Letter

Synthesis and structural analysis of CaFe₂O₄-type single crystals in the NaAlSiO₄-MgAl₂O₄-Fe₃O₄ system

TAKAYUKI ISHII^{1,*}, GIACOMO CRINITI^{2,*}[†], XIAOYU WANG², KONSTANTIN GLAZYRIN³, AND TIZIANA BOFFA BALLARAN²

¹Center for High Pressure Science and Technology Advanced Research, Beijing 100094, China ²Bayerisches Geoinstitut, University of Bayreuth, 95440 Bayreuth, Germany ³Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, 22607 Hamburg, Germany

ABSTRACT

Orthorhombic CaFe₂O₄-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 NaAlSiO₄, NaAlSiO₄-MgAl₂O₄, NaAlSiO₄-MgAl₂O₄-Fe₃O₄, and NaAlSiO₄-MgAl₂O₄-Fe₃O₄-H₂O at 23–26 GPa and 1100–2200 °C. Under dry conditions, single crystals of Cf-type phase up to 100–150 µm 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 Fe²⁺ and partially disordered Al and Si in the octahedral sites. Iron-bearing Cf-type phases have 32–34% Fe³⁺ that is hosted both in the octahedral sites and in the eightfold-coordinated site. In NaAlSiO₄-MgAl₂O₄-Fe₃O₄-H₂O 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