Growth and characterization of bulk AlN substrates grown by PVT

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Recent major developments in GaN semiconductor technology have driven the interest towards aluminum nitride (AlN) and gallium nitride (GaN) bulk crystals, which hold promise to be ideal substrates for III-nitride epitaxy. Up to now the potential of these materials in substrate applications has been disadvantaged by the lack of sufficiently large and perfect single crystals. In this context, preparation of AlN crystals by physical vapor transport (PVT) seems to be very promising. By sublimating AlN powder at 2000...2300°C and subsequent condensation of vapor species we have achieved preparation of dense, polycrystalline material containing single-crystalline grains as well as freestanding single crystals exceeding 100 mm^3 in volume (see Fig. 1). The grown material is single-phase wurtzite AlN containing about 100 ppm wt of oxygen; transition metals are present only in the sub-ppm range.

In this study, we present our recent results on the growth of AlN substrates by PVT and we emphasize on the news results we have achieved. Then we present a detailed investigation of optical and electrical properties of such bulk AlN crystals. We have performed measurements of optical absorption, FT-IR reflectance, cathodoluminescence, thermal conductivity and electrical resistivity on samples grown at different temperatures in order to get information about incorporation of impurities and formation of intrinsic defects. Additionally, impurity concentrations were measured by GDMS and SIMS.

It turns out that these properties depend significantly on growth parameters such as temperature and crystal orientation/polarity in respect to temperature gradient. An example is shown in Fig. 2: crystals grown at different temperatures exhibit different optically excited transitions, showing up as broad absorption bands in UV range optical absorption. Another example is cathodoluminescence, where the position and strength of the broad UV luminescence band of freestanding crystals strongly depend on the crystal orientation. We attribute this to orientation-dependent impurity incorporation and defect formation. This result is validated by AFM and SEM microscopy in conjunction with EDX analysis and SIMS performed on crystal surfaces.

All presented results can lead the way towards a better understanding of electronic levels in bulk AlN and the influence of crystal growth on impurity concentration and intrinsic defect formation.

Fig. 1 caption:
Freestanding AlN single crystals grown by the PVT technique (shown on 1 mm grid).

Fig. 2 caption:
Optical absorption spectra of bulk AlN crystals grown at different temperatures. Top region and seeding region denote the location of the absorption measurement in the crystals, respectively.