

## Phase relation in the $\text{Ca}^{2+}\text{Ti}^{4+}\text{O}_3\text{-Y}^{3+}\text{Ga}^{3+}\text{O}_3$ system

Satoko MOTAI, Takaya NAGAI\* and Yusuke SETO

Department of Natural History Sciences, Faculty of Science, Hokkaido University, Sapporo, Hokkaido 060-0810, Japan

### Introduction

The  $\text{ABO}_3$  compounds with the perovskite structure have been focused due to their unique electro-optical, thermo-mechanical and catalytic properties. Materials with the perovskite structure are also important in geoscience, since  $\text{MgSiO}_3$  perovskite is the most major constituent mineral in the Earth's lower mantle. Recent experimental studies indicated that  $\text{Mg}^{2+}\text{Si}^{4+}\text{O}_3$  perovskite incorporates significant amount of trivalent cations such as  $\text{Al}^{3+}$  and  $\text{Fe}^{3+}$  [e.g.,1,2]. Because the perovskite structure can tolerate structural distortions within its framework, cations of variety of sizes and charges can occupy the A and B sites. Consequently the various physical and/or chemical properties could be changed depending on the chemical compositions. Thus, it is not surprising that the incorporation of trivalent cations into  $\text{MgSiO}_3$  perovskite greatly influences on its elastic property [3]. However, it is unclear what kind of mechanism controls the incorporation of trivalent cations into  $\text{A}^{2+}\text{B}^{4+}\text{O}_3$  perovskite. In the present study, we investigated the phase relation in the  $\text{Ca}^{2+}\text{Ti}^{4+}\text{O}_3\text{-Y}^{3+}\text{Ga}^{3+}\text{O}_3$  system at atmospheric pressure, 1 GPa and 2 GPa. It is noted that  $\text{CaTiO}_3$  perovskite is stable at atmospheric pressure. On the other hand,  $\text{YGaO}_3$  perovskite is stabilized at a high pressure [4].

### Experimental

Samples were synthesized from the oxide mixture using a muffle furnace at about 1720K and atmospheric pressure for more than 80 hours. High pressure synthesis was performed by using a piston-cylinder apparatus at about 1670K and 1GPa and 2GPa for 48 hours. The powder X-ray diffraction measurements were carried out at BL-18C in PF using an imaging plate. The incident X-ray beam was monochromatized to wavelengths of 0.6161 Å and collimated to 100 μm in diameter. Two-dimensional X-ray diffraction patterns were analyzed by the PDI software, which was originally programmed [5]. A scanning electron microscope (SEM, JEOL JSM-5310) equipped with an energy dispersive X-ray spectrometer (EDS, OXFORD LINK-ISIS) used to analyze micro-texture and chemical compositions of the recovered samples.

### Results and Discussion

Cations of  $\text{Y}^{3+}$  and  $\text{Ga}^{3+}$  are incorporated into  $\text{Ca}^{2+}\text{Ti}^{4+}\text{O}_3$  perovskite as  $\text{YGaO}_3$  component up to 40 mol % at atmospheric pressure. The solubility of  $\text{YGaO}_3$  component greatly increases with pressure and about 80 mol % of  $\text{YGaO}_3$  component could dissolve into  $\text{CaTiO}_3$  perovskite (Fig.1). It is expected that a complete solid solution with the perovskite structure would occur in the

$\text{Ca}^{2+}\text{Ti}^{4+}\text{O}_3\text{-Y}^{3+}\text{Ga}^{3+}\text{O}_3$  system at a higher pressure. The crystal structure of  $\text{YGaO}_3$ -bearing  $\text{CaTiO}_3$  perovskite remains orthorhombic and the lattice parameters changes almost linearly as a function of the amount of  $\text{YGaO}_3$  component (Fig.2).

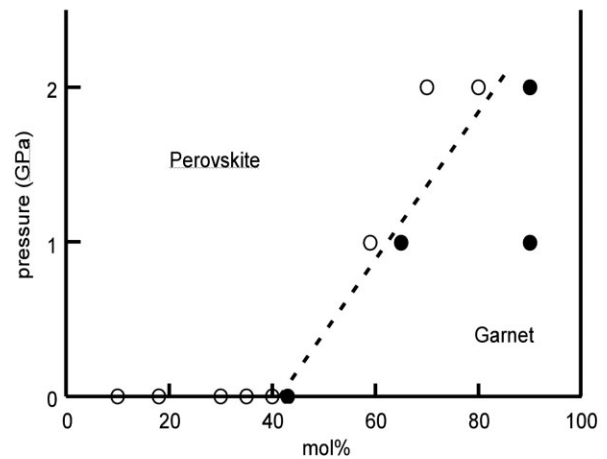


Fig.1. Phase diagram of the  $\text{Ca}^{2+}\text{Ti}^{4+}\text{O}_3\text{-Y}^{3+}\text{Ga}^{3+}\text{O}_3$  system at 1670 K. The horizontal axis represents mol% of  $\text{YGaO}_3$  component.

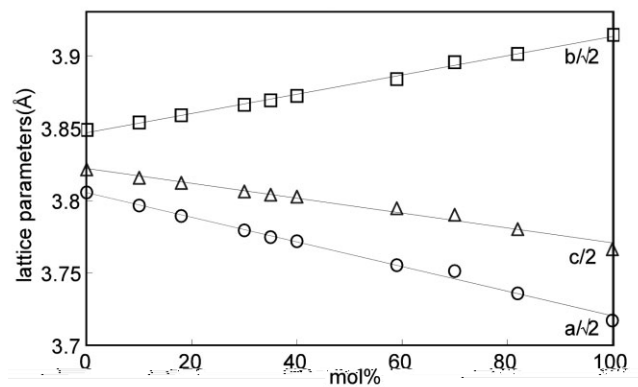


Fig.2. Variation of the lattice parameters in the  $\text{Ca}^{2+}\text{Ti}^{4+}\text{O}_3\text{-Y}^{3+}\text{Ga}^{3+}\text{O}_3$  system. The horizontal axis represents mol% of  $\text{YGaO}_3$  component.

### References

- [1] D.J. Frost and F. Langenhorst, *Earth Planet. Sci. Lett.*, 199, 227 (2002)
- [2] D. Nishio-Hamane et al., *Geophys. Res. Lett.*, 32, L16306 (2005)
- [3] J. Zhang and D.J. Weidner, *Science*, 284, 782 (1999)
- [4] M. Marezio et al., *Materials Res. Bull.*, 1, 247 (1966)
- [5] <http://mineralx.ep.sci.hokudai.ac.jp/seto/>

\* nagai@mail.sci.hokudai.ac.jp