

LETTER

Synthesis and structural analysis of  $\text{CaFe}_2\text{O}_4$ -type single crystals in the  $\text{NaAlSiO}_4$ - $\text{MgAl}_2\text{O}_4$ - $\text{Fe}_3\text{O}_4$  system

TAKAYUKI ISHII<sup>1,\*</sup>, GIACOMO CRINITI<sup>2,†</sup>, XIAOYU WANG<sup>2</sup>, KONSTANTIN GLAZYRIN<sup>3</sup>, AND TIZIANA BOFFA BALLARAN<sup>2</sup>

<sup>1</sup>Center for High Pressure Science and Technology Advanced Research, Beijing 100094, China

<sup>2</sup>Bayerisches Geoinstitut, University of Bayreuth, 95440 Bayreuth, Germany

<sup>3</sup>Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, 22607 Hamburg, Germany

ABSTRACT

Orthorhombic  $\text{CaFe}_2\text{O}_4$ -structured (Cf) Na-rich aluminous silicate (space group *Pbnm*) is a major mineral of metabasaltic rocks at lower mantle conditions and can, therefore, significantly affect the physical properties of subducted oceanic crusts. We attempted to synthesize single crystals of Cf-type phases in the systems  $\text{NaAlSiO}_4$ ,  $\text{NaAlSiO}_4$ - $\text{MgAl}_2\text{O}_4$ ,  $\text{NaAlSiO}_4$ - $\text{MgAl}_2\text{O}_4$ - $\text{Fe}_3\text{O}_4$ , and  $\text{NaAlSiO}_4$ - $\text{MgAl}_2\text{O}_4$ - $\text{Fe}_3\text{O}_4$ - $\text{H}_2\text{O}$  at 23–26 GPa and 1100–2200 °C. Under dry conditions, single crystals of Cf-type phase up to 100–150  $\mu\text{m}$  in size were recovered from 23 GPa and 2000–2200 °C. Single-crystal X-ray diffraction and composition analyses suggest that the synthesized Cf-type phases have a few percent of vacancies in the eightfold-coordinated site with Na, Mg, and  $\text{Fe}^{2+}$  and partially disordered Al and Si in the octahedral sites. Iron-bearing Cf-type phases have 32–34%  $\text{Fe}^{3+}$  that is hosted both in the octahedral sites and in the eightfold-coordinated site. In  $\text{NaAlSiO}_4$ - $\text{MgAl}_2\text{O}_4$ - $\text{Fe}_3\text{O}_4$ - $\text{H}_2\text{O}$  system, no formation of Cf-type phase was observed at 24 GPa and 1100–2000 °C due to the formation of hydrous Na-rich melt and Al-rich oxides or hydroxides, suggesting the possible absence of Cf-type phase in the hydrous basaltic crust. The single-crystal syntheses of Cf-type phases will be useful for investigating their physical properties, potentially improving models of lower mantle structure and dynamics.

**Keywords:** Calcium ferrite, single crystal, multi-anvil press, high pressure, basaltic crust