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Compressibility and high-pressure structural behavior of $Mg_2Fe_2O_5$

NICKI C. SIERSCH[1,*], TIZIANA BOFFA BALLARAN[1], LAURA UENVER-THIELE[2], AND ALAN B. WOODLAND[2]

[1]Bayerisches Geoinstitut, Universität Bayreuth, D-95440 Bayreuth, Germany
[2]Institut für Geowissenschaften, Goethe-Universität Frankfurt, Altenhöferallee 1, D-60438 Frankfurt am Main, Germany

ABSTRACT

The compressibility and structural behavior of the novel $Mg_2Fe_2O_5$ oxide has been investigated by in situ single-crystal X-ray diffraction in a diamond-anvil cell up to a pressure of 17 GPa. The bulk compressibility of $Mg_2Fe_2O_5$ can be described using a second-order Birch-Murnaghan equation of state (BM2 EoS) with V_0 = 352.4(2) Å^3 and K_0 = 171(4) GPa. Three linear BM2 EoS were used to describe the axial compressibility of $Mg_2Fe_2O_5$, which was found to be highly anisotropic. The *a* and *b* lattice parameters have very similar compressibilies, with a_0 = 2.8917(11) Å and linear modulus M_a = 572(16) GPa and b_0 = 9.736(3) Å and linear modulus M_b = 583(15) GPa, respectively. The *c*-axis is the most compressible direction as indicated by the smaller linear modulus [c_0 = 12.520(15) Å and M_c = 404(28) GPa]. The $Mg_2Fe_2O_5$ structure consists of edge-sharing octahedra alternating with layers of trigonal prisms. The compression behavior of the M-O bonds of the M1 and M2 octahedra and of the M3 prisms depend on their location in either an edge-sharing environment, which makes them stiffer, or a corner-sharing environment where they have more freedom to distort and compress. The main compression mechanism consists of a polyhedral tilting around the M2-O1-M2 angle, which decreases with increasing pressure. $Mg_2Fe_2O_5$ has recently been added to the list of stable end-members of phases with M_4O_5 stoichiometry, making it a potentially relevant phase in the Earth's upper mantle and transition zone. To develop thermodynamic activity-composition models for high-pressure phases, it is crucial to know the accurate elastic parameters of each individual end-member. Currently these have only been measured for $Mg_2Fe_2O_5$ (this study) and Fe_4O_5.

Keywords: $Mg_2Fe_2O_5$, Fe_4O_5, transition zone, high-pressure, compressibility, crystal structure