

Pressure-temperature stability studies of FeOOH using X-ray diffraction

A.E. GLEASON,^{1,*} R. JEANLOZ,¹ AND M. KUNZ²

¹Department of Earth and Planetary Science, University of California, Berkeley, McCone Hall 4767, Berkeley, California 94720, U.S.A.

²Advanced Light Source, Lawrence Berkeley National Laboratory, 1 Cyclotron Road, Berkeley, California 94720, U.S.A.

ABSTRACT

The Mie-Grüneisen formalism is used to fit a Birch-Murnaghan equation of state to high-temperature (T), high-pressure (P) X-ray diffraction unit-cell volume (V) measurements on synthetic goethite (α -FeOOH) to combined conditions of $T = 23$ – 250 °C and $P = 0$ – 29.4 GPa. We find the zero-pressure thermal expansion coefficient of goethite to be $\alpha_0 = 2.3 (\pm 0.6) \times 10^{-5} \text{ K}^{-1}$ over this temperature range. Our data yield zero-pressure compressional parameters: $V_0 = 138.75 (\pm 0.02) \text{ \AA}^3$, bulk modulus $K_0 = 140.3 (\pm 3.7) \text{ GPa}$, pressure derivative $K'_0 = 4.6 (\pm 0.4)$, Grüneisen parameter $\gamma_0 = 0.91 (\pm 0.07)$, and Debye temperature $\Theta_0 = 740 (\pm 5) \text{ K}$. We identify decomposition conditions for $2\alpha\text{-FeOOH} \rightarrow \alpha\text{-Fe}_2\text{O}_3 + \text{H}_2\text{O}$ at 1–8 GPa and 100–400 °C, and the polymorphic transition from $\alpha\text{-FeOOH}$ ($Pbnm$) to $\varepsilon\text{-FeOOH}$ ($P2_1mn$). The non-quenchable, high-pressure $\varepsilon\text{-FeOOH}$ phase P - V data are fitted to a second-order (Birch) equation of state yielding, $K_0 = 158 (\pm 5) \text{ GPa}$ and $V_0 = 66.3 (\pm 0.5) \text{ \AA}^3$.

Keywords: Goethite, XRD data, diamond-anvil cell, compressibility measurements