

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

**F. NESTOLA,^{1,*} T. BOFFA BALLARAN,² T. BALIC-ZUNIC,³ F. PRINCIVALLE,⁴ L. SECCO,¹
AND A. DAL NEGRO¹**

¹Dipartimento di Geoscienze, Università di Padova, Corso Garibaldi 37, I-35137 Italy

²Bayerisches Geoinstitut, University of Bayreuth, Universitaetstrasse 37, D-95447 Germany

³Geological Institute, University of Copenhagen, Oester Volgade 10, DK-1350 Denmark

⁴Dipartimento di Scienze della Terra, Università di Trieste, Via E. Weiss 8, I-34127 Italy

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_{T_0} , and its first pressure derivative, K' , were simultaneously refined using a third-order Birch-Murnaghan equation of state, giving the following coefficients: $V_0 = 529.32(2) \text{ \AA}^3$, $K_{T_0} = 193(1) \text{ GPa}$, $K' = 5.6(3)$ for the ordered sample and $V_0 = 528.39(2) \text{ \AA}^3$, $K_{T_0} = 192(1) \text{ GPa}$, $K' = 5.4(3)$ 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