Orientation-Dependent Properties of Aluminum Nitride Single Crystals

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Recent major developments in nitride semiconductor technology have driven the interest towards aluminum nitride (AlN) as substrate employed in III-nitride epitaxy e.g. for deep-UV optoelectronic applications and high-power microwave devices. In this context, preparation of AlN crystals by physical vapor transport (PVT) seems to be very promising. Recently, we described a process for the preparation of self-nucleated AlN crystals. As these crystals were grown with minimal contact with crucible walls or other crystals, they show a natural growth habit with many observable facets. Identification of the most stable (slowly growing) faces in actual growth conditions is very important since they are favorable for high-quality seeded growth.

In this study, we investigate different as-grown facets as well as on oriented, polished cuts of several self-nucleated AlN single crystals. First, we show that Raman and Fourier transform infrared spectroscopy provide means to evaluate crystalline quality as well as to detect the orientation of any AlN facet. Such local, nondestructive technique is very useful for selecting and evaluating samples of single crystalline AlN. Second, we describe how optical absorption and luminescence depend on sample orientation. Correlating these properties to optical and atomic force microscopy of as-grown surfaces, we conclude that defect formation and incorporation of impurities into the growing crystal depend strongly on the respective surface orientation. Third, we evaluate micro-hardness measurements performed on different crystal facets in terms of crystallographic structure and impurity incorporation.

In summary, impurity incorporation and/or intrinsic defect formation strongly depends on the crystallographic orientation of the facet. As a result, single-crystalline freestanding AlN exhibits a non-conventional asymmetric growth habit and a pronounced zonal structure. Apart from determining crystal orientations that are promising for seeded growth of AlN, information on orientation-dependent properties can provide a deeper understanding of typical defects and impurities in bulk AlN.



Fig. 1: Raman spectra taken in normal incidence on different as-grown facets of a self-nucleated AlN single crystal. The orientation of any AlN facet can be unambiguously determined by the presence and position of different TO and LO phonon bands .



Fig. 2: Cathodoluminescence spectra taken at room temperature on different as-grown facets of a self-nucleated AlN single crystal. Luminescence in the 5.5–6.2 eV energy range is attributed to bound exciton decay. Luminescence at lower energies is presumably impurity and/or defect related and strongly varies with facet orientation.