International Workshop

on

Nuclear Resonant Inelastic Scattering

May 14-15, 2007

SPring-8

Committee

Host

CREST* research group for "Studies on Nuclear Resonant Scattering Methods for Materials Science"

Co-host

Japan Synchrotron Radiation Research Institute (JASRI)

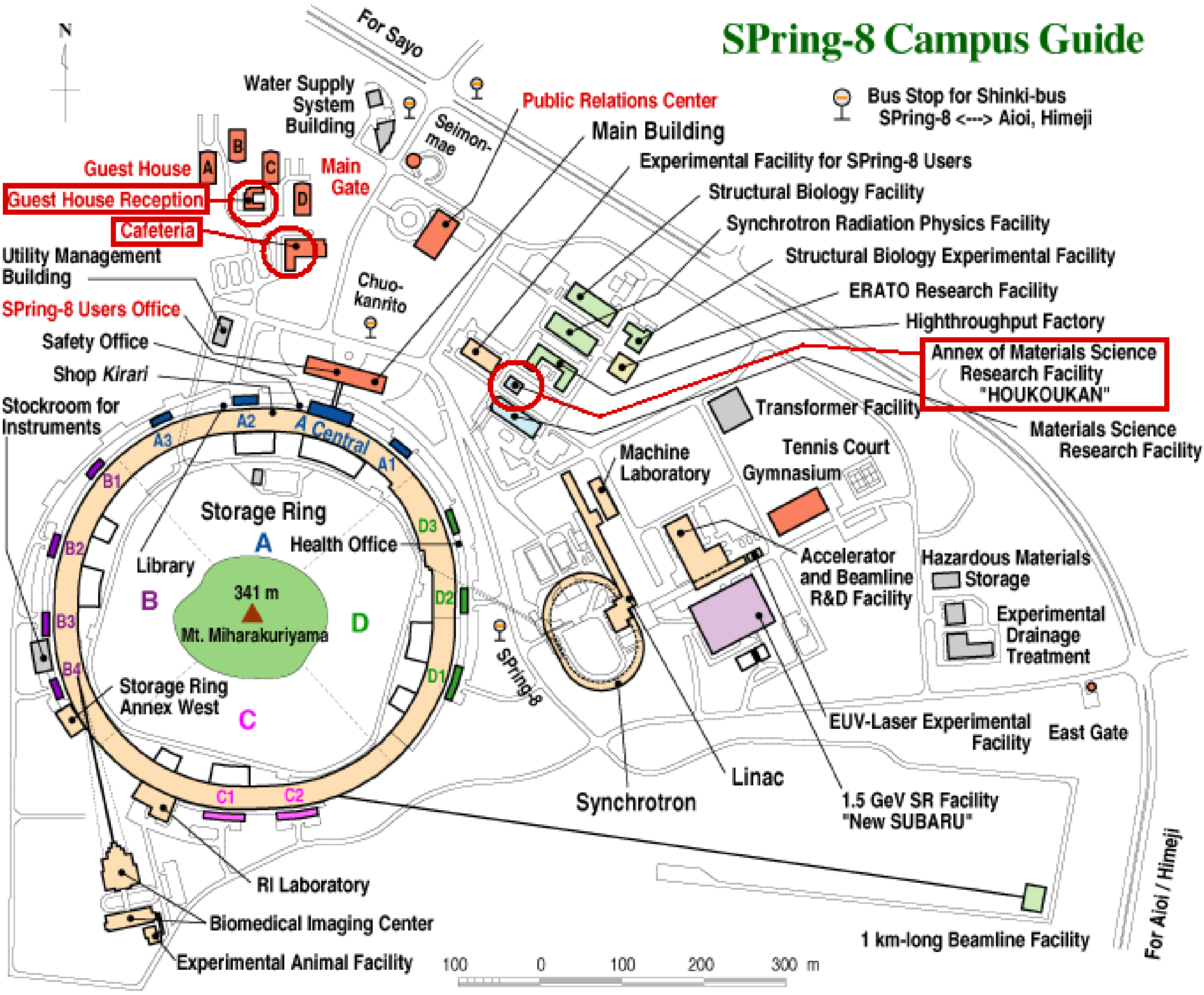
Local Committee

CREST research group members:

