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Comparative compressibility and structural behavior of spinel $MgAl_2O_4$ at high pressures: The independency on the degree of cation order

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Abstract

The equation of state and the crystal structure evolution with pressure were determined for two single crystals of pure natural $MgAl_2O_4$ spinels with different degrees of order. The two samples studied were cut from a larger single crystal and one of them was experimentally disordered at high temperature. The two crystals, showing an inversion parameter x of 0.27 and 0.15 at ambient conditions, were loaded together in a diamond anvil cell and their unit-cell edge was measured up to about 7.5 GPa at 14 different pressures. The unit-cell volume, V_0, the bulk modulus, K_{T0}, and its first pressure derivative, K', were simultaneously refined using a third-order Birch-Murnaghan equation of state, giving the following coefficients: $V_0 = 529.32(2)$ Å^3, $K_{T0} = 193(1)$ GPa, $K' = 5.6(3)$ for the ordered sample and $V_0 = 528.39(2)$ Å^3, $K_{T0} = 192(1)$ GPa, $K' = 5.4(3)$ for the disordered one. Complete intensity data were collected at 0, 0.44, 2.92, 7.34, and 8.03 GPa in a separate experiment. For the ordered and disordered samples the oxygen atomic coordinate u remains practically unchanged inside the investigated pressure range with an average value of 0.2633(5) and 0.2614(2), respectively. As a consequence, the polyhedral compressibilities are similar and are not influenced by the Mg/Al distribution over the two crystallographic sites. This also suggests that pressure has little or no influence on the degree of order in the $MgAl_2O_4$ spinel.

Keywords: X-ray single-crystal diffraction, spinel, cation ordering, high pressure