

## **The high-pressure phase transformation and breakdown of $\text{MgFe}_2\text{O}_4$**

**SOFIA WINELL,<sup>1,\*</sup> HANS ANNERSTEN,<sup>1</sup> AND VITALI PRAKAPENKA<sup>2</sup>**

<sup>1</sup>Department of Earth Sciences, Uppsala University, SE 752 36 Uppsala, Sweden

<sup>2</sup>Consortium for Advanced Radiation Source (CARS), University of Chicago, Chicago, Illinois 60637, U.S.A.

### **ABSTRACT**

The high-pressure transformation of  $\text{MgFe}_2\text{O}_4$  was studied by Mössbauer and Raman spectroscopy and synchrotron X-ray diffraction using the DAC technique and laser annealing at temperatures of 1500–2000 K. The high-pressure phase of  $\text{MgFe}_2\text{O}_4$  was observed from in situ Mössbauer spectra at  $17 \pm 1$  GPa after laser annealing by the appearance of two quadrupole doublets. This indicates a disordered distribution of Mg and Fe in an early stage. The displacive nature of the transformation of the spinel into its high-pressure polymorph was shown at increasing pressure by the redistribution of iron into only one site. After decompression Mössbauer spectroscopy revealed the presence of  $\text{Fe}_2\text{O}_3$  in the sample. This was further confirmed by Raman spectroscopy at ambient conditions and by in situ high-pressure XRD, indicating a partial breakdown of the spinel into its constituent oxides MgO and  $\text{Fe}_2\text{O}_3$ . The XRD pattern of the high-pressure phase of  $\text{MgFe}_2\text{O}_4$  can be indexed in agreement with the  $\text{CaMn}_2\text{O}_4$ -type structure, with cell parameters  $a = 2.775(2)$ ,  $b = 9.283(16)$ , and  $c = 9.446(5)$  Å at  $23 \pm 2$  GPa. The multiphase spectra from all three analytical methods suggests that inhomogeneous conditions prevailed in the DAC experiments, resulting in two different reactions at high pressure and temperature, i.e.,  $T < 1800$  K:  $\text{MgFe}_2\text{O}_4 \rightarrow \text{Fe}_2\text{O}_3 + \text{MgO}$  and  $T > 1800$  K:  $\text{MgFe}_2\text{O}_4 \rightarrow \text{hp-MgFe}_2\text{O}_4$ .

**Keywords:** High-pressure studies, magnesioferrite, phase transition, Mössbauer spectroscopy, XRD data