C1

High resolution Compton scattering

BL08W

Keywords: Electron orbital states, Fermi surface

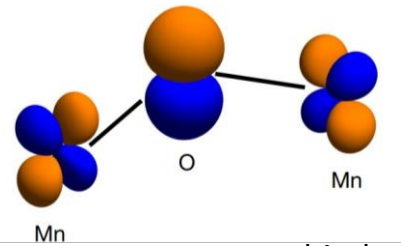
- Features

Electronic orbitals and Fermi surface are important for material properties. Lithium-ion batteries, for example, have the redox properties determined by the electronic orbitals that transfer electrons, while superconducting transitions, electric conduction and alloy regularization are affected by the shape of Fermi surfaces. High-resolution Compton scattering can visualize electron orbitals and Fermi surfaces, and extract related physical observables by measuring the electron density distribution in momentum space.

- Examples

Measurement of bulk states without surface effects

Mechanism of anion charge compensation (O^{2-}/O^{-}) of large-capacity cathode material $Li_xTi_{0.4}Mn_{0.4}O_2$



π-type Mn t_{2g} - O $2p$ orbitals

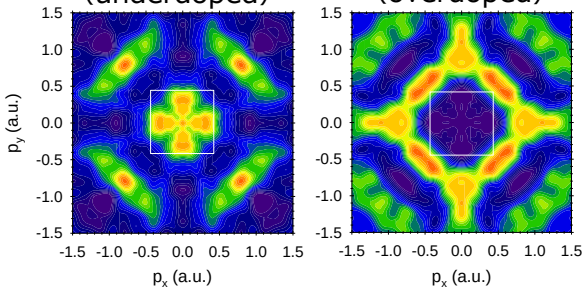
Nature **594**, 213(2021)

Measurement under electromagnetic fields and variable temperature

Visualization of hole states of high-Tc superconductor $La_{2-x}Sr_xCu_4O_4$

Hole creating superconductivity (underdoped)

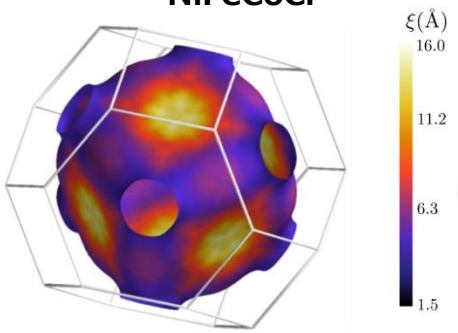
Hole breaking superconductivity (overdoped)



Science **332**, 698 (2011)

In situ measurement under ambient conditions or in solution

Fermi surface and electronic coherent length of random alloys NiFeCoCr



Phys. Rev. Lett. **124**, 046402 (2020)

- Towards SPring-8-II

High-resolution Compton scattering can measure bulk electronic states without interrupted by surface conditions. This method will promote fundamental understanding of the mechanism of high-capacity Li ion batteries, and contribute to the development of carbon-neutral materials.

C1

Magnetic Compton Scattering

BL08

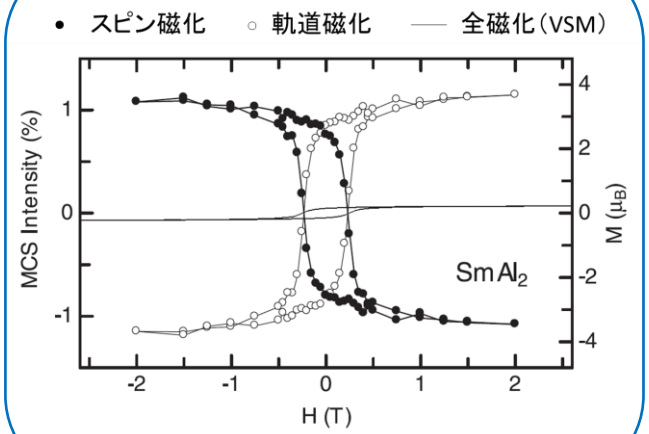
Keywords: Magnetic material, Magnetic property

- Features

Magnetic materials are important components in industry including development of electric vehicles. The magnetism has its origin in quantum phenomena, but it is difficult to evaluate on a microscale because most experimental methods can only extract total magnetization. To measure physical observables directly related to the electronic wavefunctions by spin states, magnetic Compton scattering is useful.

