Experimental evidence for the survival of augite to transition zone depths, and implications for subduction zone dynamics

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ABSTRACT

(Ca,Mg)-rich clinopyroxenes are abundant in Earth’s upper mantle and subduction zones. Experimental studies on the thermoelastic properties of these minerals at simultaneous high pressure and high temperature are important for constraining of the composition and structure of the Earth. Here, we present a synchrotron-based single-crystal X-ray diffraction study of natural diopside-dominated augite ([Ca0.66Na0.05Mg0.60](Mg0.74Fe0.11Al1.18Ti0.67)(Si1.06Al0.1)O6.06) at P and T to ~27 GPa and 700 K. The experiment simulates conditions in cold subducting slabs, and results indicate that augite is stable over this pressure and temperature range. A third-order high-temperature Birch-Murnaghan equation was fit with the pressure-volume-temperature data, yielding the following thermoelastic parameters: $K_0 = 111(1)$ GPa, $K'_0 = 4.1(1)$, $(\partial K_0/\partial T)_0 = -0.008(5)$ GPa/K and $\alpha_T = 4(1) \times 10^{-5}$ K$^{-1}$ +2(3)×10$^{-8}$ K$^{-2}$. A strain analysis shows that the compression along the three principal stress directions is highly anisotropic with $\varepsilon_1: \varepsilon_2: \varepsilon_3 = 1.98: 2.43: 1.00$. Additionally, high-pressure structural refinements of room-temperature polyhedral geometry, bond lengths and O3-O3-O3 angle were investigated to ~27 GPa and 700 K. The experiment simulates conditions in cold subducting slabs, and results indicate that augite is stable over this pressure and temperature range. A third-order high-temperature Birch-Murnaghan equation was fit with the pressure-volume-temperature data, yielding the following thermoelastic parameters: $K_0 = 111(1)$ GPa, $K'_0 = 4.1(1)$, $(\partial K_0/\partial T)_0 = -0.008(5)$ GPa/K and $\alpha_T = 4(1) \times 10^{-5}$ K$^{-1}$ +2(3)×10$^{-8}$ K$^{-2}$. A strain analysis shows that the compression along the three principal stress directions is highly anisotropic with $\varepsilon_1: \varepsilon_2: \varepsilon_3 = 1.98: 2.43: 1.00$. Additionally, high-pressure structural refinements of room-temperature polyhedral geometry, bond lengths and O3-O3-O3 angle were investigated to ~27 GPa at ambient temperature. Pressure dependences of polyhedral volumes and distortion indicate that the substitution of Al$^{3+}$ for Si$^{4+}$ significantly changes the compressional behavior of the TO$_4$-tetrahedron in augite. Density calculations of this augite along a subducting slab geotherm suggest that augite as well as other common clinopyroxenes would promote slab stagnations at transition zone depths if they are metastably preserved in significant quantities.

Keywords: Pyroxenes, augite, high pressure and temperature, single-crystal X-ray diffraction, subduction zone

INTRODUCTION

Pyroxenes are among the most important rock-forming minerals and are commonly found in both igneous and metamorphic rocks. Oceanic lithosphere consists of about 40% pyroxenes and garnet (Frost 2008). It was believed that pyroxenes transform into denser majorite garnet while oceanic crust subducts into the mantle (Akaogi and Akimoto 1977). However, recent studies imply that this reaction is inhibited under cold slab conditions, so pyroxenes may survive in deeper parts of the mantle than was previously thought (Nishi et al. 2008, 2013; Van Mierlo et al. 2013). Surviving metastable pyroxenes might cause stagnations of some slabs at depths along the 660 km discontinuity, due to their lower densities compared to garnet and broader metastability range compared to the metastable olivine (Agrusta et al. 2014; King et al. 2015; Nishi et al. 2013; Van Mierlo et al. 2013). Therefore, knowledge of the properties of pyroxenes to transition zone pressures (≥25 GPa) is very important in modeling the subduction zone environments.

Among the pyroxene group minerals, augite is the most common species and occurs in basalts and gabbros, which are major components of the oceanic crust. Augite is also commonly found in andesites, diorites, peridotites, and pyroxenites. Augite is monoclinic (C2/c space group) and has relatively complex crystal chemistry. Pyroxenes have a general formula of $M_2M_1T_2O_6$. In augite, $M_1$ sites are usually filled with Mg$^{2+}$, Fe$^{3+}$, Ti$^{4+}$, and Al$^{3+}$; $M_2$ are larger polyhedral sites that commonly accommodate Ca$^{2+}$, Na$^+$, Fe$^{2+}$, and Mg$^{2+}$; while T$^2$ sites are occupied predominantly by Si$^{4+}$, but typically contains some Al$^{3+}$ (Clark et al. 1969). In contrast with augite, diopside [CaMgSi$_2$O$_6$] and hedenbergite [CaFeSi$_2$O$_6$] are usually Al free. Although pyroxene minerals have been extensively investigated at high pressures with the discovery of several new polymorphs (Dera et al. 2013a; Finkelstein et al. 2014; Plonka et al. 2012; Zhang et al. 2012), studies of augite at high pressures and temperatures have been limited. Augite is important to the petrology of subducted slabs, therefore it seems urgent to fill the gap in understanding of the compressional behavior of this mineral at simultaneous high pressures and temperatures. In this study, single-crystal X-ray diffraction measurements of natural augite were conducted at 0–26.65(2) GPa at ambient temperature and the crystal structures were refined. The $P-V-T$