Crystals and Substrates for Next-Generation Oxide Semiconductor Devices

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The growth of oxide single crystals from the melt at high temperatures is a core activity at IKZ. While the growth process largely depends on thermochemical behavior and thus must be adapted to each desired compound, the underlying technologies are useful for different crystals regardless of the application. In this talk, we will report on our work on preparation of different oxide crystals and substrates for novel wide band-gap oxide semiconductors.

2-inch diameter gallium oxide (β-Ga2O3) 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. 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 [6].

Rutile GeO_2 is another novel wide band-gap oxide semiconductor (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 [7]. 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 [8], 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 $LaInO_3$ [9], which leads to improved crystalline quality of the $BaSnO_3$ films when the substrate surface is well prepared [10]. As alternatives, Ba_2ScNbO_6 [11] as well as $(Nd,La)(Lu,Sc)O_3$ [12] 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.

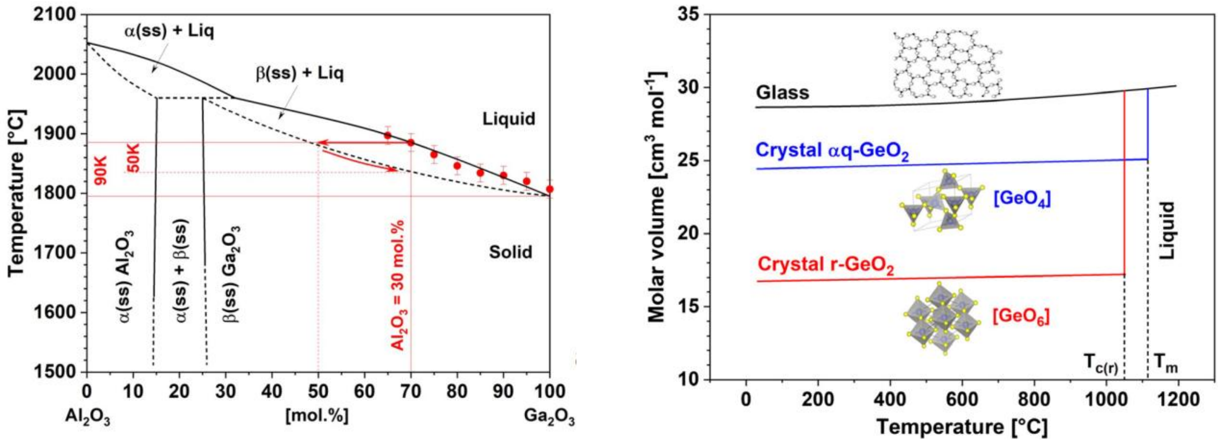

Fig. 1: Phase diagram (sketch) of Al_2O_3–Ga_2O_3 (left) [5] and phase transitions upon cooling of GeO_2 (right) [7].

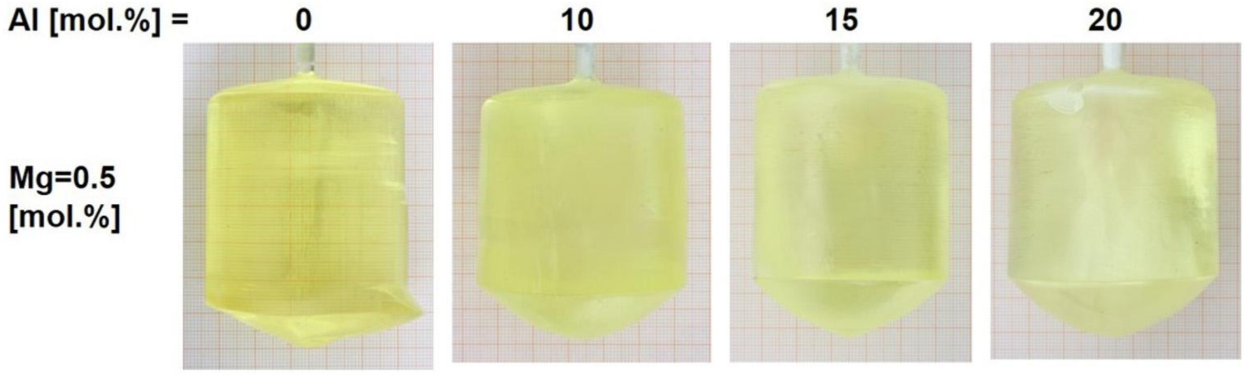

Fig. 2: 2-inch diameter β-$(Al_xGa_{1-x})_2O_3$ crystals with x = 0–0.2 and Mg = 0.5 mol. % in the melt [5]

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