Makoto Seto (Kyoto Univ., SPring-8/JAEA)
Yoshitaka Yoda (SPring-8/JASRI)
Shunji Kishimoto (KEK)
Hisao Kobayashi (Univ. of Hyogo)
Ko Mibu (Nagoya Institute of Technology)
Takaya Mitsui (SPring-8/JAEA)
Yasuhiko Imai (SPring-8/JASRI)
Shinji Kitao (Kyoto Univ.)
Yasuhiro Kobayashi (Kyoto Univ.)

*CREST, or Core Research for Evolutional Science and Technology, is a team of researchers to promote fundamental project of science and technology supported by Japan Science and Technology Agency (JST) in Japan.

Map of SPring-8



Workshop is held at HOUKOUKAN in the SPring-8 campus.

Get-Together Party is held at the Cafeteria.

Check-in is needed at the Guest House Reception for stay at the Guest House.

Useful Information

Reception Desk

Reception desk is open at HOUKOUKAN at 8:30-9:00 on May 14. During the workshop, Reception desk will be kept open until 12:00 on May 15.

Guest House Reception

All visitors of the Guest House need to check in at the Guest House Reception between 16:00 and 22:00. You must check out before 10:00. Guest House fee (2000 Yen / night) should be paid at the Guest House Reception when you check out.

Cafeteria

Every user of Cafeteria needs the Cafeteria Prepaid Card. With this card, all menus are offered at half price. The card is offered at Get-Together Party on May 13 or in front of the Guest House Reception (only at 7:50-8:00 on May 14).

Before using, load money onto the card by the machine located just inside the Cafeteria entrance in this way:

1. Insert your card into the machine,
2. Insert bill(s) into the machine,
3. Choose the amount you would like to load on your card and press the button, and
4. Receive your card with a new balance.

The money loaded on the card can be refunded. Note that you won't get the card back, if you withdraw the entire balance by using the machine. Please make sure that the refund should be done only when you never use the card in future.

Program of International Workshop on Nuclear Resonant Inelastic Scattering

May 13, 2007 (Sun)

17:30-19:30	Get-Together party	Cafeteria

May 14, 2007 (Mon)

8:30-9:00	Reception	Reception Desk at HOUKOUKAN
9:00-12:30	Scientific Session	HOUKOUKAN

< Chair: Ko Mibu >

1	9:00-9:15	Research Project on Nuclear Resonant Scattering in Japan	Makoto Seto	p.8
2	9:15-9:30	Status of BL09XU	Yoshitaka Yoda	p.9
3	9:30-10:00	Detectors for Nuclear Resonant Scattering Experiments	Shunji Kishimoto	p.10
4	10:00-10:30	Some APD Detectors: Implementation and Application	Alfred Baron	p.11
		Coffee Break		
5	10:55-11:00	Status of ESRF	Aleksandr Chumakov	
6	11:00-11:30	Phonons at the Fe(110) Surface	Aleksandr Chumakov	p.12
7	11:30-12:00	Nuclear Inelastic Scattering Studies of Lattice Dynamics in Thermoelectric Materials	Raphael Hermann	p.13
8	12:00-12:30	High-Resolution Monochromators for High Energy Region	Yasuhiko Imai	p.14

12:30-13:45	Lunch break	
13:45-14:30	Facility tour	BL09XU, etc
14:30-17:25	Scientific Session	HOUKOUKAN

< Chair: Hisao Kobayashi >

9	14:30-15:00	High-Resolution Monochromators	Thomas Toellner	p.15
10	15:00-15:30	Phonon Density of States in $L1_0$-Type PtFe Thin Films	Yorihiko Tsunoda	p.16
		Coffee Break		

