MS15-P31 High-temperature synthesis of the new strontium borogermanate $Sr_{3-x/2}B_{2-x}Ge_{4+x}O_{14}$ (x = 0.32)

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The strontium borogermanate $Sr_{3-x/2}B_{2-x}Ge_{4+x}O_{14}$ (x = 0.32) [1] (Figure 1) was synthesized by high-temperature solid-state reaction of SrO, GeO_2, and H_3BO_3 in a NaF/KF flux system using platinum crucibles. The structure determination revealed that $Sr_{3-x/2}B_{2-x}Ge_{4+x}O_{14}$ (x = 0.32) crystallizes in the trigonal space group *P*321 (No. 150) with the parameters *a* = 800.7(2) and *c* = 488.8(2) pm, with *R*1 = 0.0281, *wR*2 = 0.0671 (all data), and Z = 1. The crystal structure of $Sr_{3-x/2}B_{2-x}Ge_{4+x}O_{14}$ (x = 0.32) consists of distorted SrO_8 cubes, GeO_6 octahedra, GeO_4 tetrahedra, and BO_4 tetrahedra. In addition to the structural investigations, Raman and IR-spectroscopic investigations were carried out. Taking into account that $Sr_{3-x/2}B_{2-x}Ge_{4+x}O_{14}$ (x = 0.32) is isotypic to $Ca_3Ga_2Ge_4O_{14}$ [2,3] this compound represents the first boron-containing member of the family of langasites ($La_3Ga_5SiO_{14}$) possessing the general composition $A_3XY_3Z_2O_{14}$.[4] This class of compounds is highly interesting concerning their piezoelectric properties because nearly all 140 known member crystallize in the trigonal noncentrosymmetric space group *P*321.[5, 6] As several members of the langasite family are already promising piezoelectric materials, the herein reported compound leads to a wider range of compositions which might lead to better piezoelectric properties of potential materials.

[1] B. Petermüller, L. L. Petschnig, K. Wurst, G. Heymann, H. Huppertz, *Inorg. Chem.* 53, 9722 (2014)

[2] E. L. Belokoneva, M. A. Simonov, A. V. Butashin, B. V. Mill, N. V. Belov, *Dokl. Akad. Nauk SSSR* 255, 1099 (1980)

[3] E. L. Belokoneva, N. V. Belov, *Dokl. Akad. Nauk SSSR* 260, 1363 (1981)

[4] B. V. Mill, E. L. Belokoneva, T. Fukuda, *Russ. J. Inorg. Chem.* 43, 1168 (1998)

[5] B. V. Mill, B.A. Maksimov, Yu. V. Pisarevskii, N. P. Danilova, A. Pavlovska, S. Werner, J. Schneider, *Kristallografiya* 49, 60 (2004)

[6] H. Ohsato, T. Iwataki, H. Morikoshi, *Trans. Electr. Electron Mater.* 13, 51 (2012)

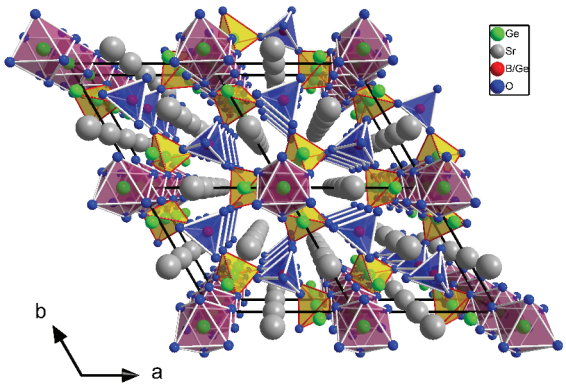

Figure 1. Crystal structure of $Sr_{3-x/2}B_{2-x}Ge_{4+x}O_{14}$ (x = 0.32) down [001] exhibiting channels created through the GeO_4-B/GeO_4 network an occupied by Sr atoms (grey)

Keywords: Piezoelectricity, Langasite, Synthesis