Poster Presentation

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Nanoindentation and ellipsometry of $Li_2ZnTi_3O_8$ & Zn_2TiO_4 single crystals

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Spinel-type $Li_2ZnTi_3O_8$ and Zn_2TiO_4 are useful for various industrial applications due to their interesting chemical and physical properties, for example, as promising anode materials in Li-ion batteries or as components in dielectric devices [1]. Since $Li_2ZnTi_3O_8$ and Zn_2TiO_4 are expected to have high refractive indices (n calc. = 2,33 and 2,26) we tried to characterize these materials in more detail including single-crystal X-ray diffraction, nanoindentation, spectroscopic ellipsometry and electron microprobe analysis. Single crystals of $Li_2ZnTi_3O_8$ and Zn_2TiO_4 were grown directly from melt at 1723 K and 1873 K, respectively. Fragments of sintered polycrystalline $Li_2ZnTi_3O_8$ and Zn_2TiO_4 precursors were placed on an iridium sheet and fired in a muffle furnace from 1273 to 1723/1873 K with a heating ramp of 15 K/min. After a dwell time of 3 min the melt was cooled down to 1473 K with a ramp of 10 K/min and subsequently quenched in water. Structural investigations of the $Li_2ZnTi_3O_8$ and Zn_2TiO_4 single crystals resulted in the following basic crystallographic data: cubic, $P4_332$, a = 8.3697(2) Å, V = 586.31(3) Å^3, Z = 4 and Fd-3m, a = 8.46230(17) Å, V = 605.99(2) Å^3, Z = 8, respectively. Nanoindentation experiments were performed with a Berkovich diamond indenter tip to determine the hardness and elastic modulus of Zn_2TiO_4 and $Li_2ZnTi_3O_8$. For sample preparation the single crystals were embedded in resin and polished to a mirror-like surface finish. More than 150 indents with a distance of 10 µm were made with a maximum load of 20 mN. Analysis of the load-displacement curves for Zn_2TiO_4 revealed a hardness of 10.51 ± 0.39 GPa and a reduced elastic modulus of 180.90 ± 3.92 GPa. Atomic force micrographs displayed indents with a max. depth of 288 ± 5 nm. $Li_2ZnTi_3O_8$ exhibited a hardness of 6.86 ± 0.45 GPa and a reduced elastic modulus of 148.88 ± 6 GPa. Zn_2TiO_4 showed a dispersion of 0.09 due to the variation of the refractive index from 2.24 (430,8 nm, Fraunhofer G line) and 2.15 (686,7 nm, B line).

[1] *Z. Hong, M. Wei, X. Ding, L. Jiang, K. Wei, Electrochemistry Communications, 2010, 12, 720-723*

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