11	15:55-16:25	Nuclear Resonant Inelastic X-ray Scattering from ^{83}Kr	Jiyong Zhao	p.17
12	16:25-16:55	Nuclear Resonant Inelastic X-ray Scattering Studies of Kr Clathrate Hydrates	Dennis Klug	p.18
13	16:55-17:25	Recent Nuclear Resonant Inelastic Scattering Studies of Filled Skutterudites and Related Compounds	Satoshi Tsutsui	p.19

17:30-22:00 Banquet Hotel Seashore at Mitsu

May 15, 2007 (Tue)

9:00-12:00 Scientific Session HOUKOUKAN

< Chair: Shunji Kishimoto >

14	9:00-9:30	Vibrational Studies of Single Crystal Biological Model Compounds	Ercan Alp	
15	9:30-10:00	Nuclear Resonant Vibrational Spectroscopy (NRVS) of Nitrogenase and Hydrogenase	Stephen Cramer	p.20
		Coffee Break		
16	10:25-10:30	Status of APS	Wolfgang Sturhahn	
17	10:30-11:00	Geophysics Studies with Nuclear Resonant Spectroscopy	Wolfgang Sturhahn	p.21
18	11:00-11:30	Vibrational Properties on $CuFeS_2$ Under High Pressure	Hisao Kobayashi	p.22
19	11:30-12:00	Discussion & Closing Remarks		

12:00-16:00 Optional Excursion (Lunch included) Engyoji Temple in Mt. Shosha

Research Project on Nuclear Resonant Scattering in Japan

M. Seto[1,2,3]

[1]*Research Reactor Institute, Kyoto University, Kumatori-cho, Sennan-gun, Osaka 590-0494*

[2]*Japan Atomic Energy Agency, Sayo-cho, Sayo-gun, Hyogo 679-5148*

[3]*CREST, Japan Science and Technology Agency, Kawaguchi, Saitama 332-0012*

Recently, the advent of third generation synchrotron radiation sources permitted us to use high-quality X rays, which cannot be obtained with previous X-ray sources. We, therefore, started a research project titled “Studies on nuclear resonant scattering methods for materials science”, which is performed in the program of CREST (Core Research for Evolutional Science and Technology) of JST (Japan Science and Technology Agency). In this research, we develop advanced nuclear resonant scattering methods and instruments such as high-resolution monochromaters, detectors for high-energy regions, nuclear monochromaters generating high-intensity X-rays with the order of neV width. Using the methods, precise element- and site-specific studies on multi-extreme conditions, nano-materials, ultra-trace constituents in materials can be performed.

Present Status of Nuclear Resonant Scattering beamline, BL09XU at SPring-8

Yoshitaka Yoda[1,2]

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10 years has passed since the nuclear resonant scattering beamline BL09XU in SPring-8 started its operation in October 1997. The CREST project headed by Prof. Seto has started from the autumn of 2005. Target research of its project in JASRI/SPring-8 is "Development of advanced optics for nuclear resonant scattering". The following activities supported by the CREST project will be discussed in my talk.

1. New experimental hutch build last winter
2. Liquid nitrogen cooled high heat-load monochromator
3. High resolution monochromators

