

EXPLORATION, CRYSTAL STRUCTURE AND PROPERTIES OF NEW FUNCTIONAL BORATE MATERIALS

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Borates have played an important role among the resource of functional materials due to their rich varieties in crystal structure, wide optical transmittance with high damage threshold, and wide band gaps. They are potential new non-linear optical crystals, birefringent crystals, laser crystals and luminescent materials, and received the increasing interests. During recent years, a series of excellent optical crystals have been found successively of BBO, LBO, CBO, CLBO, KBBF, SBBO and YCOB. Even though, new potential functional crystals are expected to be discovered due to their structural complexity. Therefore, further effort is still needed to perform the exploration.

To explore new optical and electrical functional materials, phase relations for ternary borate systems have been investigated in our research group since 1997. Over 30 new compounds were found and their structures were determined successfully by X-ray powder or single crystal diffraction data. New methods of structural analysis from the powder diffraction data have been developed. From 2000 to 2007, high quality patterns of powder X-ray diffraction data of 100 new compounds have been submitted to ICDD (International Center for Diffraction Data) as the standard PDF files. More recently, we have studied the phase relations between the alkali/alkali-earth metal oxides and trivalent metal borates. A systematic survey of the $\text{Li}_2\text{O-RE}_2\text{O}_3\text{-B}_2\text{O}_3$ (RE=Nd, Sm, Eu, Er, Tm) system and the $\text{BaO-R}_2\text{O}_3\text{-B}_2\text{O}_3$ (R=Sc, In, Bi) system has led to the discovery of two kinds of new borates, potential superionic ion conductors $\text{Li}_6\text{REB}_3\text{O}_9$ (RE=Nd, Sm, Eu, Er, Tm) and promising scintillators $\text{RBA}_3\text{B}_9\text{O}_{18}$ (R = Sc, In, Bi).

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