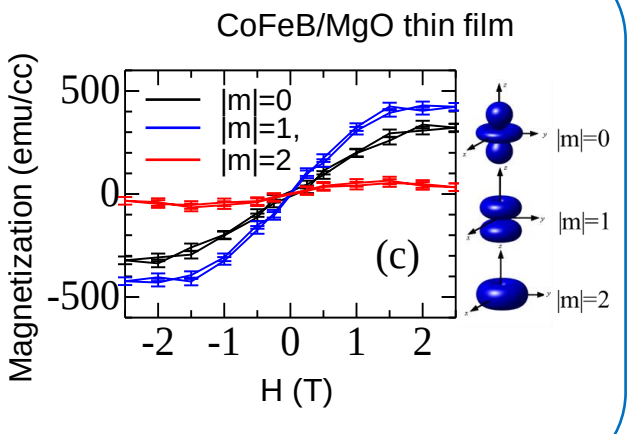
- Examples

Magnetization measurement with separated spin/orbital components



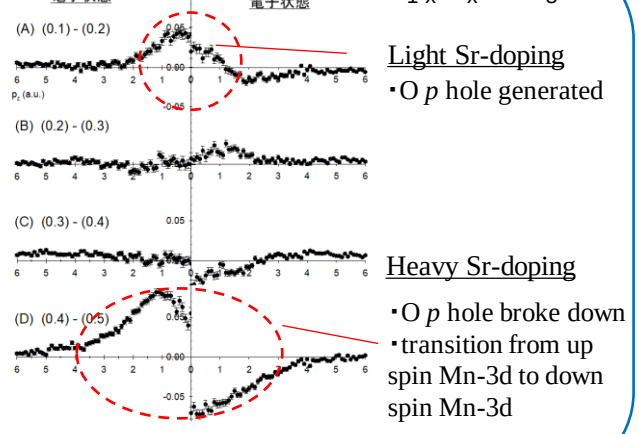
Appl. Phys. Lett. **102**, 082403 (2013)

Separated magnetization measurement by magnetic quantum number m



J. Phys.: Condens. Matter **28**, 436001 (2016)

Electronic states by up/down spin



Appl. Phys. Lett. **98**, 052107 (2011)

- Towards SPring-8-II

Magnetic Compton scattering uses high-energy X-rays having excellent penetration that enables evaluation of bulk properties free from surface states. The new source will realize high-speed mapping of magnetic properties inside magnetic materials/devices and at interfaces.

C2

Nuclear Resonance Vibrational Spectroscopy - Active site of the enzyme -

BL35XU, BL19LXU

- Features

Keyword: Element specific

Nuclear resonance vibrational spectroscopy is sensitive only to specific isotopes and provides information about their vibrational states. It is particularly useful for enzymes, because it can extract the vibrations of exactly the metals at the active center from a huge background. Combined with sophisticated simulations this provides valuable information about the structure of active centers of enzymes.

- Gallery

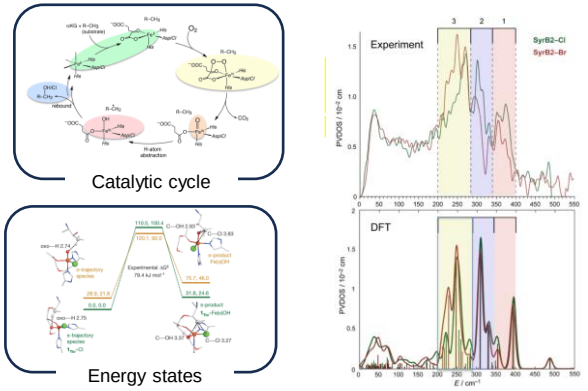
Average of 3 high impact (IF>12) publications every year

List of recent publications

[1] Nature Chem. Biol. (2023) https://doi.org/10.1038/s41589-022-01226-w.
[2] Inorg. Chem. 62 (2023)
[3] Faraday Discuss. 243 (2023).
[4] Biophys. J., 121 (2022) 346a.
[5] Proc. Natl. Acad. Sci. U.S.A., 118 (2021).
[6] J. Am. Chem. Soc., 143 (2021).
[7] Angew. Chemie Int. Ed., 60 (2021).
[8] J. Am. Chem. Soc., 143 (2021).
[9] Inorg. Chem., 60 (2021).
[10] Chem. Sci., 12 (2021).
[11] Biochemistry, 60 (2021).
[12] Angew. Chemie Int. Ed., 59 (2020).
[13] ACS Catal., 10 (2020).
[14] J. Am. Chem. Soc., 142 (2020).
[15] J. Am. Chem. Soc., 142 (2020).
[16] Chem. Sci., 11 (2020).

