

Poster Presentations

[MS20-P06] Structural properties of mullite-type $\text{Pb}(\text{Al}_{1-x}\text{Mn}_x)\text{BO}_4$.

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We report on the structural characterization and the pressure- and temperature-dependent behavior of the two end-members of the mullite-type $\text{PbAl}_{1-x}\text{Mn}_x\text{BO}_4$ solid solution [1, 2]. Investigations were carried out using neutron, synchrotron and in house X-ray powder diffraction, Raman spectroscopy and density functional theory (DFT) calculations. Polycrystalline mullite-type PbMBO_4 (M = Al and Mn) samples were produced following the glycerin method [3]. The crystal structure was refined in the space group Pnam in the mullite-type standardized setting [4]; therefore, the edge-sharing MO₆ octahedral

chains run parallel to the crystallographic c-axis. They are connected by BO₃ groups and stabilized by PbO₄E building units. The planar geometry of the BO₃ group changes only slightly over the whole composition range of the solid solution. The very small deviations from a three-fold local symmetry of the BO₃ group could well be monitored from the recorded infrared and Raman spectra using DFT calculated mode assignments. The rigidity of the BO₃ group plays the dominant roles in the thermal contraction in the a-direction and the expansion in the b- and c-directions, leading to a correlation a·b/c ~ unity. The unit-cell volume at zero-pressure and 0 K was obtained and as well evaluated as the isothermal bulk-modulus experimentally from pressure dependent synchrotron X-ray diffraction using a diamond anvil cell and theoretically from DFT calculation. The pressure-dependent data were modeled using higher-order Birch-Murnaghan equations of state [5, 6] Thermal first-order Gruneisen approximation for the zero-pressure equation of state. We used the double-Debye-double-Einstein-Anharmonicity model [7] to calculate the temperature-dependent internal energy of the crystalline end members. The simulation helped to understand the anisotropic thermal expansion and together with the experimental and calculated bulk moduli to approximate the thermodynamic Gruneisen parameters.

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