Using Brilliant X-Rays to Study Iron

Challenge

In the search to understand the makeup of Earth's core, scientists have struggled to find methods with which to simulate the high pressures and temperatures believed to exist at the center of the Earth. Without accurate experimental tools, theories about the true nature of Earth's core elements cannot be proved or disproved.

Argonne's Answer

Argonne National Laboratory's Advanced Photon Source (APS) is allowing a team of scientists from several different institutions to simulate conditions at the core of the Earth on samples of iron and iron-containing compounds, allowing them to see how experimental results compare with current theoretical understanding about the elements found in the center of our planet.

Using the APS to perform nuclear resonant inelastic x-ray scattering (NRIXS), the scientists examined samples of iron (Fe) under ultrahigh pressures previously achievable only with smaller-than-practical samples of material. This capability allowed measurements to 153 GPa — a dramatic increase in pressure over previous Fe analyses based on ultrasonic measurements at 16.5 GPa and radial x-ray diffraction measurements at 20–39 GPa.

Approach: Using NRIXS to Analyze Iron

NRIXS uses ultrahigh-intensity x-ray beams to facilitate measurement of the vibrational, elastic, and thermodynamic properties of the element analyzed. Parameters that can be measured include:

- Temperature
- Heat capacity
- Mean square displacement
- Shear modulus
- Compressional and shear velocity
- Zero-point energy
- Kinetic energy
- Average force constant
- Partial photon density of states
- Debye sound velocity
- Specific heat
- Entropy

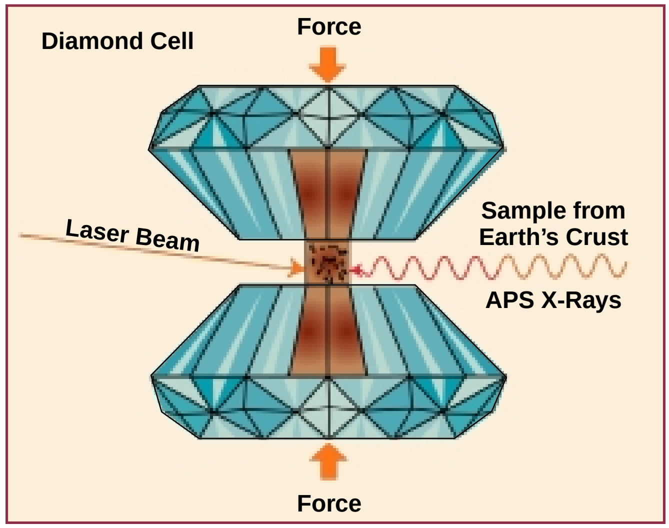

Figure 1. How the diamond anvil cell works.

To analyze Fe, the scientists used a diamond anvil cell (Figure 1), which consists of two gem-quality diamonds mounted between screws in a press. The researchers placed a very small sample between the diamonds, then compressed the sample between the diamonds by tightening the screws. The cell was then placed into the experimental setup shown in Figure 2, and ultrahigh pressure was applied. Extremely brilliant and monochromatic x-ray beams were used to excite the Fe nuclei; as these nuclei decayed, they provided a delayed signal that could be separated from the signal

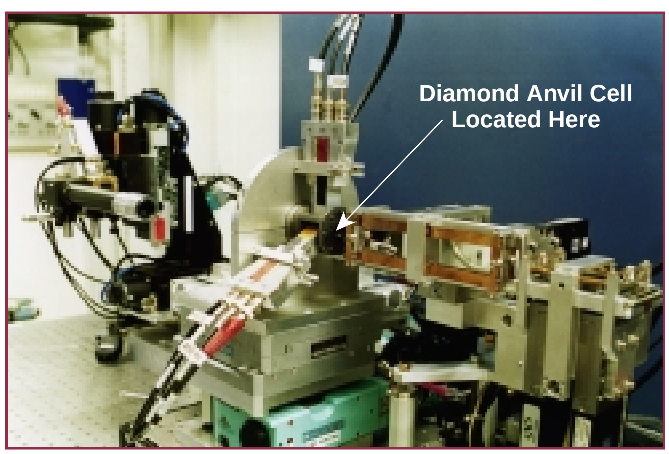

Figure 2. Photo shows the experimental setup at Sector 3 of the APS Synchrotron Radiation Instrumentation Collaborative Access Team (SRI-CAT) and indicates the position of the diamond anvil cell.

produced by the initial excitation by the x-ray pulse. NRIXS data were collected by recording the delayed signal versus the energy of the incident x-rays on the sample (Figure 3). A computer program known as PHOENIX was used to extract data and calculate the partial phonon (vibrational energy) density of Fe states.

