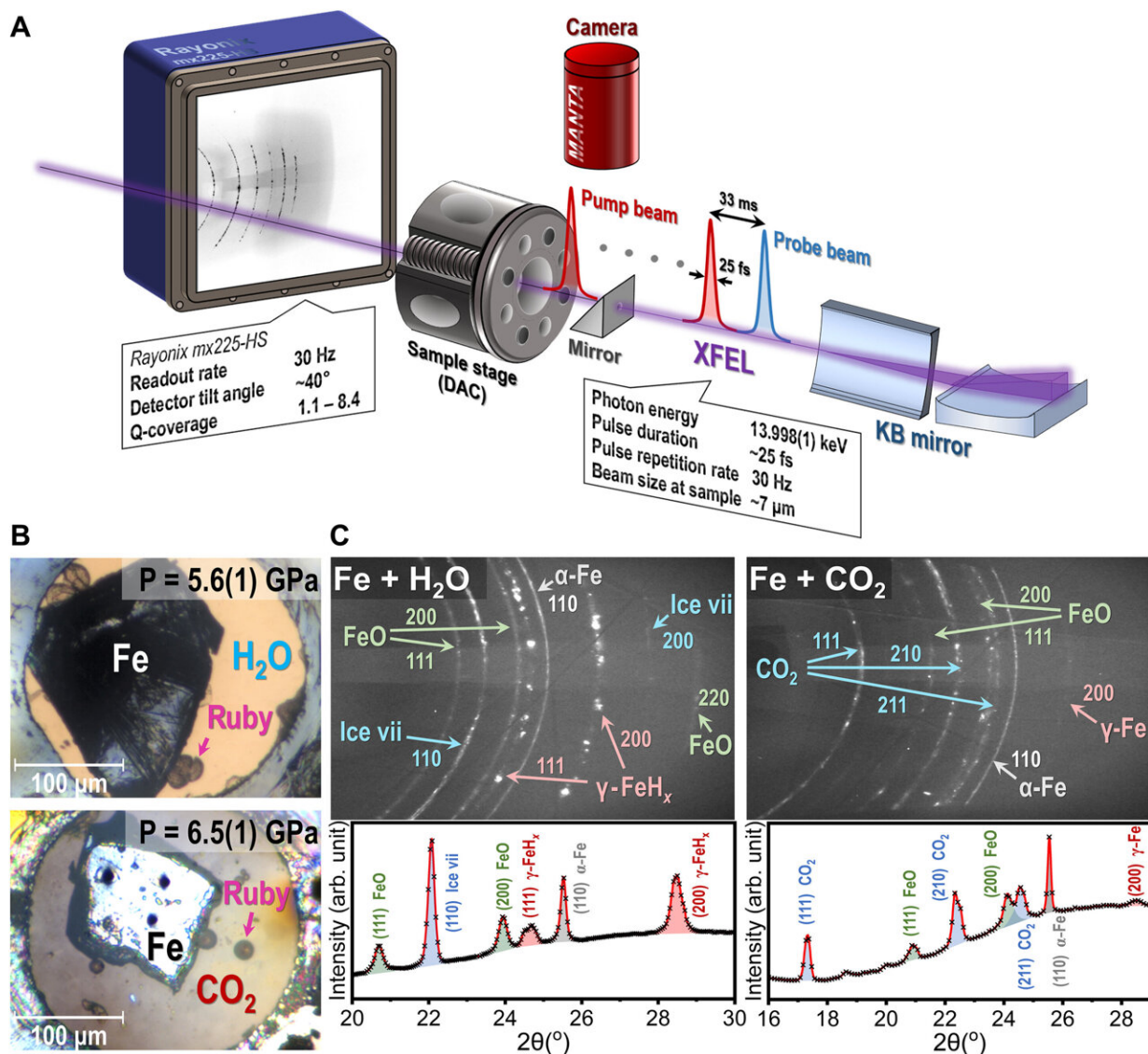


Planetary scientists simulate oxidation of iron by giant impact during atmospheric evolution of early Earth

December 20 2023, by Thamarasee Jeewandara



Schematics of XFEL pump-and-probe experiment on a precompressed sample in a diamond anvil cell. (A) Geometry of XFEL pump-and-probe experiment. (B) Photographs of iron foil with 4- μm thickness inside DAC with surrounding volatile fluids: H_2O (top) and CO_2 (bottom). (C) XRD images and patterns under XFEL-induced reaction in the $\text{Fe} + \text{H}_2\text{O}$ (left) and $\text{Fe} + \text{CO}_2$ (right) systems. Credit: *Science Advances*, doi: 10.1126/sciadv.adi6096

Giant-impact driven redox processes in the atmosphere and magma ocean may have played crucial roles during the evolution of the Earth. However, the absence of rock records from the time or era makes it challenging to understand these processes.