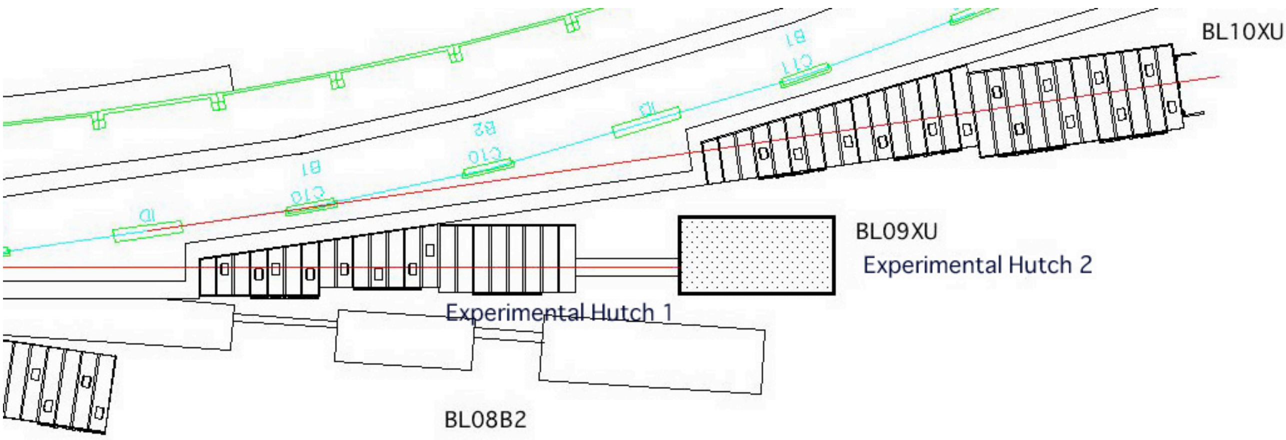

Figure The new experimental hutch built after the first experimental hutch.

Detectors for nuclear resonant scattering experiments

Shunji Kishimoto[1,2]
[1]Photon Factory, High Energy Accelerator Research Organization
[2]CREST/JST

Silicon avalanche-photodiode (Si-APD) timing detectors have been developed for nuclear resonant scattering using synchrotron X-rays. The Si-APD detector shows a good time resolution of 50 ps to 1 ns, and a wide dynamic range of count-rate, 10^9 -10^{10}. Nuclear resonant scattering using synchrotron X-rays is now extending its application to a higher energy region of nuclear levels. However, due to a small photoabsorption cross section of Si (Z=14) at energies higher than 10 keV, the detector efficiency sharply decreased to less than 1% for a 100-μm thick APD at 50 keV, for example. To improve the efficiency for a high-energy photon, we can use Si-APDs with a stacked and/or inclined arrangement. A scintillation detector with a fast light-emission is also expecting for timing measurements. In scintillators by exciton recombination in semiconductors, the lead-halide based perovskite-type organic-inorganic hybrid compound has a sub-nanosecond decay component and a relatively high light output, about 10% of NaI(Tl), even at room temperature. We are now investigating its property with synchrotron X-rays. The results in the test measurements will be presented at the workshop.

APD Detectors: Implementation and Applications

Alfred Q.R. Baron
SPring-8: RIKEN & JASRI

The use of APD detectors will be discussed both in general [1] and in the context of two recent applications [2][3]. The general comments focus on the need for multi-element detectors, and, the electronics to handle many channels in parallel. Several detectors will be described (including 8 and 16 element detectors), and the present status of work in collaboration with the ESRF [4]. The talk will then focus on applications, including nuclear inelastic scattering with ^{201}Hg [2] which has a very short (< 1ns) lifetime and nuclear forward scattering and relaxation in Dy spin-ice where the hyperfine beat frequency becomes rather fast (beat periods < 1ns) [3].

[1] A. Q. R. Baron, S. Kishimoto, J. Morse, and J.-M. Rigal, Journal of Synchrotron Radiation **13**, 131 (2006).

[2] D. Ishikawa, A. Q. R. Baron, and T. Ishikawa, Physical Review B **72**, 140301(R) (2005).

[3] J. P. Sutter, S. Tsutsui, R. Higashinaka, Y. Maeno, O. Leupold, and A. Q. R. Baron, Physical Review B **75**, 140402(R) (2007).

[4] T. Deschaux and the Nuclear Resonance Group.

Phonons at the Fe(110) surface

T. Ślęzak,[1,2] J. Łażewski,[3] S. Stankov,[4] K. Parlinski,[3] R. Reitinger,[5] M. Rennhofer,[5] R. Rüffer,[4] B. Sepiol,[5] M. Ślęzak,[2] N. Spiridis,[1] M. Zając,[2] A. I. Chumakov,[4] R.Röhlsberger[6], M.Sladecek[5], G.Vogl,[5] and J. Korecki.[1,2]

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[4] *European Synchrotron Radiation Facility, BP220, F-38043 Grenoble, France*

[5] *Scattering and Spectroscopy group, Faculty of Physics, University of Vienna, A-1090 Wien, Austria*

[6]*Deutsches Electronen Synchrotron DESY, Notkestr. 85, 22607 Hamburg, Germany*

We studied atomic vibrations of a clean Fe (110) surface. The samples were prepared, characterized, and measured *in situ* in ultra-high vacuum conditions. The density of phonon states $g(E)$ was measured separately for the first, second, and further atomic monolayers using nuclear inelastic scattering of synchrotron radiation.

