### Using X-Ray Absorption Spectroscopy to Study Iron Oxides at Extreme Compressions





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*χ*: Isolated EXAFS modulations *μ*: Absorption coefficient XANES: X-ray absorption near edge spectroscopy EXAFS: Extended x-ray absorption fine structure

#### Summary

## X-ray absorption spectroscopy (XAS) was used to characterize the electronic and crystal structure of compressed $Fe_2O_3$

- XAS characterizes the temperature, density and complex chemistry of iron oxides at planetary core conditions
- A high resolution flat crystal x-ray spectrometer has been developed with an estimated  $E/\Delta E > 2000^*$  to study compressed iron oxides
- With the increased spectral resolution, a XANES feature in Fe<sub>2</sub>O<sub>3</sub> was measured above 500GPa

The XANES feature will be used to characterize the spin transitions in Fe<sub>2</sub>O<sub>3</sub>



#### **Collaborators**

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#### Iron oxides under extreme environments influence the evolution of the Earth and super-Earths



- Due to its high reactivity, iron influences the oxygen and hydrogen cycles in the mantle of Earth and Super Earths<sup>\*</sup>
- The composition and effects of light elements in the predominately iron and nickel Earth core remains an open question\*\*

#### XAS was used to characterize the behavior of iron oxides under extreme conditions



Image: M. Williams, "What are the Earth's Layers?," Universe Today, 7 December 2015, <u>https://phys.org/news/2015-12-earth-layers.html</u>

<sup>\*</sup>Q. Hu *et al.*, Nature <u>534</u>, 241 (2016). <sup>\*\*</sup>K. Hirose *et al.,* Annu. Rev. Earth Planet. Sci. <u>41</u>, 657 (2013).

# XAS presents features near an x-ray absorption edge that can be used to deduce the electronic density of state and atomic structure of matter





International X-ray Absorption Society, Fe2O3 Data, M. Newville, Rev. Min. Geo. <u>78</u>, 33 (2014) https://xaslib.xrayabsorption.org

### XANES and EXAFS spectroscopy can reveal the states and structure of materials at extreme conditions





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<sup>\*</sup>M. Newville, Rev. Mineral. Geochem. <u>78</u>, 33 (2014).<sup>†</sup>J.J. Rehr et al., Phys. Chem. Chem. Phys., <u>12</u>, 5503-5513 (2010). <sup>\*\*</sup>A. Sanson et al., Phys. Rev. B <u>94</u>, 014112 (2016).

### A resolution better than 1400 $E/\Delta E$ is required to preform ambient XANES measurements of Fe<sub>2</sub>O<sub>3</sub>



Ambient Fe<sub>2</sub>O<sub>3</sub> XAS data was degraded with gaussians of different FWHM to simulate the spectrum at different resolutions



International X-ray Absorption Society, Fe2O3 Data, https://xaslib.xrayabsorption.org B. Ravel and M. Newville, J. Sync. Rad. <u>12</u>, 537-541 (2005).

#### We designed, built, tested and deployed a new high resolution x-ray spectrometer (EFX) for XAS measurements on OMEGA EXAFS Flat Crystal (EFX) Spectrometer External tungsten to reduce background Light-tight image plate cassette Adjustable front filter pack to provide on Internal fluorescence shot energy calibration shielding to reduce lines background

Flat Si 111 crystal with narrow rocking curve for high spectral resolution





### A front end filter pack provides calibration of the energy dispersion relation on all shots





## EFX is expected to have a resolution (E/ $\Delta$ E) > 2000 at 7.5keV with a source size of 50 $\mu$ m



0 7450 7500 7550 Energy (eV)

\*Resolution at 7.5keV



## XAS data of compressed $Fe_2O_3$ has been measured at the OMEGA laser facility with EFX above 500GPa





### The measured EFX spectrum captures the main features of the simulated EFX spectrum



- Ambient BCC Fe EXAFS spectra was simulated using FEFF<sup>\*</sup>
- The simulated spectra was degraded using the EFX response given an implosion backlighter





### With the increased resolution of EFX, we measured a XANES feature in $Fe_2O_3$ compressed above 500GPa



The pre-edge feature will be used to characterize the spin transitions



Pressures obtained with HYADES simulations

B. Ravel and M. Newville, J. Sync. Rad. <u>12</u>, 537-541 (2005). A. Sanson *et al.*, Phys. Rev. B 94, 014112 (2016).

#### Conclusions

### X-ray absorption spectroscopy (XAS) was used to characterize the electronic and crystal structure of compressed Fe<sub>2</sub>O<sub>3</sub>

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### EFX has a peak sensitivity of 3eVnsr/pix and an average dispersion of 14.8eV/mm





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