In a report [published](#) in *Science Advances*, Jinhuyuk Choi and a research team of planetary scientists in Seoul, Germany, and Korea, presented experimental results that can simulate giant impact-driven reactions between [iron](#) and volatiles, using [X-ray free electron lasers](#).

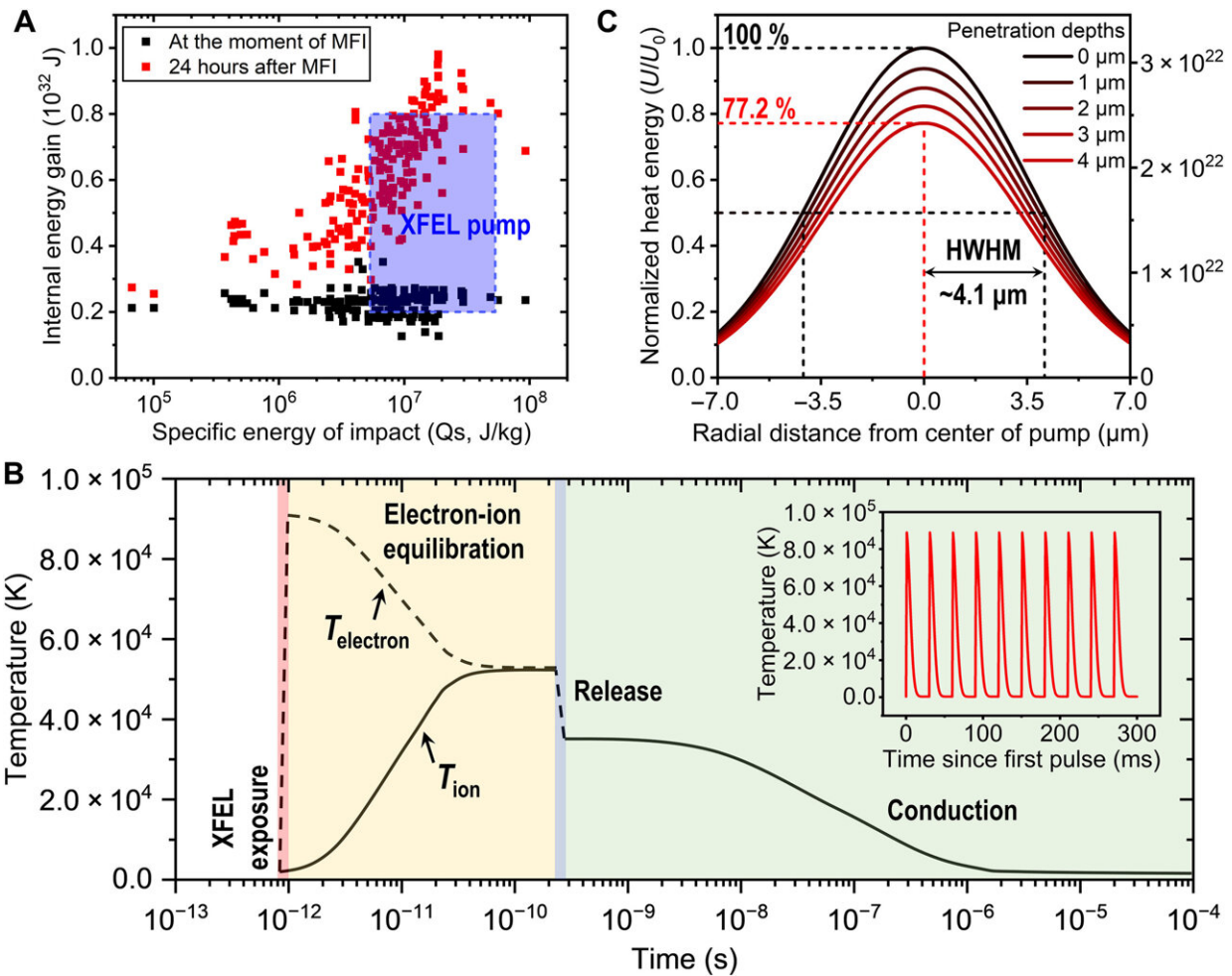
The scientists used the X-ray [free electron](#) laser pump to oxidize iron to [wüstite](#) and reduced the volatiles to hydrogen and [carbon monoxide](#). The iron oxidation proceeded to form hydrides and [siderites](#) to imply a redox boundary. The findings shed light on the process of creating a reduced atmosphere that underlies the emergence of prebiotic organic molecules on the early Earth.

