Equation of state and phase transition in KAlSi$_3$O$_8$ hollandite at high pressure

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ABSTRACT

The tetragonal hollandite structure (KAlSi$_3$O$_8$ hollandite) has been studied up to 32 GPa at room temperature using high-pressure in-situ X-ray diffraction techniques. A phase transformation from tetragonal $I4/m$ phase to a new phase was found to occur at about 20 GPa. This transition is reversible on release of pressure without noticeable hysteresis and hence this new high-pressure phase is unquenchable to ambient conditions. The volume change associated with the transition is found to be small (not measurable), suggesting a second order transition. The diffraction pattern of the high-pressure phase can be indexed in a monoclinic unit cell (space group $I2/m$), which is isostuctural with BaMn$_6$O$_{16}$ hollandite. The $\gamma$ angle of the monoclinic unit cell increases continuously above the transition. A Birch-Murnaghan equation of state fit to pressure-volume data obtained for KAlSi$_3$O$_8$ hollandite yields a bulk modulus $K_0 = 201.4$ (7) GPa with $K_0'' = 4.0$.

INTRODUCTION

KAlSi$_3$O$_8$ hollandite, orthoclase, is one of the abundant minerals found in the crust. It is an important host mineral of potassium at near-surface conditions of the Earth and is transported into the deeper part of the mantle as one of the components of subducting slabs. However, the nature of potassium-bearing minerals in the deep mantle is still a matter of debate. When KAlSi$_3$O$_8$ hollandite is subjected to high pressure, it first decomposes into a three-phases assemblage (wadeite-type K$_2$Si$_4$O$_9$ + Al$_2$SiO$_5$ kyanite + SiO$_2$ coesite) at ~6 GPa and then recombines to form a hollandite-structured phase (KAlSi$_3$O$_8$, hereafter) above ~9 GPa. For depths lower than 100 km, Wendland and Eggler (1980) suggested that kalsilite (KAlSiO$_4$) is stable instead of sanidine (a GPa. For depths lower than 100 km, Wendland and Eggler (1980)

These measurements provide new constraints on the KAlSi$_3$O$_8$ hollandite compression curve is also very important to the understanding the dynamics of subducted continental slab. To constrain the mineralogy and density of subducted slabs through the 670 km discontinuity, the equation of state (EOS) and physical properties of their main constituents must be known. The isothermal bulk modulus of KAlSi$_3$O$_8$ hollandite was measured by Zhang et al. (1993) using single-crystal X-ray diffraction; however, their study was limited to pressures up to 4.5 GPa, which is too low to make reliable extrapolations to the deep mantle.

In the present paper, we present new high-pressure measurements performed up to 32 GPa in the diamond anvil cell at room temperature, using hydrostatic pressure transmitting media. These measurements provide new constraints on the KAlSi$_3$O$_8$ hollandite EOS. We also report the first evidence of a structural phase transition occurring at ~20 GPa.

EXPERIMENTAL METHOD

Powder X-ray diffraction data were collected at both the Institute for Solid State Physics, University of Tokyo, using MoK$\alpha$ radiation (rotating anode) and at the BL13-A beam line of the Photon Factory, KEK (synchrotron source). We used modified Mao-Bell type diamond anvil cells, with anvils having culet diameters of 450 $\mu$m. Rhenium gaskets were pre-indentsted to 11 GPa and drilled to a diameter of 180 $\mu$m. Experiments below 10 GPa were carried out using a methanol-ethanol (4:1) mixture as a pressure-transmitting medium. For higher pressure, He gas was loaded using a system similar to the one described by Yagi et al. (1996). Starting sample was a pure KAlSi$_3$O$_8$ hollandite with hollandite structure. It was prepared from an isochemical mixture of K$_2$CO$_3$, Al$_2$O$_3$, and SiO$_2$, fired in air for degassing and then converted to hollandite structure at 20 GPa and 1500 °C in a "Kawai-type"...