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Crystal growth, electronic structure and optical properties of $\text{Sr}_2\text{Mg}(\text{BO}_3)_2$

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Abstract

Single crystals of $\text{Sr}_2\text{Mg}(\text{BO}_3)_2$ (SMBO) were grown by Kyropoulos method. X-ray powder diffraction (XRD) analysis, transmission spectrum, thermal properties, band structure, density of states and charge distribution as well as Raman spectra of SMBO were described. The as-grown SMBO crystals show wide transparency range with UV cut-off below 180 nm. A direct band gap of 4.66 eV was obtained from the calculated electronic structure results. The calculated band structure and density of states results indicated the top valence band is determined by O 2p states whereas the low conduction band mainly consists of Sr 5s states. Twelve Raman peaks were observed in the experimental spectrum, fewer than the number predicted by the site group analysis. Raman peaks of SMBO were assigned combining first-principle calculation and site group analysis results. The strongest peak at 917 cm^{-1} in the experimental spectrum is assigned to symmetric stretching mode $A_1'(v_1)$ of free BO_3 units. SMBO is a potential Raman crystal which can be used in deep UV laser frequency

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