Active site in the enzymes

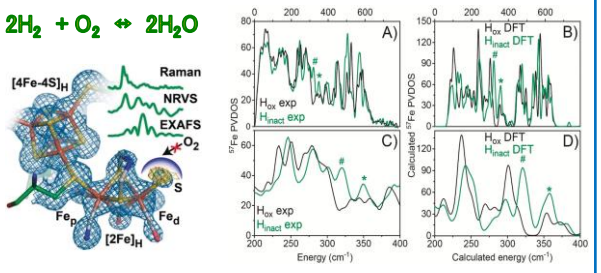
Elucidation of the Fe(IV)=O intermediate in the non-haem iron halogenase



Nature, 499 (2013) 320. doi:10.1038/nature12304

Enzyme for hydrogen: Hydrogenase

Crucial insight into O_2 stability mechanisms in the active site of the enzyme, hydrogenase



Angew. Chemie Int. Ed. **59**, 16786 (2020).
https://doi.org/10.1002/anie.202005208

- Toward SPring-8-II

Smaller samples will be possible with a small beam size at SP8-II. We also hope to improve the resolution using the improved brilliance. Research of the artificial catalysts and material science, especially earth science, will be accelerated by these features.

C2

Energy domain Mössbauer Spectroscopy - Complex materials -

BL35XU, BL19LXU

- Features

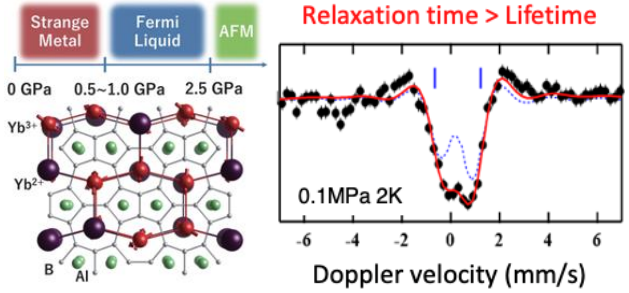
Keyword: Local electronic states

Energy domain Mössbauer spectroscopy at synchrotron radiation can investigate element-specific local electronic states with small beam size and without radioisotopes. This technique is especially useful for analyzing complex materials. Small beam size enable the study under the extreme conditions such as high pressure and/or high temperature easily. Basically this is hyperfine spectroscopy but with a much expanded range of resonances: e.g. Fe, Eu, Sm, Sn, Dy, K, Ge, Ni, Ir, Yb.

- Gallery

Charge fluctuations by ^{174}Yb EDMS

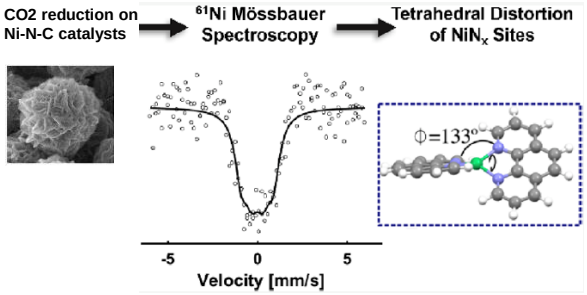
Observation of the charge fluctuations in a strange metal



Science **379**, 908 (2023).
DOI: 10.1126/science.abc478

Carbon Electrocatalysts by ^{61}Ni EDMS

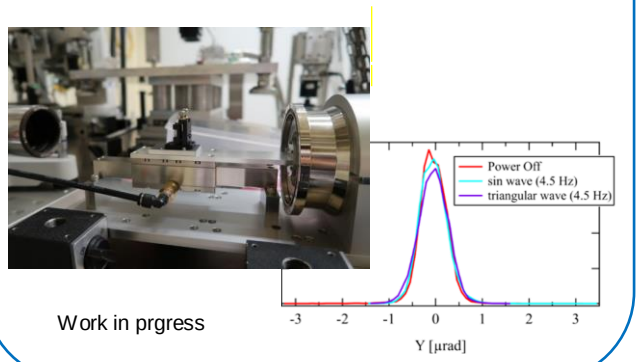
Investigation of the Structure of Atomically Dispersed NiNx Sites in Ni and N-Doped Carbon Electrocatalysts



J. Am. Chem. Soc. 144, 21741 (2022).
https://doi.org/10.1021/jacs.2c09825

Synchrotron Mössbuer Source

Synchrotron Mössbauer source of ^{57}Fe is under development with special device for public use



Work in prgress

- Toward SPring-8-II

Better spatial resolution can be obtained due to the higher brilliance. A synchrotron Mössbauer source of ^{57}Fe is under development for the public use at SPring-8-II. We hope to have a nm-scale beam size. Also, x-ray polarization analysis will become easier.

