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Crystals and substrates for next-generation oxide semiconductor devices

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The growth of volume crystals of oxides and fluorides has a long tradition at the IKZ but is also characterized by modern topics with outstanding international visibility. One striking example is the preparation of novel ultra-wide band-gap (UWBG) semiconductor materials. 2-inch diameter gallium oxide (β-Ga_2O_3) bulk crystals grown from melt by the Czochralski method have been developed at IKZ[1–3]. Mg-doped semi-insulating as well as Si-doped electrically conducting substrates are demanded for lateral and vertical power transistor devices that exhibit the highest breakdown fields and enable miniaturization of power electronics[4].

In the meantime, we have extended our research to develop the corresponding ternary compound β-$(Al_xGa_{1-x})_2O_3$ (AlGaO) that will allow for band-gap tuning and electron confinement. Single crystals are needed to determine reliable electronic and structural properties and to assess the solubility limits in near-equilibrium conditions[5], but also as lattice-adapted substrates for films or film stacks of different composition[6]. We obtained and investigated single AlGaO crystals in the range from $x = 0$ to $x = 0.4$, and also ones doped with Mg or Si. While the monoclinic structure is retained up to $x = 0.4$, the electrical conductivity in the samples deteriorates for $x > 0.15$, while the thermal conductivity suffers even from low amounts of aluminum due to impurity scattering[7].

Rutile GeO_2 is another novel UWBG material (bandgap 5.0–5.5 eV) with promising properties for power electronics applications significantly exceeding those of β-Ga_2O_3. We have prepared the world's first bulk single crystals with good structural quality and high electrical conductivity when lightly doped with Sb (0.02–0.2 % at.). The melting point of GeO_2 is only 1115°C. However, the bulk crystal growth is exceedingly difficult due to high viscosity of the melt, glass formation, and a phase transition. Thus, we utilized alkaline carbonate fluxes for TSSG growth[8]. While the results are encouraging, this material is still in an early stage regarding epitaxy and device development.

Finally, the case of substrates for $BaSnO_3$ is considered. $BaSnO_3$ is a wide band-gap (about 3 eV) oxide semiconductor of perovskite structure with an exceptionally high electron mobility at high carrier densities (e.g., 320 V/cm·s at $8 \cdot 10^{19}$ cm^{-3}), and proper interfaces could even enable a 2DEG formation. We have grown $BaSnO_3$ single crystals at IKZ using directional solidification[9], but the size is very difficult to scale up and heterointerfaces could introduce additional functionality. We have thus also developed bulk growth of the lattice-matched compound $LaInO_3$[10], which leads to improved crystalline quality of the $BaSnO_3$ films when the substrate surface is well prepared[11]. As alternatives, Ba_2ScNbO_6[12] as well as (Nd,La)(Lu,Sc)O_3[13] crystals have been grown, the latter even by the Czochralski method. However, the very high melting temperature of these compounds (about 2150°C) makes preparation challenging.

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