Evolution of the Earth and the origin of life

The early giant impact that led to the formation of the moon more than 4.5 billion years ago was a catastrophic determinant in the [evolution of the Earth](#). The global chemical mixing and redox process that occurred in the steam atmosphere and magma ocean due to this giant impact effect led to out-gassing and interim formation in the reduced

atmosphere; [a prerequisite to the origin of life.](#)

While a variety of studies have proposed plausible scenarios underlying redox processes of the early mantle and atmosphere on Earth, researchers have attributed the formation of prebiotic organic species to the [low oxygen fugacity](#) of the planet. The Earth's mantle was oxidized to the present-day level since the Archean age to contain [water, carbon dioxide, and nitrogen](#). To conduct [numerical simulations](#) that reproduce the early Earth conditions, the researchers needed to develop appropriate experimental methods to validate the giant impact-induced reactions.



Energy distribution and temporal evolution of pressure and temperature by

XFEL pump pulse. (A) Comparison of the MFI-induced energy, i.e., specific energy by impact in diverse models versus corresponding internal energy gain of proto-Earth as adopted from Carter et al. (25), to the peak energy delivered by the XFEL pump used in this study. The area surrounded by a blue rectangle indicates the condition achieved by the XFEL pump used in this study. (B) Schematics of temperature evolution of iron by XFEL pump, modified from Husband et al. (39). Numbers at the top of the diagram indicate (i) isochoric heating occurring within a picosecond, (ii) electron-ion equilibration where the excitation of electron transfers heat to ions composing the lattice, (iii) isentropic release, and (iv) isobaric cooling. An inset shows noncumulative nature of heat by XFEL pumps in 30-Hz repetition rate used in this study. (C) Distribution of heat energy around the center of the XFEL pump as a function of radial distance and penetration depth in α -Fe. HWHM, half width at half maximum. Credit: *Science Advances*, doi: 10.1126/sciadv.adi6096

The [moon forming impact](#) can have vaporized the bulk silicate Earth to form a steam atmosphere and expanded the magma ocean to cause global mixing between the materials from proto-Earth and the differentiated impactor. Planetary scientists postulate that the moon forming impact would have induced vigorous chemical reactions between the differentiated compounds of the impactor and proto-Earth—leading to early life.

X-ray free electron lasers as a structural probe

Since X-ray free electron lasers are the brightest artificial light source in the energy regime of X-rays produced from [undulator magnets](#). The team incorporated laser-like ultrashort pulsed structures generated from self-amplified spontaneous emission.

In this work, Choi and colleagues used X-ray free electron lasers to pump and probe a pre-compressed mixture of heavy iron, and volatile

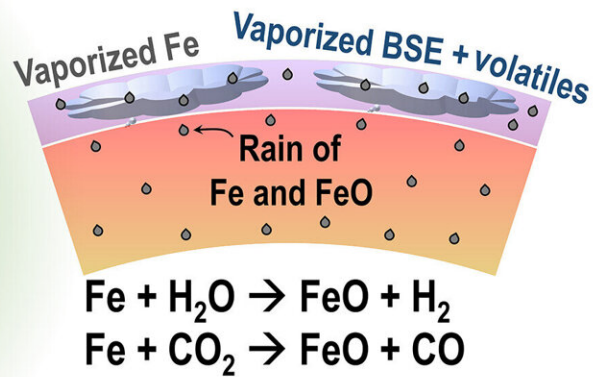
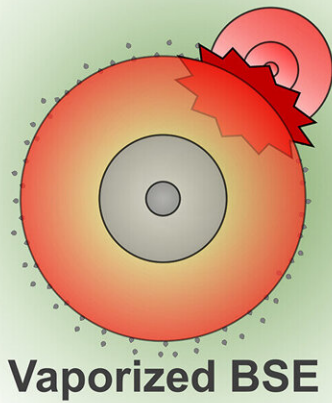
water and [carbon dioxide](#) to simulate chemical reactions between the metallic core of the impactor, and volatiles present in the proto-Earth. The results provided experimental evidence for the giant impact-driven oxidation of iron, leading to the early evolutionary pathways required for the origin of life.

