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Equation of state and phase transition in $KAlSi_3O_8$ hollandite at high pressure

Tristan Ferroir,[1] Tsuyoshi Onozawa,[2] Takehiko Yagi,[2,*] Sebastien Merkel,[2] Nobuyoshi Miyajima,[2] Norimasa Nishiyama,[3] Tetsuo Irifune,[3] and Takumi Kikegawa[4]

[1]Ecole Normale Superieure de Lyon, 69364 Lyon cedex 07, France
[2]Institute for Solid State Physics, University of Tokyo, Kashiwa, Chiba 277-8581, Japan
[3]Geodynamics Research Center, Ehime University, Matsuyama 790-8577, Japan
[4]Photon Factory, KEK, Tsukuba, Ibaraki 305-0801, Japan

Abstract

The tetragonal hollandite structure ($KAlSi_3O_8$ 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 *I*4/*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 *I*2/*m*), which is isostructual with $BaMn_8O_{16}$ hollandite. The γ angle of the monoclinic unit cell increases continuously above the transition. A Birch-Murnaghan equation of state fit to pressure-volume data obtained for $KAlSi_3O_8$ hollandite yields a bulk modulus $K_0 = 201.4$ (7) GPa with $K_0' = 4.0$.