C2

BL35XU, BL19LXU

Time Domain Interferometry - Slow Dynamics -

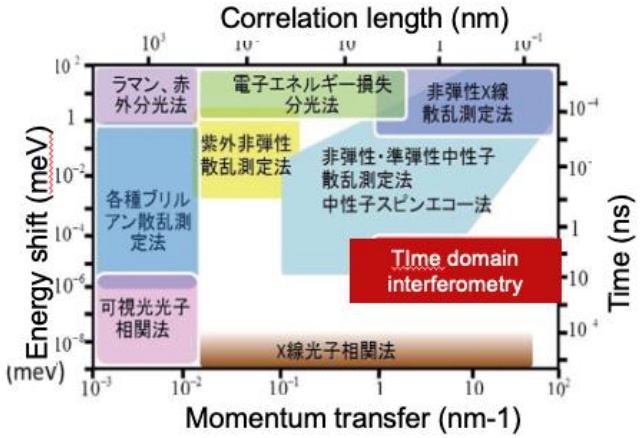
- Features

Keyword: Slow dynamics

Time Domain Interferometry (TDI) gives us the information of nanoscale dynamics from nsec to μsec. It can be applied to the soft materials such as ion liquid, ion conducting glass, rubber, liquid crystal and Membrane protein. This is basically the only alternative to Neutron Spin Echo (NSE) spectroscopy and is in fact better because it allows new access to materials with hydrogen and small samples.

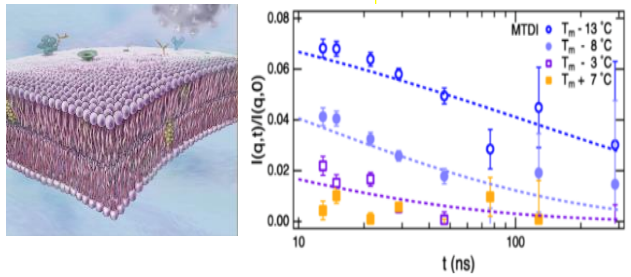
- Gallery

Energy and momentum region



Biomembranes

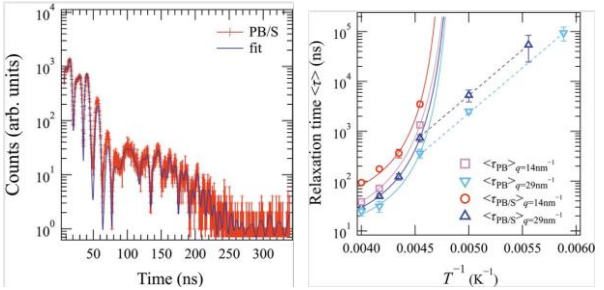
Better understanding properties of biomembranes essential for life activities



Phys. Rev. Lett. **127**, 078102 (2021).
https://doi.org/10.1103/PhysRevLett.127.078102

Tire Rubber

Microscopic observation of the effects of elongation on the polymer chain dynamics of crosslinked polybutadiene



J. Synchrotron Radiat. 29, 1180 (2022).
https://doi.org/10.1107/S1600577522007998

- Toward SPring-8-II

Better spatial resolution can be obtained due to the higher brilliance. The gamma ray quasi-elastic scattering in energy domain is also under development by SACLA/SPring-8 Basic Development Program.

C3

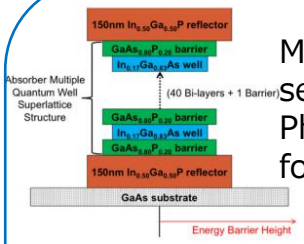
Thermal conduction and phonons BL35XU, BL43LXU

- Features

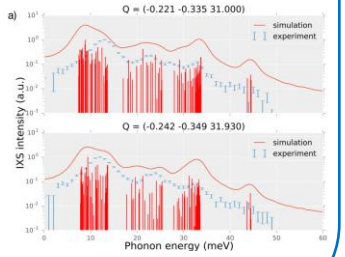
Thermal conduction in solids is carried out by electrons and phonons. Thermoelectric materials are required to exhibit high electrical conductivity but low thermal conductivity. Conversely, electrical insulators with high thermal conductivity are needed in, e.g., electronic circuits. In designing such materials, inelastic X-ray scattering is used to evaluate phonon properties. Such materials are sometimes synthesized in thin films, where IXS is one of the few probes that may be utilized.

