ESRF	**Experiment title:** Structure and stability of iron fluoride at the Earth's lower mantle conditions: Implication for fluorine reservoirs in deep Earth	**Experiment number**: ES-916
Beamline:	**Date of experiment**: from: 03 Feb 2021 to: 06 Feb 2021 and a makeup experiment at 08-May 2021	**Date of report**: 18-August 2021
Shifts:	**Local contact(s)**: Davide Comboni (email: davide.comboni@esrf.fr) Gaston Garbarino (email: gaston.garbarino@esrf.fr)	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Qingyang Hu*, Center for High Pressure Science and Technology Advanced Research

Yanhao Lin, Center for High Pressure Science and Technology Advanced Research

Ho-kwang Mao, Center for High Pressure Science and Technology Advanced Research

Report:

We have conducted 9-shift beamtime at ESRF and accomplished four related projects. After the experiment, we submitted one manuscript and it was now under review by *Science Bulletin*. We also finished two manusciprts that will be submitted soon. In addition, we collected very promising results on FeF_3 but may need additional experiment to finish it in the next run. The results are summarizd below. We would like to mention that within 9 shifts beamtime, at least 3 manuscripts have be produced and we also have the chance to resolve a long-pursuit question in Earth sciences. ESRF beamline scientsts will be co-authors in all the above-mentioned works.

1. We discovered a high-pressure hexagonal structured Fe_3F phase at above 200 GPa. This is the main results fully matching our proposal. We found oxygen can partially or fully replace the site of F to make $Fe_3(F, O)$. An XRD pattern obtained at ESRF is shown below (Figure 1). The results can explain the density deficiency in the core.

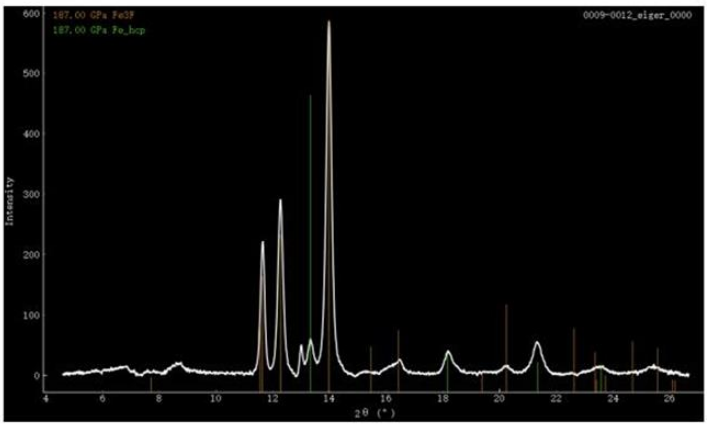

Figure 1. The X-ray diffraction pattern of Fe_3F synthesized at 190 GPa and 2400 K. It coexisted with hcp-Fe.

2. We submitted a manuscript titled "Evidence for scattered water transportation spots in the mid-lower mantle" and was curently under review by *Science Bulletin*. This work uncovered the water storage in the mid-lower mantle by combined XRD, electrical conductivity and seismic velocity experiment in iron oxide. Dr. Gaston Garbarino is a co-author of this work. The abstract is pasted below:
   "Water in Earth's transition zone and the core-mantle boundary plays a key role in its stratification, volatile cycling, and core formation. If water transportation is sustained between the aforementioned layers, the lower mantle should contain water channels with distinctive seismic and/or electromagnetic signatures. Here, we investigated the electrical conductivity and sound velocity of ε-FeOOH up to 70 GPa and 1800 K and compared results with global tomography data. A 3-order abrupt jump of electrical conductivity was observed above 50 GPa, reaching 1.24±0.19 × 103 S/m at 61 GPa. Meanwhile, longitudinal sound velocity dropped by ~20% in responding to the high-to-low spin transition of Fe3+. The high-conductivity and low-sound velocity of ε-FeOOH reproduce the seismic wave scatterings in the mid-lower mantle. Such unique properties of hydrous ε-FeOOH, or possibly other Fe-enriched phases can be detected as evidences for active water transportation in the mid-lower mantle."

3. We completed a manuscript titled "Experimental and theoretical evidence for the pressure-induced decomposition of silver iodide" and will be submitted to *PRL* in summer. We discovered the pressure induced decomposition of AgI to single elements. Dr. Gaston Garbarino is a co-author of this work.
4. We are preparing a manuscript titled "Mixed water storage mechanism the stability of ultrahydrous SiO_2" and plan to submitted to a geophyical journal by the end the year. Here, we verified the exisiting problem on the phas transition boundary of hydrous stishovite. We also revealed the water incorportation mechanism through combined single-crystal XRD and first-principles simulations. Dr. Davide Comboni and Dr. Michael Hanfland from ESRF will be co-authors.