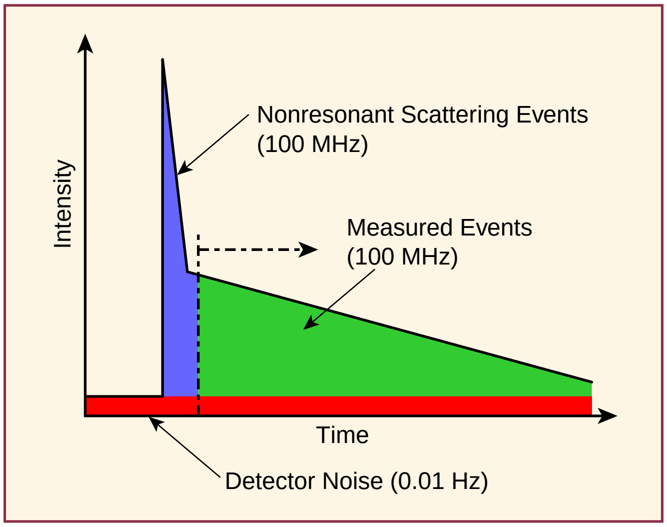

Figure 3. The principle of NRIXS time discrimination measurement.

The data obtained with NRIXS and PHOENIX were compared with seismic and theoretical data. Results suggest that an alloy of Fe and 5-10% nickel (Ni) will produce a match between theoretical hypotheses, seismic data, and experimental outcomes (Figure 4).

Impact

This pioneering project demonstrates the unique value of Argonne's APS in performing nuclear resonant inelastic x-ray scattering, which can be used to study the lattice dynamics of materials such as iron under extreme conditions by means of the diamond anvil cell. The high-resolution results can be used to improve theoretical models, especially for extrapolations to high temperatures. The NRIXS technique can be applied to a wide range of materials to obtain high-pressure and high-temperature data that were previously unobtainable in the experimental realm.

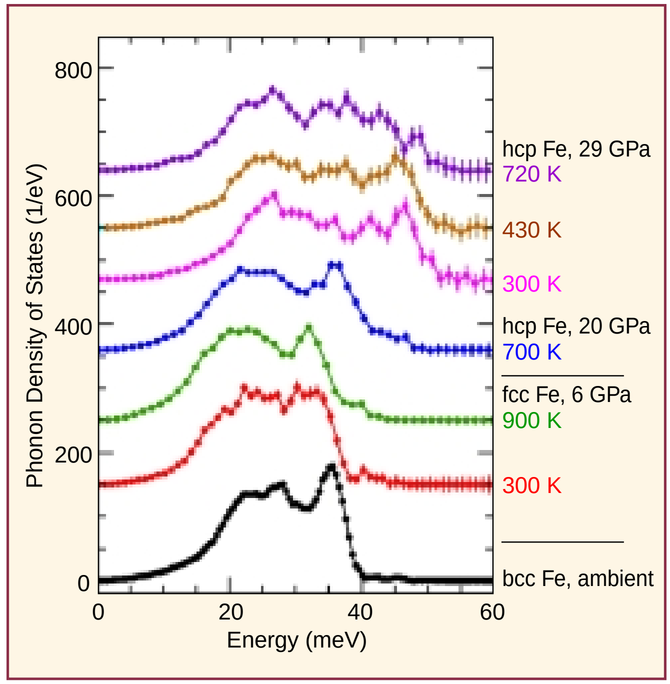

Figure 4. Vibrational energy (phonon) density of states for Fe at elevated temperatures. The Fe sample was heated by an electric current and the temperature was determined directly from the "detailed balance" of the NRIXS raw data with an accuracy of ~10%.

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