- Examples

Phonons in multilayers



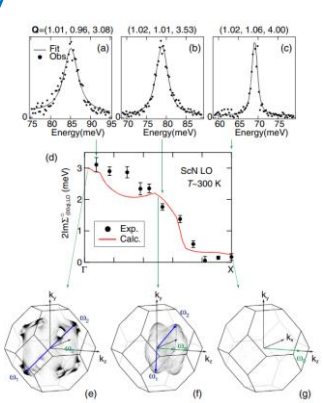
Multilayer thinfilm of semiconductors
Phonon engineering for thermo-electrics

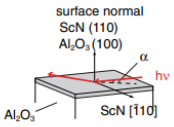


Consistency between calculations (red) and experiments (blue)

Appl. Phys. Lett. **110**, 043102 (2017)

Phonon Life time in ScN thin film



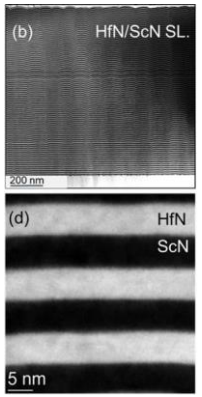


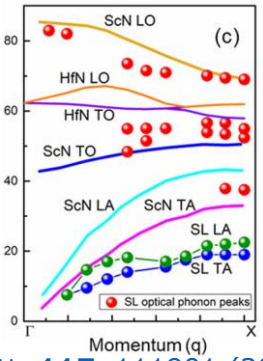
Measured phonon linewiths of ScN thin film can be explained 3-phonon model.

Phys. Rev. Lett. **120**, 235901 (2018)

Kohn anomaly in supper lattice

Kohn anomaly which is not observed in balk samples





Appl. Phys. Lett. **117**, 111901 (2020)

- Toward SPring-8-II

The high brilliance of SPring-8-II makes the measurements easier: the footprint the beam on the sample becomes smaller and the beam becomes more collimated. Consequently, it more sophisticated experiments may be realized, and, in particular, the region of total external reflection may be used to provide information with ~1nm sensitivity.

C3

Dynamics of Complex Materials

BL35XU, BL43LXU

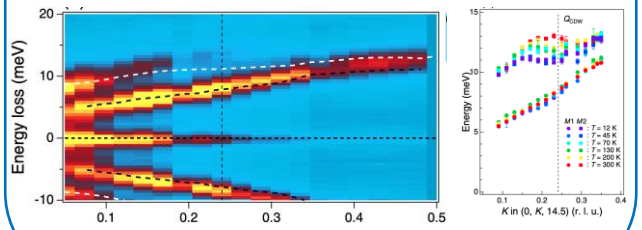
- Features

IXS serves a diverse community that investigates the interplay different degrees of freedom in complex materials: the properties of many interesting and technologically relevant materials arise from the interplay of lattice dynamics with electronic order, magnetic order, structure and thermal condutivity. The small x-ray small beam size allows investigations of phonons in samples that can not be measured by other methods.

- Examples

Common Softening in Cuprates

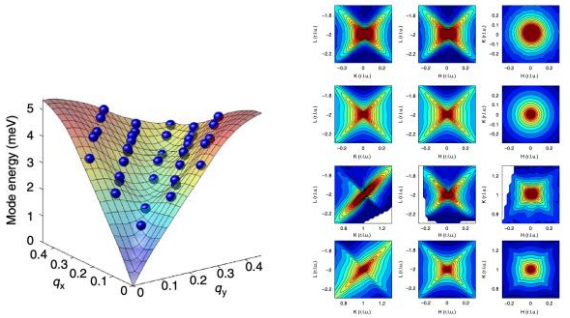
CDW instability, and related phonon softening is present in multiple families of cuprate superconductors



Phys. Rev. X **8**, 011008 (2018)

Microscopic Mechanism of Anti-Ferroelectricity

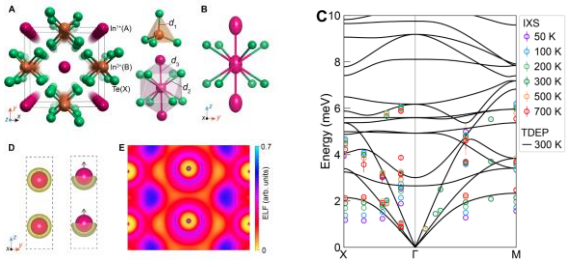
Phonon softening and diffuse scattering show antiferro-electricity come from a missed phase transtion.



Nature Comm. **4**, 2229 (2013)

Electrons Stopping Phonons

Combined structural/dynamics study shows lone pair electrons cause anharmonicity and reduced thermal conductivity



Angew. Chemie **62**, e202218458 (2023)

- Toward SPring-8-II

Smaller, faster, more extreme: The reduced beam size at SPring-8-II will make smaller samples easier to measure and permit access to different and potentially more extreme (higher temperatures, high pressures) conditions.

