Structural Design, Crystal Growth and Optical Properties of $Sr_2Be_2B_2O_7$-type Deep-UV Birefringent Materials

Ruixin Guo[1,2,3]*, Shu Guo[1,2]

*Ruixin Guo: guorx@sustech.edu.cn
1 Shenzhen Institute for Quantum Science and Engineering, Southern University of Science and Technology, Shenzhen 518055, China
2 International Quantum Academy, Shenzhen 518048, China
3 Beijing Center for Crystal Research and Development, Key Laboratory of Functional Crystals and Laser Technology, Technical Institute of Physics and Chemistry, Chinese Academy of Sciences, Beijing 100190, China

Designing and synthesis of functional materials is one of the most challenging goals for both chemistry and materials science communities. Beryllium borates have been widely studied for the potential application in the deep-UV region as the nonlinear optical (NLO) materials or birefringent materials. As one of the famous NLO materials, $Sr_2Be_2B_2O_7$ (SBBO), was first reported and characterized by Chen et al. in 1995. Structurally, it features 2D $[Be_6B_6O_{15}]_\infty$ double-layers in the *ab* plane [1]. Owing to the excellent structure-based optical performances (Δn = 0.062 @1064 nm; UV absorption edge down to 165 nm; nonlinear optical coefficient up to 5~6 × KH_2PO_4), SBBO could be considered as an ideal structural motif for further exploring new functional materials [1,2].

In this work, we will present crystal structure, single crystal growth, and optical properties of several SBBO-type materials, including $NaMgBe_2B_2O_6F$, $BaMBe_2(BO_3)_2F_2$ (*M* = Cd, Zn), and $Ba_{1.09}Pb_{0.91}Be_2(BO_3)_2F_2$ [3, 4]. These compounds are promising deep-UV birefringent materials with the short UV absorption edges (λ < 200 nm) and moderate birefringence (~0.06 @ 589 nm). Meanwhile, the structural and optical properties comparison of SBBO-type materials will be compared and discussed to elucidate the role of cation size in modulating the magnitude of birefringence in materials. Our results will provide a useful strategy to carefully control the magnitude of birefringence under certain structural motifs.

References

[1] Chen CT et al. Design and synthesis of an ultraviolet-transparent nonlinear optical crystal $Sr_2Be_2B_2O_7$. Nature 1995; 373: 322−324.
[2] Lin ZS et al. Mechanism for linear and nonlinear optical effects in crystals of the Sr2Be2B2O7 family. J. Appl. Phys. 2003; 93: 9717−9723.
[3] Guo RX et al. Realization of enlarged birefringence from $BaCdBe_2(BO_3)_2F_2$ to $NaMgBe_2(BO_3)_2F$ via the cation size effect as a potential deep-ultraviolet birefringent material. Inorg. Chem. 2022; 61: 7624-7630.
[4] Guo RX et al. $BaZnBe_2(BO_3)_2F_2$: a novel zinc-beryllium borate with SBBO-type structure overcoming the polymorphism problem. Dalton T. 2021; 50: 2138-2142.