Supplementary information

A New Reference for the Thermal Equation of State of Iron

Experimental Data and EoS with Pressures Measured according to the MgO Calibration from Tange et al. 2009 [1]

The experimental data pressures were calibrated with MgO equations of state from Speziale et al. 2001 [2] and from Tange et al. 2009 [1]. At 100 GPa, a 4 GPa difference exists between the two calibrations. At higher pressures, the room-temperature Fe EoS extrapolated from the points calibrated with the MgO EoS from Tange et al. 2009 [1] fails to reproduce the experimental volumes determined by Dewaele and co-authors (2006) [3]. Conversely, the Fe EoS extrapolated from the data calibrated with the MgO EoS of Speziale and co-authors (2001) [2] reproduces the points from Dewaele et al. (2006) [3] and the experimental points at higher pressures from Mao et al. 1990 [4], Tateno et al. 2010 [5] and Sakai et al. 2014 [6] (exception made for their point with the calibration P1). Accordingly, the MgO EoS from Speziale et al. 2001 [2] was used as the reference for the calibration of the experimental data.

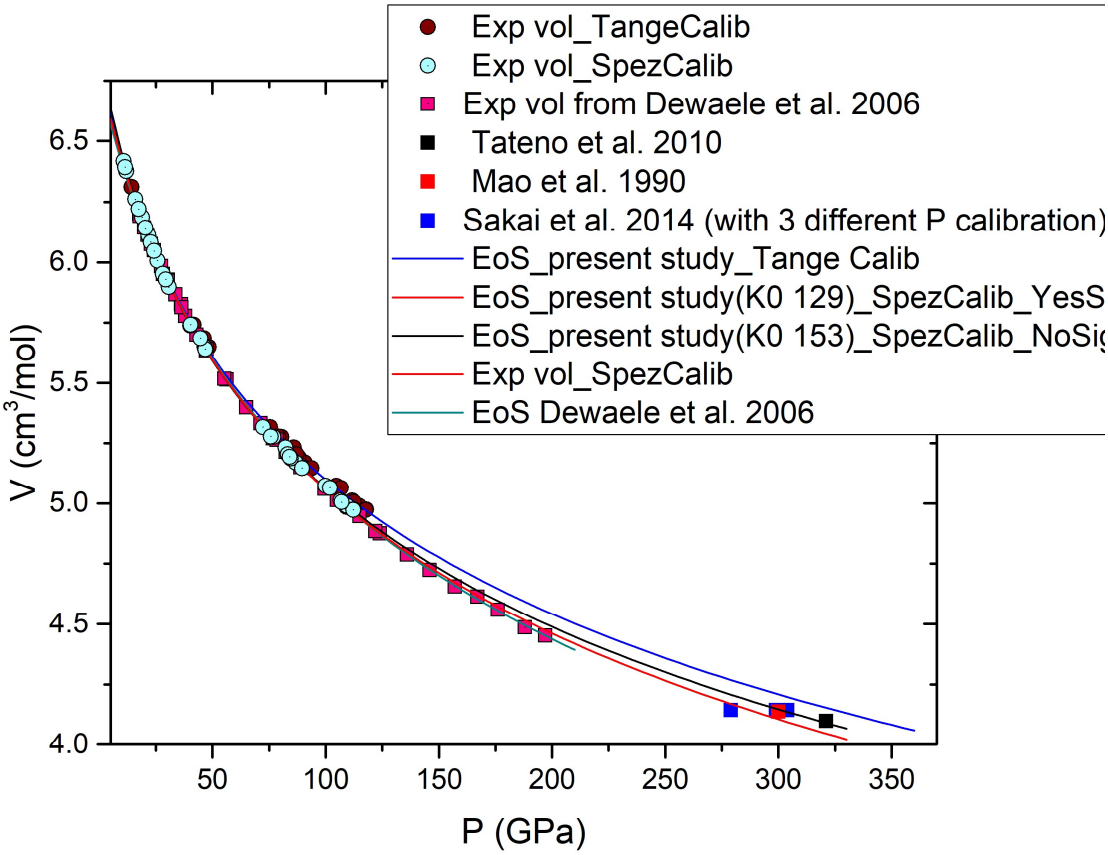

Figure S1. Compression data at room temperature with fitted equation of state. The experimental points from the present study have been calibrated with two different equations of state for MgO (Speziale et al., 2001 [2]; Tange et al., 2009 [1]) and compared with the experimental data from (Dewaele et al., 2006 [3]). Fitted equations of state are presented for both the pressure calibration, in particular, for the data calibrated with (Speziale et al., 2001 [2]) a refinement without taking in account uncertainties in pressure is shown as well. The experimental points available at extremes pressures (Mao et al., 1990 [4]; Sakai et al., 2014 [6]; Tateno et al., 2010 [5]) were used as a reference to estimate the reliability of the fitted EoS.

