

Thermal equation of state of manganite

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Manganese(III) oxide hydroxide is found in nature as the minerals groutite (alpha-MnOOH), feitknechtite (beta-MnOOH), and manganite (gamma-MnOOH). Manganite is one of the naturally occurring polymorphs of Mn³⁺-OOH with an InOOH-related structure. The oxide hydroxides of trivalent cations have an InOOH-related structure, in which the trivalent cation is octahedrally coordinated by oxygen. InOOH, beta-CrOOH, epsilon-FeOOH, and delta-AlOOH have orthorhombic unit cells. However, manganite is monoclinic because of the Jahn-Teller distortion. Here we report the pressure-volume-temperature relation of gamma-MnOOH. The aim of this study was to determine the compression behavior of an oxide hydroxide with an InOOH-related structure.

The high-pressure X-ray diffraction study was carried out at the station NE7A at the Photon Factory Advanced Ring (PF-AR) in High Energy Acceleration Research Organization (KEK). The PF-AR operates at 6.5 GeV with an injection current of 60 mA. We used a Kawai-type multianvil apparatus driven by a large volume press, MAX-III. Tungsten carbide cubes (Tungaloy grade F) of 22 mm edge length were used for high-pressure generation.

Experiments were performed up to a pressure of 18.0 GPa and a temperature of 700K. The pressure-volume data were fitted by a third-order Birch-Murnaghan equation of state with the following parameters: $V_0 = 135.22(8) \text{ \AA}^3$, $K_0 = 77(2) \text{ GPa}$ and $K_{0T} = 12.0(5)$. The temperature dependence of the bulk modulus was determined to be $dK/dT = -0.022(6) \text{ GPa/K}$. This study shows that the most compressible axis is the b-axis. The beta angle in the monoclinic unit cell decreases with increasing pressure.

Keywords: X-ray diffraction, Equation of state, High pressure, MnOOH, Synchrotron radiation, Hydrous mineral