Crystal Structure Determination of Ba2MgSiO7 by Neutron Diffraction

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The emission depends on the environment of the emission ion site in the host lattice. The silicate phosphors have relatively strong and rigid characteristics of partly covalent Si-O bond. In addition, rigid frameworks often provide relatively distorted coordination around the emission ion. Therefore, strong crystal fields were observed in many silicate phosphors. Alkaline earth silicate phosphor, M2MgSi2O7 (M = Ca, Sr and Ba) are expected as high luminance phosphor. However, the crystal structure of Ba2MgSi2O7 has not been reported up to now. The powder XRD pattern of Ba2MgSi2O7 differs from that of single crystal Ba2MgSi2O7. In this study, we show the crystallographic date on Ba2MgSi2O7 refined from the neutron powder diffraction patterns.

Crystal structures of Ba2MgSi2O7, were first reported by M. Shimizu et al. [1]. They refined Ba2MgSi2O7 on the basis of a tetragonal system with space group P-421m (a = 0.8425 nm). The crystal structure of Ba2MgSi2O7 differs from the tetragonal symmetry. Indexing of the XRD pattern for the powder sample, Ba2MgSi2O7 has monoclinic system with space group C2/c (a = 0.8426 nm). However, since these structures were deduced only from the electron and powder X-ray diffractions, the information on light elements, especially for oxygen atom, was quite poor.

Figure 1 and Table 1 shows the powder neutron diffraction pattern fitting and structural parameters for the Ba2MgSi2O7. All of the diffraction peaks were well indexed on monoclinic system C2/c. A good fitting profile were obtained with Rwp = 5.65 %.

Tetragonal and monoclinic structures take similarly layered structures with different barium coordination environments. It is considered that the synthesis temperature and annealing time are most important factors whether Ba2MgSi2O7 take the two-type structure, tetragonal or monoclinic.

[1] Y. Lin, C. W. Nan, X. Zhou, J. Wu, H. Wang, D. Chen, S. Xu. Mater. Chem. Phys., 82 (2003) 860-863.

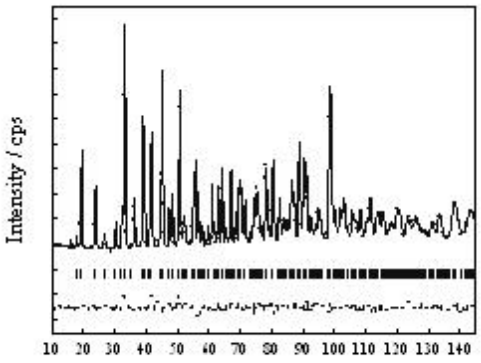

Fig. 1 Powder neutron fitting of $Ba_2MgSi_2O_7$.

Table 1 Structural parameter of $Ba_2MgSi_2O_7$.

Atom	Site	x	y	z	B / nm^2
Ba	8f	0.272(5)	0.044(1)	0.476(1)	0.0084(4)
Mg	4e	0.000	0.744(1)	0.250	0.009(2)
Si	8f	0.111(1)	0.282(5)	0.133(1)	0.007(1)
O(1)	8f	0.100(1)	0.142(1)	0.120(2)	0.015(3)
O(2)	8f	0.303(1)	0.342(1)	0.235(1)	0.003(1)
O(3)	8f	0.479(1)	0.149(1)	0.042(1)	0.001(4)
O(4)	4e	0.000	0.334(1)	0.250	0.009(4)

C 2/c (A-15), a = 0.8425(8) nm, b = 1.0732(8) nm, c = 0.8454(8) nm, Rwp = 5.65 %, Rp = 4.34 %, RR = 9.84 %, Re = 4.57 %, S = 1.23

Fig. 1.