

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

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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-Murnaghan equations of state (EOS) using the parameters: volume of $V_0 = 415.4$ (5) \AA^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) \AA^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 $K_T = K_0 + (\partial K_T / \partial T)_P (T - 300)$, $K'_T = K'_0$, $V_T = V_0 [\exp(\int_{300}^T \alpha(T) dT)]$, where thermal expansivity $\alpha(T)$ is $a_0 + a_1 T$. The parameters are $V_0 = 405.0$ (2.6) \AA^3 , $K_0 = 106.9$ (25.9) GPa, $K'_0 = 5.3$ (3.9), $a_0 = 2.01$ (44) $\times 10^{-5} \text{ K}^{-1}$, $a_1 = 2.10$ (1.1) $\times 10^{-8} \text{ K}^{-2}$, 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.