Phase transitions and electronic properties of Fe2O3 under laser compression by ultrafast in-situ X-ray absorption spectroscopy

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Understanding the structural changes of hematite (α-Fe2O3) under extreme conditions of pressure and temperature is crucial for gaining insights into the physical properties of planetary interiors such as Earth and super-Earths (2 to 10 times more massive). At ambient conditions, hematite is a rhombohedral structured antiferromagnetic insulator [1,2]. Its high-pressure behaviour has been largely studied over the past decades using static compression [1,3,7]. Several phase transitions were reported but particular attention was given to the structural, electronic and magnetic changes occurring ∼50 GPa: a 10% volume cell drop accompanied by a change of crystal symmetry corresponding to a distorted perovskite (ζ-Fe2O3) [3], a Mott insulator-metal transition and the collapse of the iron magnetic moments corresponding to the high-spin (HS) to low-spin (LS) electronic phase transition [3-7]. However the exact nature of the phase transition in this pressure area remains controversial [4,6,7]. The question of which transition drives the other one, electronic or structural, is still under debate.

Here, we report ultrafast time-resolved X-ray Absorption Near Edge Spectroscopy (XANES) measurements obtained on laser-compressed Fe_2O_3 at the High Power Laser Facility (HPLF) of ESRF-ID24 beamline [8]. Our XANES data provide information on time-resolved structural transformations by showing changes in the pre-edge, the white line and the 1st Extended X-Ray Absorption Fine Structure (EXAFS) oscillation within hundreds of ps after the shock breakout from the samples. More severe spectral changes are observed at longer delays between the X-ray probe and the shock, during its thermodynamic release. We will present a detailed time-resolved study of the XANES changes as a function of pressure and temperature, along the Fe_2O_3 Hugoniot thermodynamic path and release. For further understanding of the XANES features, preliminary FDMNES [9] and Quantum Espresso [10] ab-initio calculations will also be presented.

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