C3

Dynamics of Disorder

BL35XU, BL43LXU

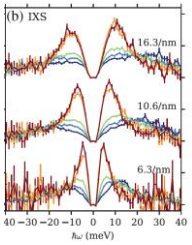
- Features

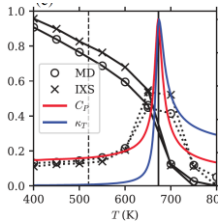
Disorder remains one of the frontiers of science. Materials, such as liquids and glasses, that are not periodic, are technologically important and poorly understood. At large length scales, they can be treated as continua, but as one approaches atomic length scales, the ”mesoscale”, such treatments fail. Inelastic X-Ray scattering with extremely high resolution ($\Delta E/E<10^{-7}$) provides a unique window on this region, unmatched by any other technique. It promotes new understanding of the mesoscale, including both identification of commonalities in behavior and discovery of new scienfic concepts.

- Examples

Gas-like liquids and liquid-like gases

Liquid near the critical point has regions that are dynamically gas-like



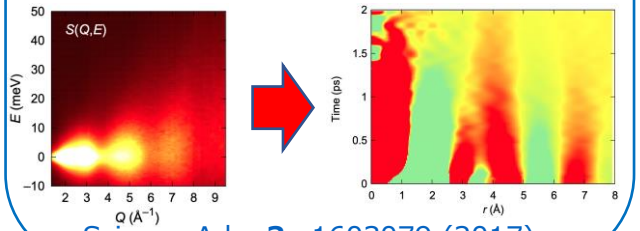


In water, this can be related to the hydrogen bonds

Phys. Rev. Lett. **125**, 256001 (2020)

Space-Time View of Liquids

A new approach show shows how looking at dynamics directly in real space allows on to gain inight – in this case the interaction of neighboring water molecules

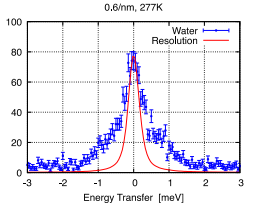


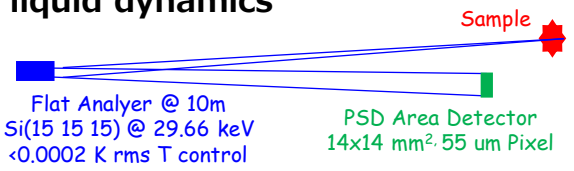
Science Adv. **3** e1603079 (2017)

Measuring where no one has measured befor

XIXS: Extreme Resolution IXS

0.38 meV FWHM World leading energy resolution for meso-scale liquid dynamics





Work in Progress

- Toward SPring-8-II

Extreme resolution will bridge the gap: Despite great effort, there is now no technique that bridges the gap between the length scale of ~60 nm (light scattering) and ~6 nm (IXS). The improved source characteristics at SPring-8-II will allow IXS to approach the light-scattering limit and provide access to dynamics that have been impossible to measure previously.

C3

Deep Earth Investigations

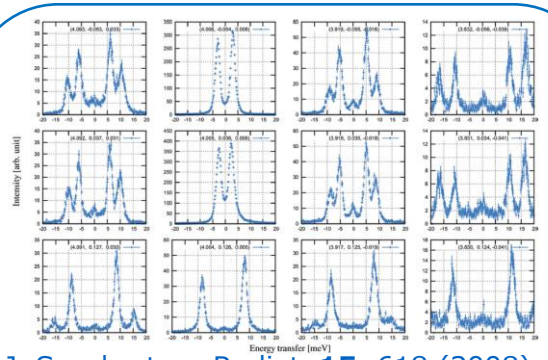
BL35XU, BL43LXU

- Features

The detailed chemical composition and temperature conditions of the Earth's interior are constrained by comparing the density and elastic wave velocity of candidate materials under high temperature and high pressure conditions in the laboratory with the observed values of the Earth. In order to do so, the technique to measure precise velocities under extreme conditions and pressure scales are required.

