MS16-04 | Structural Control of thermomechanical Properties of Monoclinic Rare-Earth Calcium Oxoborates

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Monoclinic rare-earth calcium oxoborates (*RCOB*), $RCa_4O(BO_3)_3$ recently gathered interest as candidates for high-temperature piezoelectric sensing applications since they combine favorable properties like high melting point at around 1770 K, no reported structural phase transitions, high piezoelectric sensitivity and high electric resistivity. Since the *RCOB* structure offers different possibilities for cation substitution, tuning of physical properties is principally possible.

Large single crystals of *RCOB* (*R* = Er, Y, Dy, Gd, Sm, Nd, La) were grown from melt using the Czochralski method. Their structural properties were studied at ambient conditions on as cast and on annealed and subsequently quenched samples using X-ray diffraction methods. Dilatometry and resonant ultrasound spectroscopy were employed to investigated their thermo- and electromechanical properties between 100 K and 1473 K.

Substitution of rare earth cations with larger size leads to a decrease in the bulk modulus, whereas the maximum value of the piezoelectric effect increases. Contrary to the reported lack of phase transitions, the investigated physical properties undergo reproducible discontinuities between 900 K and 1300 K which are characteristic for a glass-like transition. Structural investigations indicate a correlation with dynamic disorder of *R* and Ca on the independent cation sites at higher temperatures. The transition temperature as well as the specific type of disorder are both related to size of the rare earth ion.

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