

Crystal chemistry of compounds in Fe-O system at conditions of Earth's lower mantle

E. BYKOVA^{1,2*}, M. BYKOV², H.-P. LIERMANN¹, M. HANFLAND³, V. PRAKAPENKA⁴, L. DUBROVINSKY²

¹ P02.2, DESY, Hamburg, D 22607, Germany

(*correspondence: elena.bykova@desy.de)

² Bayerisches Geoinstitut, University of Bayreuth, Bayreuth, D 95440, Germany

³ ID15B, ESRF, Grenoble, F 38043, France

⁴ 13-IDB, APS, Argonne, IL 60437, USA

Oxides of iron are widely studied in geosciences as potential phases during the Earth's accretion as well as components of materials forming present day mantle and core-mantle boundary. Despite several decades of research the structure, properties and high-pressure and high-temperature (HPHT) behaviour of compounds in Fe-O system remain controversial. Establishing of phase relations in Fe-O system would create solid basis for analysis of effects of oxygen fugacity on chemical reactions at deep Earth's interiors and for development geodynamic models of these most remote region of our planet.

We applied methods of single-crystal X-ray diffraction and Mössbauer spectroscopy in laser-heated diamond anvil cells to study phase transformations, chemical stability and crystal chemistry of compounds belonging to Fe-O system at pressures up to 140 GPa and temperatures over 3000 K.

We observed that conventional iron oxides (FeO, Fe₃O₄ and Fe₂O₃) exhibit rich polymorphism at HPHT which is in significant degree governed by magnetic and electronic changes in Fe atoms. Moreover, none of these oxides remain chemically stable at certain *PT* conditions corresponding to Earth's deep mantle- and core-mantle boundary, forming under decomposition new compounds with unusual stoichiometry like Fe₅O₇ and Fe₂₅O₃₂.