Phase stability and elastic properties of the NAL and CF phases in the NaMg2Al5SiO12 system from first principles

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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 NaMg2Al5SiO12 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 seismically 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

INTRODUCTION

As mid-ocean ridge basalt (MORB) is produced via partial melting of mantle peridotite at mid-ocean ridge, it is enriched in iron, aluminum, and other incompatible elements with large ionic radii (e.g., Hofmann 1994). Since the subduction of MORB at plate convergence zones makes the mantle chemically heterogeneous, it is important to study the fate of the basaltic materials for understanding the chemical evolution of the Earth (Christensen and Hofmann 1994).

The main host of aluminum in a mantle transition zone of peridotitic (pyrolic) composition is majorite garnet (Irfune and Ringwood 1987). It decomposes into an assemblage of Mg-perovskite (MgPv) and Ca-perovskite (CaPv) at 26 GPa in the uppermost lower mantle (Irfune and Ringwood 1987). For the pyrolitic composition, Al2O3 is accommodated mostly in MgPv and no separate aluminous phase is observed after the decomposition of majorite (Irfune 1994). In contrast, for the aluminum-rich basaltic composition, a separate aluminous phase is formed at lower mantle condition (Irfune and Ringwood 1993). This aluminous phase, called the “Al-rich phase,” has a crystal structure similar to the calcium ferrite (CF) structure. Later, this Al-rich phase was proposed to be a new hexagonal aluminous (NAL) phase (Miyajima et al. 2001; Akaogi et al. 1999; Sanehira et al. 2005) or a CF-type phase (Kesson et al. 1998; Hirose et al. 1999; Ono et al. 2001). Studies on the phase relations of natural MORB reported that both NAL and CF coexist up to about 50 GPa but NAL disappears above 50 GPa (Perrillat et al. 2006; Ricolleau et al. 2008, 2010). It was also observed that as the volumetric fraction of NAL decreased with increasing pressure, the fraction of MgPv increased. It is therefore still unclear whether the disappearance of the NAL phase is due to the high-pressure stability relation between the NAL and CF phases or alternatively the NAL dissolves into MgPv (Ricolleau et al. 2010). Studies on the phase relations along the NaAlSiO4-MgAl2O4 join using diamond-anvil cell techniques suggested that the CF phase can be recognized as the high-pressure phase of the NAL phase (Imada et al. 2011). In contrast to the phase stability, the elasticity of these phases and its pressure dependence has not yet been studied.

In this study, we investigate the high-pressure stability of the NAL and CF phases and their high-pressure elasticity by means of the ab initio density functional computation method. First, we describe models for the crystal structure of the NAL and CF phases in the NaMg2Al5SiO12 system. Second, we introduce details of first-principles computations. Third, we show results for the stability and elasticity including anisotropic properties. Finally, we discuss these geophysical implications for subducted basaltic slabs.

CRYSTAL STRUCTURE MODELS

The NAL phase has a hexagonal crystal structure with the space group P63/m with a chemical formula of XY3Z2O12, where X is a large monovalent or divalent cation such as Ca2+, Na+, and...