Poster Presentation

MS01.P02

High-pressure behavior of Fe_2O_3

E. Bykova[1,2], M. Bykov[2], V. Prakapenka[3], Z. Konôpková[4], H. Liermann[4], N. Dubrovinskaia[2], L. Dubrovinsky[1]
[1]University of Bayreuth, Bavarian Research Institute of Experimental Chemistry and Geophysics, Bayreuth, Germany, [2]University of Bayreuth, Laboratory of Crystallography, Bayreuth, Germany, [3]University of Chicago, Center for Advanced Radiation Sources, Chicago, USA, [4]DESY Photon Science, Deutsches Electronen Synchrtron, Hamburg, Germany

High pressure behavior of Fe_2O_3 has been a long-standing subject of research due to its high importance for understanding Earth's interiors. At pressures from 40 to 60 GPa it undergoes a series of transformations, such as structural changes with a large volume discontinuity (~10 %), a drop of the resistivity, a spin crossover of Fe^{3+}, and a disappearance of the ordered magnetic state. The crystal structure of the phase(s) observed on compression at ambient temperature above 50 GPa is still under question since only powder X-ray diffraction (XRD) data were available so far. Mössbauer and Raman spectroscopy studies cannot provide definitive structural information. Applying laser heating to Fe_2O_3, compressed up to 70 GPa and above, results in a distinct reconstructive phase transition to the $CaIrO_3$-type structure, according to powder XRD. Poverty of the available structural data encouraged us to perform a series of high-pressure and high-temperature XRD experiments on single crystals of Fe_2O_3 in diamond anvil cells. We have studied the behavior of Fe_2O_3 at pressures up to 100 GPa and temperatures up to 2500 K. Here we report crystal structures of two novel high-pressure Fe_2O_3 polymorphs, as well as the relations between a spin state of iron atoms and the crystal chemistry of the iron compound. In our compression experiments initially hematite-structured Fe_2O_3 transformed to a new phase at ~54 GPa with 10 % of the volume reduction. This phase has a triclinic distorted perovskite-type structure. The second reconstructive transition occurred at 66–70 GPa with 3 % of the volume discontinuity and resulted in formation of an orthorhombic phase. Laser heating to ~2100±100 K at pressures above 70 GPa promoted a transition to a Cmcm $CaIrO_3$-type phase, whose crystal structure was refined by means of single crystal XRD to R_1 ~ 9.7 %. Decompression experiments showed that the Cmcm phase transforms back to hematite at pressures between ~25 and 15 GPa.

Keywords: high-pressure, phase transition, synchrotron single-crystal X-ray diffraction