The results show that atoms of the first layer vibrate with frequencies significantly lower and amplitudes much larger than those in the bulk. Furthermore, the surface atoms reveal a remarkable difference in vibrational spectra along two perpendicular in-surface directions. These vibrational anomalies are localized strictly on the surface, i.e., the vibrations of the second monolayer are already very close to those of the bulk. The softening of vibrations does not change the Debye-like behavior $g(E) \propto E^2$ of the DOS at low energies.

The experimental observations are in excellent agreement with the first principles calculations. Strong enhancement of the surface DOS at low frequencies arises from the surface phonon modes and from an overall softening due to missing neighbors. The broken translational symmetry along the surface normal is reflected as in plane anisotropy of elastic properties.

Nuclear inelastic scattering studies of lattice dynamics in thermoelectric materials

R. P. Hermann

Institut für Festkörperforschung, Forschungszentrum Jülich GmbH, D-52425 Jülich, Germany

Measurements of the phonon density of states in thermoelectric material have significantly contributed to our understanding of the origin of the low lattice thermal conductivity of these materials. Inelastic neutron scattering and heat capacity measurements were the first techniques to validate the "rattling" atom concept that is a cornerstone in this understanding. These measurements were then complemented by a determination of the element specific density of states by nuclear inelastic scattering. We have carried out phonon DOS measurements at the ^{151}Eu, ^{121}Sb, and ^{57}Fe nuclear resonances. The results from these measurements on $EuFe_4Sb_{12}$, $Eu_8Ga_{16}Ge_{30}$, and Zn_4Sb_3 will be presented in parallel with inelastic neutron scattering results.
[The European Synchrotron Radiation Facility is acknowledged for provision of the synchrotron radiation facility at beamlines ID18 and ID22N. The European Community - Access to Research Infrastructure action of the Improving Human Potential Programme HPRI-2001-00175 is acknowledged for provision of neutron scattering beam time at the FRJ-II research reactor in Jülich, Germany.]

High-Resolution Monochromators for High Energy Region

Yasuhiko Imai [1,2], Makoto Seto [2,3], Yoshitaka Yoda [1,2], Shinji Kitao [2,3], Ryo Masuda [2,3], Satoshi Higashitaniguchi [2,3], Chika Inaba [2,3]

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[3] *Research Reactor Institute, Kyoto University, Kumatori-cho, Sennan-gun, Osaka 590-0494, Japan*

High-resolution monochromators (HRMs) for Mössbauer nuclei with excitation energies less than 30 keV have been developed successfully using high angle diffractions by silicon crystals. The widely used silicon crystal, however, is not suitable for high efficient HRM at higher energy region because of the high symmetry of the crystal structure and the low Debye temperature. The high symmetry of the crystal structure gives a small number of permitted diffraction planes due to the extinction rule, which make it difficult to select a diffraction plane that has a Bragg angle near $\pi/2$ at a specific energy of X-ray. The low Debye temperature gives a low Debye-Waller factor at a high Bragg angle, and so a reflectivity becomes low even at low temperature. Therefore, the other crystals having a low symmetry of a crystal structure, a high Debye temperature and a high perfection are required for HRMs at high energy region. An α-sapphire is the most promising crystal. Consequently, quality assessment of a α-sapphire crystal has been performed in order to find better crystals and achieve better energy resolutions.

