



Characterization of ferropériclase under extreme condition using shock wave experiments carried at European XFEL utilizing DiPOLE 100-X drive laser

Carolina Camarda^{1,2}, Karen Appel¹, Khachiwan Buakor^{1,3}, Alexis Amouretti⁴, Celine Crepisson⁵, Marion Harmand⁶, Lea Pennacchioni⁷, Melanie Sieber⁷, and Christian Sternemann²

¹European XFEL GmbH, HED, Schenefeld-HH, Germany

²Technische Universität Dortmund, Dortmund, Germany

³Rostock University, Rostock, Germany

⁴SACLA-Japanese XFEL, Hyogo, Japan

⁵Processes and Engineering in Mechanics and Materials (PIMM), Paris, France

⁶University of Oxford, Oxford, United Kingdom

⁷Universität Potsdam, Potsdam, Germany

Ferropériclase (Mg,Fe)O, is the second most abundant mineral in the Earth's lower mantle, and its structural and electronic properties are critical for understanding the formation processes and evolutionary history of the Earth's core.

This study focuses on the behavior of ferropériclase under extreme conditions that simulate the environment near the core-mantle boundary (CMB) and within the outer core, at pressures around 130 GPa and temperatures of about 3500 K related to a depth of approximately 2800 km by using shock compression experiments. It is well-documented that FeO exhibits varying structural configurations under high pressure and temperature [1] and iron electron spin changes [2]. This study aims at deepening understanding of ferropériclase's role in geophysical processes occurring at extreme conditions within Earth's interior, ultimately contributing valuable insights into core formation theories and mantle dynamics. To investigate these properties, we synthesized ferropériclase (Fe_{0.14}Mg_{0.86}O) samples resembling pyrolytic mantle composition suitable for dynamic compression experiments. The experiments were conducted at the High Energy Density Scientific instrument at European XFEL within the scope of the DiPOLE community proposal 6656, utilizing time-resolved diagnostics to capture changes in the material's structure and electronic state. Two X-rays pulses were synchronized with a target impact, one before and another after the drive laser pulse of the DiPOLE 100-X laser, which allow us to probe the sample in a cold state and under pressure and temperature. The setup enabled us to acquire multiple datasets, including Velocity Interferometry for Any Reflector (VISAR) images, X-ray emission spectroscopy (XES), and X-ray diffraction (XRD). Data processing involved several steps: XES, spectra of Fe K $\beta_{1,3}$ lines were analyzed for both pulses separately ensuring accurate timing of X-ray arrivals. XRD data underwent flat fielding correction followed by summation of diffraction patterns to calculate unit cell parameters for ferropériclase.

The XES data reveal a clear transition from high-spin to low-spin states as a function of laser energy and delay relative to the ambient conditions. Concurrently, XRD analysis shows a notable shift to larger momentum transfer in the main Bragg peak compared to cold runs, allowing for precise calculation of unit cell dimensions under varying pressure conditions. By integrating our initial findings with established equations of state (EoS) [3] we can estimate the pressure conditions at each experimental shot, indicating the variation of pressures up to ~130 GPa, i.e. conditions at the CMB. This analysis facilitates the construction of a volume-pressure curve that elucidates spin transitions relevant to Earth's depths. Next step consists in analyze VISAR data and get the Hugoniot for this composition. Furthermore, we aim to understand the electronic structure of the melts.

[1] Ozawa et al. Spin crossover, structural change, and metallization in NiAs-type FeO at high pressure. *Phys. Rev. B* 84, 134417 (2011)

[2] Greenberg et al. Phase transitions and spin state of iron in FeO under the conditions of Earth's deep interior. *Phys. Rev. B* 107, L241103 (2023)

[3] Fei et al. Spin transition and equations of state of (Mg, Fe)O solid solutions. *Geophys. Res. Lett.*, 34, L17307 (2007)