and propagating through the growing crystal, may lead to formation of rhombohedral facets and pyramidal structures at the basal plane surface. As the incorporation of impurities (and presumably also the formation of vacancies) varies greatly on different crystallographic facets, the formation of these structures leads to inhomogeneous properties – such as deep-UV optical absorption – across the crystal volume.