We have developed a HRM for nuclear resonant scattering (NRS) of synchrotron radiation by Te-125 at 35.49 keV using the backscattering of α-sapphire (9 1 -10 68). We used a high quality α-sapphire and controlled its temperature around 217 K to diffract synchrotron radiation with a Bragg angle of $\pi/2 - 0.5$ mrad at NRS beamline BL09XU, SPring-8. The energy was tuned by changing the crystal temperature under the condition of the constant diffraction angle. We will report on the quality of the α-sapphire and experimental results.

High-Resolution Monochromators

Thomas S. Toellner

Advanced Photon Source, Argonne National Laboratory

An high-resolution monochromator is an essential component of nuclear resonant scattering measurements. Significant developments have occurred over recent years that allow the construction of 1 meV monochromators with good efficiency. These developments include weak-link mechanical assemblies, cryogenic stabilization, and novel crystal configurations. A variety of high-resolution monochromators employing different designs will be presented along with their measured performances. Prospects for future improvements in energy resolution will also be discussed.

This work is supported by the U.S. Department of Energy under contract no. W-31-109-Eng-38.

Phonon Density of States in L1_0-type PtFe thin films

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[2]*Japan Atomic Energy Agency, Kouto, Mikazuki-cho, Sayo-gun, Hyogo 678-5198*

L1_0-type PtFe thin films are considered to be an excellent candidate for ultra-high density magnetic recording media because of their distinctive features such as a large magnetic anisotropy energy, large saturation magnetization and high Curie temperature. To study characteristic feature of the thin films, phonon density of states of the L1_0-type PtFe alloy thin films was studied using nuclear resonance inelastic scattering method and the results were compared with those for a bulk single crystal and disordered powder samples. Phonons of the thin films are softer than those of bulk sample by about 15 % and atomic order parameter of the PtFe thin films prepared by the present method show smaller value than that of the furnace cooled bulk sample. The Debye temperature of Fe atom in the PtFe alloy is estimated to be about 110 K. Phonons of PtFe alloy seem to have nothing to do with the anomalous lattice contraction of the c-axis at high temperature.

Nuclear resonant inelastic x-ray scattering from ^{83}Kr

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Abstract

We have extended the technique of nuclear resonant inelastic x-ray scattering to the 9.4035-keV nuclear transition of ^{83}Kr at 3-ID beamline of the Advanced Photon Source. A 4-bounce, “in-line”, high energy-resolution monochromator with energy resolution of 1-meV has been developed using Si (8 0 0) reflections. This is combined with a microfocusing K-B optics for the experiments at high pressure using diamond anvil cell technique. Phonon density of states of ^{83}Kr has been measured on solid Kr under high pressures up to 46 GPa. Furthermore, vibrational properties of Kr-clathrate at low temperatures and under high pressures have been studied by nuclear resonant inelastic scattering and molecular-dynamics simulations. Results will be discussed during the presentation.

This work is supported by US DOE-BES Materials Science under contract number W-31-109-ENG-38.

Nuclear Resonant Inelastic X-ray Scattering Studies of Kr Clathrate Hydrates

Dennis D. Klug, John S. Tse, J.Y. Zhao, W. Sturhahn, and E.E. Alp

The understanding of the glass-like thermal conductivity of clathrate hydrates has been a subject of numerous practical and fundamental research studies. The role of the guest atoms or molecules in the clathrate hydrate in the thermal conductivity has been intensively studied by both theoretical and experimental methods. Recently it has been shown to be possible to study the dynamics both the clathrate structures stable at low pressures and also the phases that occur at high pressures. The nuclear resonant inelastic x-ray scattering method is ideal for characterization of the dynamics of the guest atom such as Kr since the method can yield the phonon densities of states for the Kr atoms. We present here our experimental and theoretical results on structures and dynamics of both the low-pressure and high pressure clathrate structures including recent variable temperature studies on the high pressure structure H clathrate as obtained at the Advanced Photon Source.

