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Oral contribution for 24. Kalorimetrietage

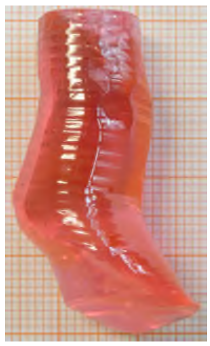
Rare-earth oxide systems for substrate and laser applications

Rare-earth scandate single crystals with orthorhombically distorted perovskite structure (P-$REScO_3$, RE = a rare-earth element from Pr–Dy) have come into the focus of interest as substrates for the epitaxial deposition of many functional oxides, and especially for strain engineering of perovskitic functional layers. The growth of such crystals in diameters beyond 30 mm is established at IKZ Berlin since two decades. The pseudocubic lattice parameters $a_{pc} \approx 4$ Å of these materials can be adjusted by an appropriate choice of the RE element occupying the larger cation site of the perovskite structure. Meanwhile also the growth of mixed crystals between two rare-earth scandates is possible and allows fine-tuning of a_{pc} [1]. Another possible field of applications for the cubic (bixbyite structure) RE_2O_3 with RE = Lu, Sc, or Y is found as excellent host materials for high-power and ultrafast lasers [2].

The pure RE_2O_3, and somewhat less also the $REScO_3$, have in common that they melt at very high temperatures beyond 2000°C, and partially even beyond 2300°C. This is very challenging because suitable crucible materials that withstand the growth conditions are scarce: Up to ca. 2250°C usually Ir is used, above sometimes Re.

Thermal analysis can help to define concentration fields in multinary RE_2O_3 based systems (so far up to four components) where liquidus temperatures are sufficiently low to allow crystal growth from the melt. In our laboratory these experiments are usually performed in a NETZSCH STA 429C with W/Re sample holders and W crucibles. Such measurements are difficult, because the load on technical components of the thermoanalytic setup is severe. Fortunately, it turns out that a thermodynamic description/assessment e.g. with FactSage is partially not very complicated, because deviations of the systems from ideality tend to be comparatively small at the highest temperatures. In the talk the following systems will be discussed in detail:

- Nd_2O_3-Lu_2O_3-Sc_2O_3 which is interesting because the perovskite phase $NdLu_{1-x}Sc_xO_3$ exists only on the scandium side [3].
- (Er)Lu_2O_3-Sc_2O_3-Y_2O_3, where for the first time the Czochralski growth of rare-earth oxide single crystals was performed recently [4].
  A photograph of $(Er_{0.07}Sc_{0.5}Y_{0.43})_2O_3$ is shown here.



- La_2O_3-Nd_2O_3-Lu_2O_3-Sc_2O_3, the first quaternary RE oxide system from which bulk crystals could be grown [5].

References:

[1] Uecker et al., Growth and investigation of $Nd_{1-x}Sm_xScO_3$ and $Sm_{1-x}Gd_xScO_3$ solid-solution single crystals, Acta Phys. Pol. A 124 (2013) 295–300.

[2] Kränkel, Rare-earth depend sesquioxides for diode-pumped lasers in the 1-, 2-, and 3-µm spectral range, IEEE J. Sec. Top. Quant. Electron. 21 (2015) 1602013.

[3] Hirsch et al., Investigation of the Nd_2O_3-Lu_2O_3-Sc_2O_3 phase diagram for the preparation of perovskite-type crystals $NdLu_{1-x}Sc_xO_3$, J. Crystal Growth 505 (2019) 38–43.

[4] Kränkel et al., Czochralski growth of mixed cubic sesquioxide crystals in the ternary system Lu_2O_3-Sc_2O_3-Y_2O_3, submitted to Acta Materialia (2021).

[5] Guguschev et al., Czochralski growth and characterization of perovskite-type (La,Nd)(Lu,Sc)O_3 single crystals with a pseudocubic lattice parameter of about 4.09 Å, J. Crystal Growth 536 (2020) 125526.