American Mineralogist, Volume 97, pages 305–314, 2012

Phase stability and elastic properties of the NAL and CF phases in the $NaMg_2Al_5SiO_{12}$ system from first principles

Kenji Kawai[1,*] and Taku Tsuchiya[2]

[1]Department of Earth and Planetary Sciences, Tokyo Institute of Technology, Ookayama 2-12-1, Meguro, Tokyo 152-8551, Japan
[2]Geodynamics Research Center, Ehime University, Bunkyo-cho 2-5, Matsuyama, Ehime 790-8577, Japan

Abstract

New hexagonal aluminous (NAL) phase and orthorhombic calcium-ferrite (CF) type phase are considered to be major mantle components of the mid-ocean ridge basalt (MORB) at pressure and temperature conditions in the lower mantle, which can potentially host alkali elements with large ionic radii. The high-pressure stability and elastic properties of both NAL and CF phases are therefore of fundamental importance for understanding the fate of subducted MORB. Here we report those properties of the $NaMg_2Al_5SiO_{12}$ system studied by means of the first-principles computation method. NAL was found to transform to the CF phase at 39.6 GPa, accompanied by discontinuities in density (+1.8%), as well as compressional wave (–0.2%), shear wave (+0.9%), and bulk sound (–1.0%) velocities. The property of subducted MORB was evaluated using these results, and the velocity contrast between pyrolite and MORB of ~–5% was found to be quite comparable to the shear velocity anomaly observed for seismic scatterers at depths from 1100 to 1800 km. However, since the transformation of the NAL to CF phase within MORB produces insignificant increases in the seismic velocities, it would be seismologically undetectable. On the other hand, the anisotropy change associated with the phase transition is significant and could be seismically detectable using observations such as shear wave splitting measurements since the CF phase is considerably more anisotropic compared to the NAL phase.

Keywords: Elastic property, phase transition, new aluminous (NAL) phase, calcium ferrite (CF) phase, first principle