- Examples

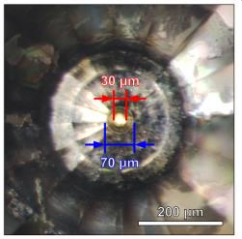
Absolute pressure scale with single crystals

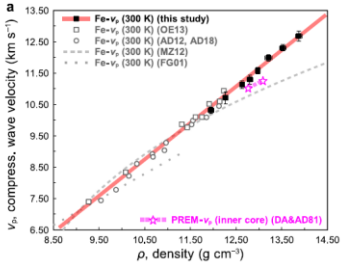


J. Synchrotron Radiat. **15**, 618 (2008)
Jpn. J. Appl. Phys. **56**, 095801 (2017)
Comptes Rendus Geosci. **351**, 236 (2019)
High Pressure Res. **40**, 465 (2020)
J. Appl. Phys. **132**, 055902 (2022)

sound velocity at pressure of earth's core

Iron at 300 GPa, the pressure at the inner core

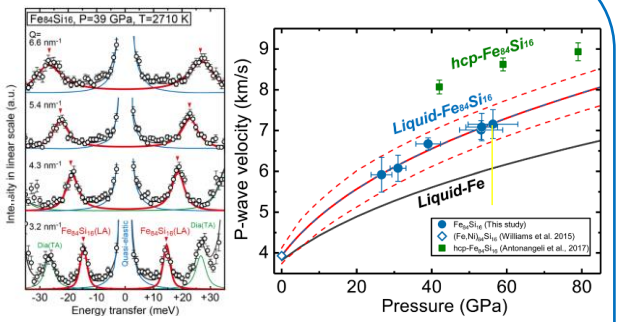




Density and longitudinal sound velocity of iron

Nature Comm. **13**, 7211 (2022)

Elastic wave velocity of Fe-alloy liquid



Silicon depleted outer core deduced from the sound velocity of Fe-Si alloy liquid

J. Geophys. Res. B **125**, 019399 (2020)

- Toward SPring-8-II

SPring-8-II will enable measurements of smaller samples and in more extreme conditions, allowing us to more close approach the conditions of Earth's core

C4

X-ray fluorescence holography

BL47XU

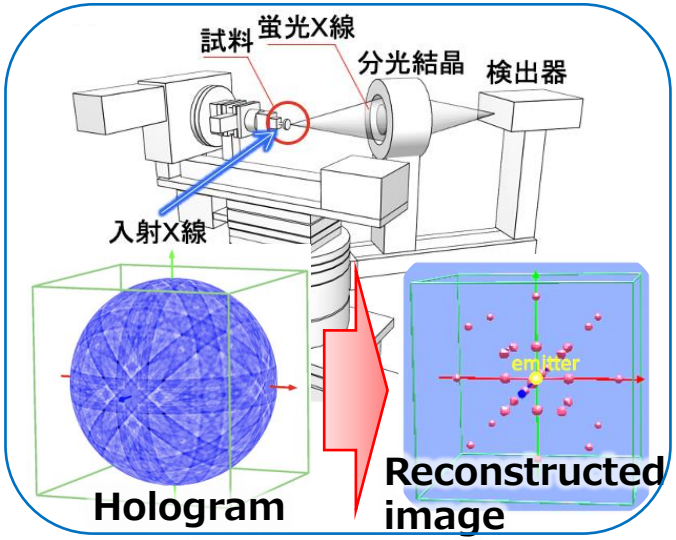
Keyword : 3D atomic image

- Features

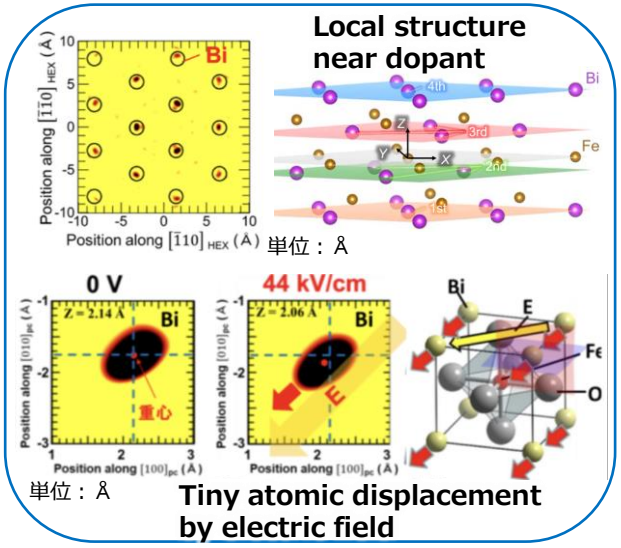
Holography has been widely used for 3D image reproduction in visible light, preventing counterfeiting of banknotes etc. Our hard X-rays enables element-selective 3D atomic images, which are used to analyze the local structure e.g. around specific additive elements in crystals of semiconductors, or around metallic elements in proteins. Our portable equipment having a large sample space is useful for detection and visualization of tiny deviations from the periodically ordered structures.