Recent Nuclear Resonant Inelastic Scattering Studies of Filled Skutterudites and Related Compounds

Satoshi Tsutsui

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Filled skutterudites are a member of clathrates with a cage structure. The presence of a localized mode has been discussed with many experiments [1-6]. However, most of experiments are indirect observations based on an Einstein model. Nuclear resonant inelastic scattering (NRIS) is only an experimental technique to measure an element specific phonon density of states directly [7]. In this sense, we can conclude that NRIS is a powerful tool to discuss the presence of localized modes.

We have carried out the NRIS of filled skutterudites and related materials for recent years. We have measured the NRIS spectra of Sm-filled skutterudites. The frequency of the Einstein-like modes shows the cage size and/or electronic state dependences [8]. The ^{149}Sm and ^{57}Fe NRIS results demonstrate the strong hybridization between the Einstein-like modes due to Sm atoms and acoustic contribution due to Fe atoms in $SmFe_4P_{12}$ [9]. We have observed a dip structure in ^{57}Fe NRIS at the same energy where the excitation due to the Sm atomic vibration is observed by ^{149}Sm NRIS. This is different from the reported results in $EuFe_4Sb_{12}$ using ^{151}Eu and ^{57}Fe NRIS [5]. Recently, we succeeded in the ^{121}Sb NRIS [10]. We have obtained the ^{121}Sb NRIS spectrum as well as ^{149}Sm and ^{57}Fe ones in $SmFe_4Sb_{12}$. Unlike the results of $SmFe_4P_{12}$, the NRIS results agree with the previous results in $EuFe_4Sb_{12}$ [5, 8].

References

[1] V. Keppens *et al*., Nature **395**, 876 (1997).
[2] R. P. Hermann *et al*., Phys. Rev. Lett. **90**, 135505 (2003).
[3] D. Cao *et al*., Phys. Rev. B **70**, 094109 (2004).
[4] E. Matsuoka *et al*., J. Phys. Soc. Jpn. **75**, 014602 (2006).
[5] G. J. Long *et al*,. Phys. Rev. B **71**, 14302 (2005).
[6] C. H. Lee *et al*., J. Phys. Soc. Jpn. **75**, 123602 (2006).
[7] M. Seto *et al*., Phys. Rev. Lett. **74**, 3828 (1995)
[8] S. Tsutsui *et al*., Physica B **383**, 142 (2006).
[9] S. Tsutsui *et al*., Hyperfine Interact. **168**, 1073 (2006).
[10] S. Tsutsui *et al*., submitted to J. Phys. Soc. Jpn.

Nuclear Resonant Vibrational Spectroscopy (NRVS) of Nitrogenase & Hydrogenase

Stephen P. Cramer, [1,2] **Yuming Xiao**, [1] **and Yisong Guo**[1]

[1]*Department of Applied Science, University of California, Davis, CA 95616*
[2]*Physical Biosciences Division, LBNL, Berkeley, CA 94720*

Our NRVS work at SPring-8 is focused on two critical enzymes – nitrogenase (N_2ase), which catalyzes the reduction of dinitrogen to ammonia, and hydrogenase (H_2ase), which catalyzes the evolution (or consumption) of dihydrogen. Nature has evolved multiple Fe-based metalloenzymes that accomplish these tasks, both with and without the assistance of a second metal (Mo, V, Ni) at the active site. N_2 fixation is the key step in the nitrogen cycle, and this biological ammonia synthesis is responsible for about half of the protein available for human consumption. H_2 catalysis is crucial for the metabolism of many anaerobic organisms, and knowledge about the mechanism of H_2 evolution may prove critical for a future 'H_2 economy'. I will present NRVS data on small molecule model compounds and the enzymes N_2ase and H_2ase, along with analyses using empirical force fields as well as DFT methods. The interaction between protein diffraction and spectroscopy will be discussed. I will finish with some discussion of what we could do with more spectral brightness.

Geophysics Studies with Nuclear Resonant Spectroscopy

Wolfgang Sturhahn

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Nuclear resonant scattering techniques at third generation synchrotron radiation facilities opened new opportunities for the study of vibrational and magnetic properties of condensed matter in research areas like geophysics, biophysics, and nano-science. In particular, the determination of the vibrational density of states with nuclear resonant inelastic x-ray scattering (NRIXS) and the study of valences and magnetic properties with synchrotron Mössbauer spectroscopy (SMS) provided remarkable results [1].

