American Mineralogist, Volume 84, pages 1588–1594, 1999

In situ X-ray diffraction study of enstatite up to 12 GPa and 1473 K and equations of state

TORU SHINMEI,[1,*] NAOTAKA TOMIOKA,[1] KIYOSHI FUJINO,[1] KOJI KURODA,[2] AND TETSUO IRIFUNE[2]

[1]Division of Earth and Planetary Sciences, Graduate School of Science, Hokkaido University, N10 W8, Kita-ku, Sapporo 060-0810, Japan
[2]Department of Earth Sciences, Faculty of Science, Ehime University, 2-5 Bunkyo-cho, Matsuyama, 790-8577, Japan

ABSTRACT

Crystal structures and phase transitions of enstatite ($MgSiO_3$) were studied by in situ X-ray diffraction experiments using synchrotron radiation and a multi-anvil high-pressure apparatus at pressures to 12 GPa and temperatures to 1473 K. Low clinoenstatite with space group $P2_1/c$ transforms to high-pressure $C2/c$ clinoenstatite at high pressures and high temperatures, accompanied by a volume reduction of about 2.5%. The β angle of this high-pressure $C2/c$ phase ranges from 101.4° to 101.7°, shows almost no variation with pressure and temperature, and is about 8° smaller than that of the high-temperature $C2/c$ phase previously reported. This confirms the suggestion (Hugh-Jones et al. 1994) that these two clinoenstatite phases differ at high pressures and high temperatures. The pressure-volume-temperature data for $P2_1/c$ and high pressure $C2/c$ clinoenstatite were fit to room-temperature third-order Birch-Murnahan equations of state (EOS) using the parameters: volume of V_0 = 415.4 (5) Å^3, isothermal bulk modulus of K_0 = 108.5 (6.4) GPa, and its pressure derivative of K_0' = 4.5 (1.3) for the $P2_1/c$ phase, and V_0 = 405.1 (1.7) Å^3, K_0 = 106.4 (17.4) GPa, and K_0' = 5.4 (2.7) for the $C2/c$ phase. These values are at ambient conditions. For the $C2/c$ phase, we determined the high-temperature EOS, expressed as $P = 3/2\ K_T\ [(V_T/V)^{7/3}–(V_T/V)^{5/3}]\{1–3/4\ (4–K_T')[(V_T/V)^{2/3}–1]\}$, where $K_T = K_0 + (\partial K_T/\partial T)_P\ (T–300)$, $K_T' = K_0'$, $V_T = V_0\ [\exp(\int_{300}^{T} \alpha(T)\mathrm{d}T)]$, where thermal expansivity $\alpha(T)$ is $a_0 + a_1\ T$. The parameters are V_0 = 405.0 (2.6) Å^3, K_0 = 106.9 (25.9) GPa, K_0' = 5.3 (3.9), a_0 = 2.01 (44) × 10^{-5} K^{-1}, a_1 = 2.10 (1.1) × 10^{-8} K^{-2}, and $(\partial K_T/\partial T)_P$ = –0.021 (10) GPa/K. Although the K_0 values are nearly the same with those of previous studies for both the $P2_1/c$ and $C2/c$ phases, the K_0' values are slightly smaller.