

A New Promising Scintillation Crystal $\text{YBa}_3\text{B}_9\text{O}_{18}$: Structure, Crystal Growth and Its Properties

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There is an increasing interest in scintillation crystals that find medical applications over the past decade, such as in computerized tomography and positron emission tomography. In order to obtain better performance, new scintillation materials should be explored. On the other hand, borates have long been a focus of research because of their rich varieties in structure, wide transmittance spectra with high damage threshold, and wide band gaps. It is possible to find some new scintillation materials in borates. Here we report the structure, the crystal growth, and the properties of a newly discovered borate $\text{YBa}_3\text{B}_9\text{O}_{18}$ which was first identified and structurally characterized by our group [1]. $\text{YBa}_3\text{B}_9\text{O}_{18}$ crystallizes in a centric space group $P6_3/m$ with lattice parameters $a = 7.1761 \text{ \AA}$ and $c = 16.9657 \text{ \AA}$. Each B atom is bonded to three O atoms, and three BO_3 groups form a planar hexagonal $[\text{B}_3\text{O}_6]^{3-}$ ring. These planar rings are parallel to each other and stack along the c-axis in the unit cell, with regular YO_6 octahedra and irregular BaO_6 and BaO_9 polyhedra in between the hexagonal $[\text{B}_3\text{O}_6]^{3-}$ rings. The substitution of lanthanides for Y results in a series of isostructural compounds $\text{REBa}_3\text{B}_9\text{O}_{18}$ (RE = Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb). $\text{YBa}_3\text{B}_9\text{O}_{18}$ single crystals with dimensions up to $13 \times 8 \times 4 \text{ mm}^3$ were successfully grown by the Czochralski pulling method and its physical properties were investigated both by experiment and theory [2]. X-ray excited luminescence measurements of $\text{YBa}_3\text{B}_9\text{O}_{18}$ showed a broad emission band in the wavelength range from 350 to 500 nm with a peak center at 400 nm. The light yield is about 6-7 times larger than that of PbWO_4 measured at nearly the same conditions. The results show that borate can also exhibit attracting scintillation properties. However, a narrow temperature range for growth and drastic anisotropy of the growth rates are the main difficulties in growing large crystals. Moreover, the crystal growth and properties of denser isostructural $\text{REBa}_3\text{B}_9\text{O}_{18}$ series deserve further investigation. This work was financially supported by the National Natural Science Foundation of China (Grant Nos. 50502039 and 50872144).

References:

- [1] X.Z. Li, C. Wang, X.L. Chen, H. Li, L.S. Jia, L. Wu, Y.X. Du, Y.P. Xu, *Inorg. Chem.* 2004, 43, 8555.
- [2] Ming He, X.L. Chen, Y.P. Sun, J. Liu, J.T. Zhao, C.J. Duan, *Crystal Growth & Design* 2007, 7, 199.