In this contribution, we discuss the combination of nuclear resonant spectroscopy with diamond anvil cell technology and its impact on the geoscientific area. We will specifically address NRIXS, a method that uses probe nuclei with suitable resonances to measure the vibrational density of states, and SMS for the determination of valences, spin states, and magnetic ordering analogous to conventional Mössbauer spectroscopy. The sensitivity of these methods in combination with the isotope selectivity allowed NRIXS and SMS investigations on materials under pressures in the mega-bar regime using diamond anvil cells and Laser heating.

Nuclear resonant spectroscopy under extreme conditions is a key method to provide sound velocities and elasticity on iron, iron alloys, and iron oxides [2,3], to study valence and high-spin to low-spin transitions in lower mantle minerals [4,5,6], and to investigate melting of iron-bearing materials [7]. Examples will illustrate the present and potential future use of nuclear resonant spectroscopy in the Earth and planetary sciences.

Even though ^{57}Fe has spawned the largest interest so far, we will review the selection of other suitable nuclear resonances that could become important for future applications. Nuclear resonant spectroscopy methods, which include NRIXS and SMS, continue to evolve with the development of new instrumentation, the improvement of synchrotron radiation sources, the increased diversity in nuclear resonant methods, and the synergy with other experimental techniques like x-ray diffraction, inelastic x-ray scattering, and x-ray fluorescence analysis. We will speculate about their potential impact on the experimental realizations and the applications of nuclear resonant spectroscopy.

This work is supported by the U. S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

References

[1] Sturhahn W. (2004) J. Phys.: Condens. Matter 16**,** S.
[2] Mao H.-K. et al. (2001) Science **292**, 914.
[3] Lin J.-F. et al. (2005) Science **308**, 1892.
[4] Jackson J.M. et al. (2005) American Mineral. **90**, 199.
[5] Lin J.-F. et al. (2006) Phys. Rev. B **73**, 113107.
[6] Lin J.-F. et al. (2006) Geophys. Res. Lett. **33**, L22304.
[7] Jackson J.M., Sturhahn W. et al. (in preparation).

Vibrational properties on $CuFeS_2$ under high pressure

Hisao Kobayashi, University of Hyogo, 3-2-1 Koto Hyogo 678-1297, JAPAN

An insulator-metal transition is one of the interesting properties in strongly correlated electron systems. At ambient pressure, $CuFeS_2$ is an antiferromagnetic semiconductor. As indicated by high-pressure resistivity measurements at room temperature, it undergoes the insulator-metal transition at 6.5 GPa with increasing pressure. Furthermore, the antiferromagnetic order disappears at this transition.

In the present study, we have measured X-ray diffraction and ^{57}Fe nuclear resonant inelastic scattering (NRIS) of $CuFeS_2$ under pressure using synchrotron radiation at SPring-8. The X-ray diffraction data were collected at room temperature with angle-dispersive techniques and an image-plate detector on BL10XU. For ^{57}Fe NRIS, the pulsed synchrotron radiation was monochromatized by the high-resolution monochromator on BL09XU. The ^{57}Fe NRIS spectra were measured by tuning the highly monochromatized X-ray beam in an energy range of about 80 meV.

Since a halo-like pattern is observed in the X-ray diffraction data above 6.3 GPa, $CuFeS_2$ undergoes a pressure-induced crystal-amorphous transition. ^{57}Fe NRIS spectra under pressure consist of large center peaks originating from elastic scattering and sidebands resulting from inelastic scattering with the annihilation and creation of phonons. The inelastic components in the spectra extract lead to the partial phonon densities of states (DOS) assuming a harmonic lattice model. There are three peaks at 10, 22 and 43 meV in the extracted partial phonon DOS below 6.0 GPa. It is noteworthy that the peak at around 10 meV in the phonon DOS stays almost unchanged up to 6.0 GPa.