Simulating the giant impact-induced environment

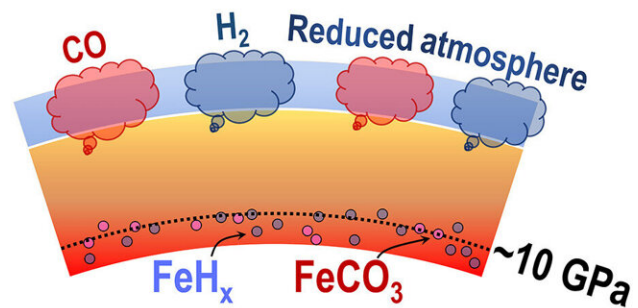
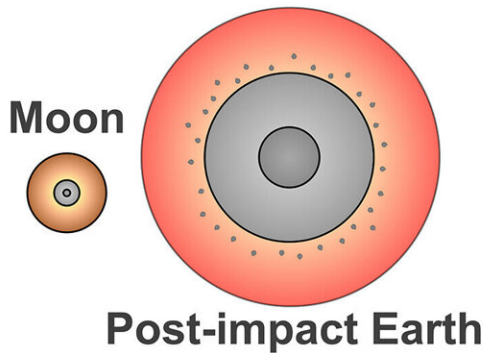
During the experiments, the scientists used a variety of materials, and estimated the temperature of the iron foil upon irradiation by a single X-ray free electron laser pulse from the deposited energy to correspond to the pulse energy absorbed by the irradiated sample. The [energy density](#) increased the instant that pressure lasted picoseconds, by [laser-shock compression](#).

While the difference in timescale between a giant impact and its experimental simulation still exist, the X-ray pump energy covered a large proportion of [giant impact-driven conditions](#).

Upon giant impact



After giant impact



A proposed scheme of the global redox reaction of the post-giant impact Earth. A schematic evolution scheme of the atmosphere and mantle in the early Earth before and after a giant impact. Credit: *Science Advances*, doi: 10.1126/sciadv.adi6096

Choi and the team additionally determined the pressure and temperature from the X-ray probe pulse and determined the effect on the iron-water system. When the team probed the samples with an additional pulse sometime after each train of pulses, the resulting reactions produced

additional hydrogen as a secondary oxidation product.

Additionally, Choi and team conducted X-ray free electron lasers on the iron-carbon dioxide system, where ferrous oxide reacted further with CO₂ to form [siderite](#) from consecutive pulses.

Microscopic observations of the recovered samples

The scientists gained further insights to the reaction pathway of the experiments after probing the cross sections of the recovered samples with [focused ion beam](#) and [electron microscopy](#).

To understand the role of silicate on the giant impact-driven reactions, the team performed an in-situ laser-heating experiment on the iron-water-silicate system. They noted how the presence of silicate did not impact the oxidation of iron or the production of reduced species. While the amount of water and carbon dioxide on bulk silicate Earth before the moon forming impact was highly controversial, an assumption exists of the reactants fully participating in the giant impact-induced reactions.

Outlook

In this way, Jinhuyuk Choi and colleagues proposed a scheme for the giant impact-driven redox processes of the early atmosphere and Earth's mantle. They observed the extent of iron oxide formation and iron hydrogenation to be inversely correlated with pressure produced from the reaction between iron and water. The X-ray free electron laser pump-probe experiments on the pre-compressed iron, mixed with volatiles experimentally simulated giant impact-driven reactions in the magma ocean.

The research team estimated the amounts of oxidized iron species and

reduced volatiles. The team supported the Theia hypothesis during the work, which describes a collision between [proto-Earth and an astronomical body called Theia](#). The outcomes explained the temporal and global conformation of the oxidized mantle and reduced atmosphere to facilitate the emergence of life on early Earth.

More information: Jinhyuk Choi et al, Oxidation of iron by giant impact and its implication on the formation of reduced atmosphere in the early Earth, *Science Advances* (2023). [DOI: 10.1126/sciadv.adi6096](https://doi.org/10.1126/sciadv.adi6096)

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