Post-Run Sample Preparation

Thin sections were prepared with a focused Ga ion beam (FIB) operating at 30 kV and currents from 20 nA to 20 pA for final surfacing. The cut is made perpendicularly to one sample surface (covered by platinum as shown in Figure S1), and across the laser-heated area and along the heating laser optical path (i.e. the axial temperature gradient). The FIB preparation allows us to carefully select the region of interest in the recovered samples. The cut is made along the infrared laser paths and the compression axis of the diamond-anvil cell. The slice is then removed in situ in the SEM chamber and welded to a copper TEM grid for further polishing and subsequent TEM observations.

Analytical Transmission Electron Microscopy

TEM observations on the FIB thin sections were performed on a JEOL 2100F microscope operating at 200 kV, equipped with a field emission gun and a high-resolution pole piece achieving a point-to-point resolution of 1.8 Å. Microstructures of the high pressure phases were obtained by conventional electron imaging and diffraction. Chemical compositions were obtained by energy dispersive X-ray spectrometry (EDXS) analyses using a JEOL detector with an ultrathin window allowing detection of light elements. The EDX spectrometer was calibrated using a series of silicates and oxides in order to obtain the corrective k-factors described in the Cliff and Lorimer method and are mandatory to obtain quantitative concentrations. Special care was taken to acquire EDX analyses at operating conditions of the TEM similar to those during the k-factor determination.

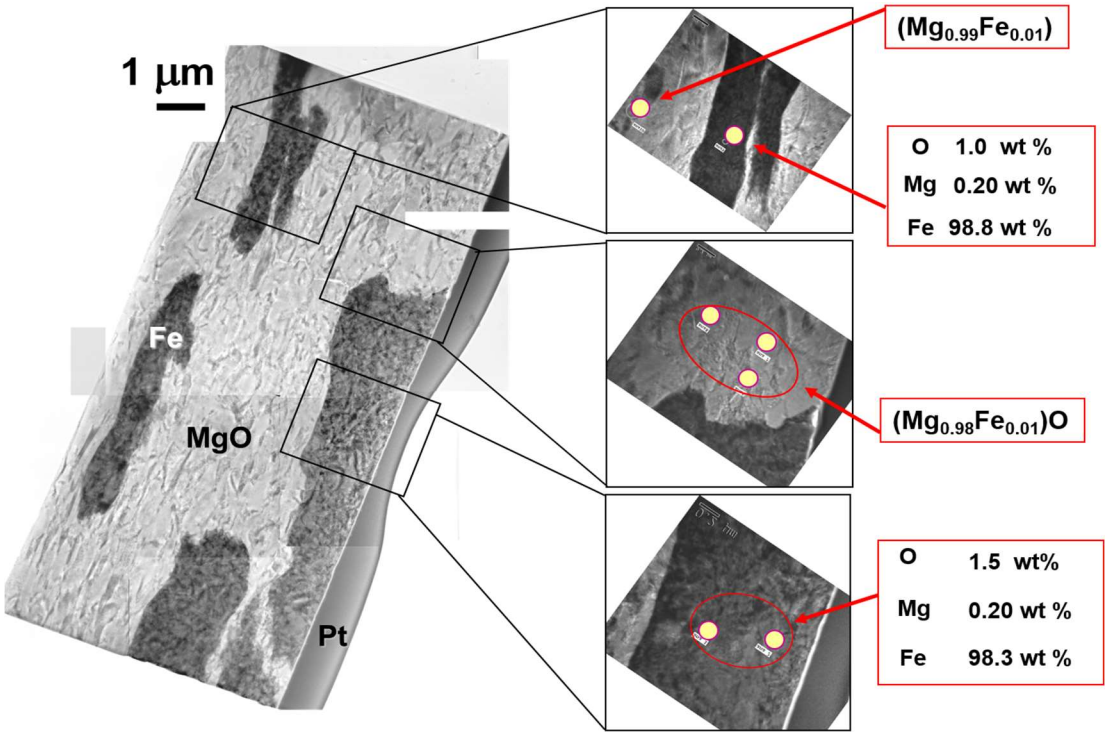

Figure S2. ATEM analyses on a FIB prepared recovered sample after diamond anvil cell experiment. The image is a combination of several high-resolution tiles. Iron appears as black areas whereas MgO is in light grey colour. Poiny analyses are represented with yellow circles on the right side. Iron grains are of the order of one to few microns along the path of X-rays and double-sided laser heating system.

References

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