American Mineralogist, Volume 87, pages 648–657, 2002

The high-temperature $P2_1/c$-$C2/c$ phase transition in Fe-free pyroxene ($Ca_{0.15}Mg_{1.85}Si_2O_6$): Structural and thermodynamic behavior

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ABSTRACT

A high-temperature in situ single-crystal X-ray diffraction study was performed from room T to 1150 °C on two crystals of Fe-free $P2_1/c$ clinopyroxenes of composition $Ca_{0.15}Mg_{1.85}Si_2O_6$ [cell parameters at room T: a = 9.651(2) Å, b = 8.846(2) Å, c = 5.202(1) Å, β = 108.38(2)°, V = 421.4 (2) Å^3] synthesized by isothermal annealing for 624 h at T = 1370 °C, P = 1 atm. A first order $P2_1/c$-$C2/c$ phase transition was found slightly below 1000 °C [T_c = 926(39) °C]. The transition was revealed by discontinuous changes in intensities and cell parameters. Prolonged heating at high temperature induced a non-reversible increase in the transition temperature up to more than 1150 °C, without apparent changes in the order of the phase transition. Coupling with strain due to incipient exsolution in a formerly almost defect-free sample is suggested to be responsible for increase in T_c. TEM observations of a sample from the same starting material after further annealing for 72 h at T = 1050 °C, P = 1 atm are consistent with the proposed incipient exsolution model. Annealing was found to induce the formation of a mottled texture oriented parallel to (101).

Results from structure refinement of data collected below the transition at T = 25, 500, 650, 800, and 1000 °C showed only minor changes in the chain configurations, which are highly differentiated up to 1000 °C, confirming the strong first-order character of the transition.