High-pressure elasticity of sodium majorite garnet, Na$_2$MgSi$_2$O$_{12}$

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ABSTRACT

Garnet is the second most abundant mineral phase in the upper mantle and transition zone settings. The crystal structure of garnet is quite flexible and hence it is able to accommodate various cations, including large incompatible cation such as sodium. We used first-principles simulation based on density functional theory and two widely used approximations—local density approximation (LDA) and generalized gradient approximation (GGA)—to explore the crystal structure, equation of state, and elasticity of sodium bearing majorite garnet with Na$_2$MgSi$_2$O$_{12}$ stoichiometry at pressures relevant to the upper mantle and transition zone. We find that the pressure-volume results based on LDA can be explained by a Birch Murnaghan finite strain equation of state with $V_0 = 1447.6$ (± 0.1) Å$^3$, $K_0 = 177.4$ (± 0.4) GPa, and $K'_0 = 3.93$ (± 0.02). The results based on GGA can be explained by a Birch Murnaghan finite strain equation of state with $V_0 = 1525.8$ (± 0.2) Å$^3$, $K_0 = 160.2$ (± 0.4) GPa, and $K'_0 = 3.96$ (± 0.02). The full elastic moduli tensor for Na-majorite with tetragonal symmetry exhibits slight deviation from the cubic symmetry with $C_{11} < C_{13}$, $C_{12} \sim C_{13}$, and $C_{44} \sim C_{66}$. The magnitude of the tetragonal strain also captures the slight deviation from the cubic symmetry. At pressures corresponding to the upper mantle and mantle transition zone, the compressional wave velocity, $v_p$, and shear wave velocity, $v_s$, for the Na-majorite garnet are fast compared to a wide variety of garnets such as pyrope, grossular, almandine, and majorite garnet. Although single-crystal anisotropy of Na-majorite is greater than pyrope, it is still low compared to the major mantle phases.

Keywords: Elasticity, equation of state, sodium majorite, mantle transition region

INTRODUCTION

In the mineralogical models of the deep Earth, garnet is a volumetrically abundant mineral phase in the upper mantle and transition zone (Ringwood 1962). In a homogenous pyrolite model, modal abundance of garnet ranges from 20 vol% at upper mantle conditions to almost 40 vol% at transition zone conditions. The thermodynamic stability of garnet enhances upon complete dissolution of the pyroxene phase at transition zone conditions. In recent studies, it has been suggested that the Earth’s mantle is far from homogenous and consists of a mixture of deformed harzburgite components and subducted oceanic crusts, or mid oceanic basalt (MORB) components (Xu et al. 2008; Stixrude and Lithgow-Bertelloni 2012). The bulk chemistry of MORB is different from deformed harzburgite and has significantly greater proportions of incompatible elements including Na$_2$O (~1.5–1.8 wt%) (Irifune and Ringwood 1993). The alkali component is likely to be incorporated into pyroxene (Angel et al. 1988) and also into garnet at higher pressures (Irifune and Ringwood 1993). Experimental studies on realistic mantle bulk compositions have shown Na-majorite to be stable at conditions relevant to the lower part of the upper mantle and transition zone (Gasparik 1990; Bindi et al. 2011; Bobrov et al. 2008a, 2008b, 2009; Dymshits et al. 2010, 2013). Sodium bearing natural garnets with (Na$_2$O > 1 wt%) have also been reported (Sobolev and Lavrentev 1971), indicating that sodium is likely to be an important component within the garnet structure at higher pressures. Na-majorite is an important host for the alkali elements and the partitioning of alkali elements might affect the relative thermodynamic stability of other alkali bearing aluminous phases such as new aluminous phases (NAL) and calcium ferrite structured (CF) phases (Dymshits et al. 2013). Owing to the importance of Na-majorite in the upper mantle and transition zone conditions, extensive studies have been conducted on phase relations (Gasparik 1990; Bindi et al. 2011; Bobrov et al. 2008a, 2008b, 2009; Dymshits et al. 2010, 2013), crystal structure determinations (Bindi et al. 2011) and high-pressure compressibility and the equation of state (Hazan et al. 1994; Dymshits et al. 2014). It is known that the bulk sound velocity i.e., compressional wave velocity, $v_p$, and shear wave velocity, $v_s$, for mineral phases and aggregates are important to relate seismological observation with the chemical composition of the mantle. The elastic moduli for majorite garnet with Na$_2$MgSi$_2$O$_{12}$ stoichiometry are important. A complete knowledge of these end-member properties is instrumental in developing a thermodynamic mixing-model that will allow predictions for the seismic velocity for complex majorite solid solutions. It will also help us to test whether these phases that host alkali elements play important role in the upper mantle and in the transition zone. Despite being important, the full elastic moduli tensor and the sound wave velocity of Na$_2$MgSi$_2$O$_{12}$ remains unknown. In this study we used first-principles method to predict crystal structure, equation of state, and full elastic moduli tensor at high pressures.

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