

Structural and Electron Density Studies of Stuffed Tridymite

Hiroshi Yamada^a, H. Kubozono^b, C. N. Xu^{ac}, ^aAIST Japan. ^bSaga University Japan. ^cJST, Japan. E-mail: hiro-yamada@aist.go.jp

Stuffed tridymite materials, MAl_2O_4 ($\text{M}=\text{Ca}, \text{Sr}, \text{Ba}$) are one of the most important matrices for luminous materials because of easily introducing various dopant ions into the framework structure and can realize various luminous colours. Utilizing these matrices, we have developed newly functional materials, which show strong mechano-, electro-, and photo-luminescence in one material [1,2]. Their physical properties are largely related to the crystal structure because the luminescent properties are strongly sensitive to its local atomic configuration and the local polarization state around dopant ions. Therefore the structural study of these materials is important for controlling their mechanical, luminescent and optical properties.

We have determined the accurate structural parameters of MAl_2O_4 ($\text{M}=\text{Ca}, \text{Sr}, \text{Ba}$) by Rietveld refinements using high resolved powder diffraction data with synchrotron X-ray radiation (SPring-8 BL02B2). It was found that their structural features were strongly dependent on cation size. The shape of AlO_4 tetrahedra that constitute of the framework structure was almost independent to the cation size meanwhile the void space around cation was variable, suggesting that the framework structure in stuffed tridymite may be easily deformed. Furthermore the charge density distribution was also calculated from the observed form factors F_O using the maximum entropy method (MEM), demonstrating that the cation ions were isolated ions meanwhile a covalent nature could be observed between Al and O.

[1] Xu C. N., *Encyclopedia of Smart Materials*, 2002, **1**, 190. [2] Liu Y., Xu C. N., *Appl. Phys. Lett.*, 2004, **84**, 5016.

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