- Examples

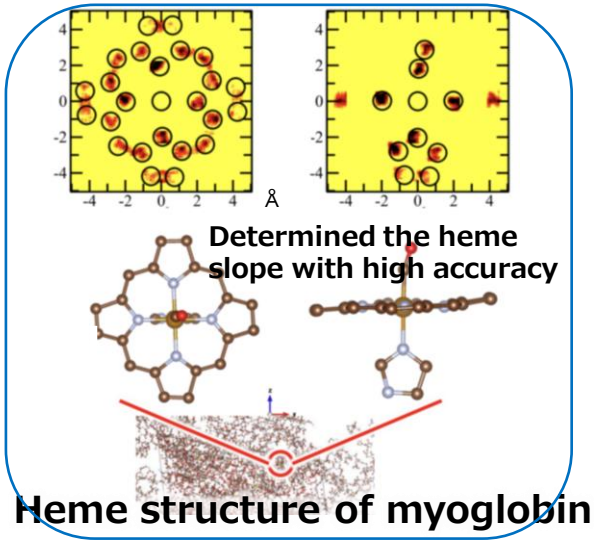
Setup for X-ray fluorescence holography



Visualization of atomic displacement around additive elements



Visualization of biosamples



- Towards SPring-8-II

Atomic scale visualization of intermediate phases between crystals and amorphous structures will contribute to creation of new functional materials. Our nanobeam will visualize local structures and structures within a single domain related to the functions of materials such as micron- and nano-sized crystal grains, porous zeolites, as well as composite defects and in crystal-like glasses.

C5

Compton scattering imaging

BL08W, BL05XU

Keywords: Operando observation, Digital twin

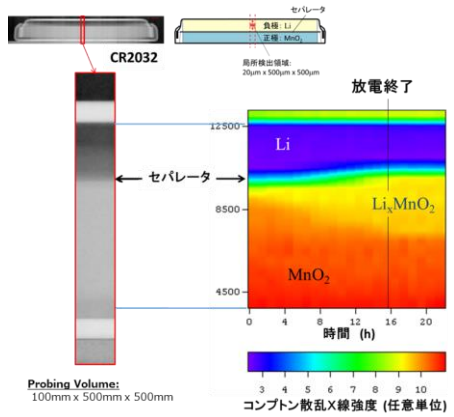
- Features

Observation of a cross-section of the object without rotation is useful in analyzing the inside of a palm-sized object. A storage battery is built into a system and is difficult to rotate and observe under operation. Compton scattering imaging enables non-destructive observation of the inside of a sample without rotation.

- Examples

Observation of a cross section of a battery without rotating it

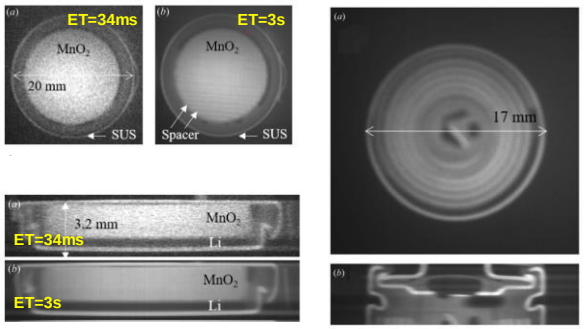
Li transfer



J. Synchrotron Rad. **22**, 161-164 (2015)

Sensitive to light elements

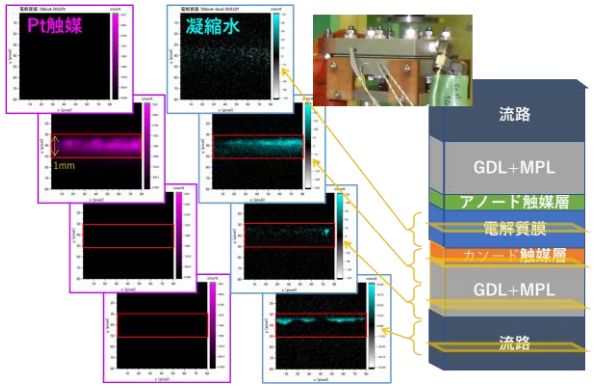
Internal structures of battery products



J. Synchrotron Rad. **28**, 1174-1177 (2021).

Simultaneous X-ray fluorescence analysis of heavy elements

Pt catalyst and water condensate distribution inside fuel cells



Appl. Sci. **13(19)**, 10753 (2023)

- Towards SPring-8-II

The new light source will enable high-speed observation that contributes to constructions of digital twin products and validation of phenomenon simulators.