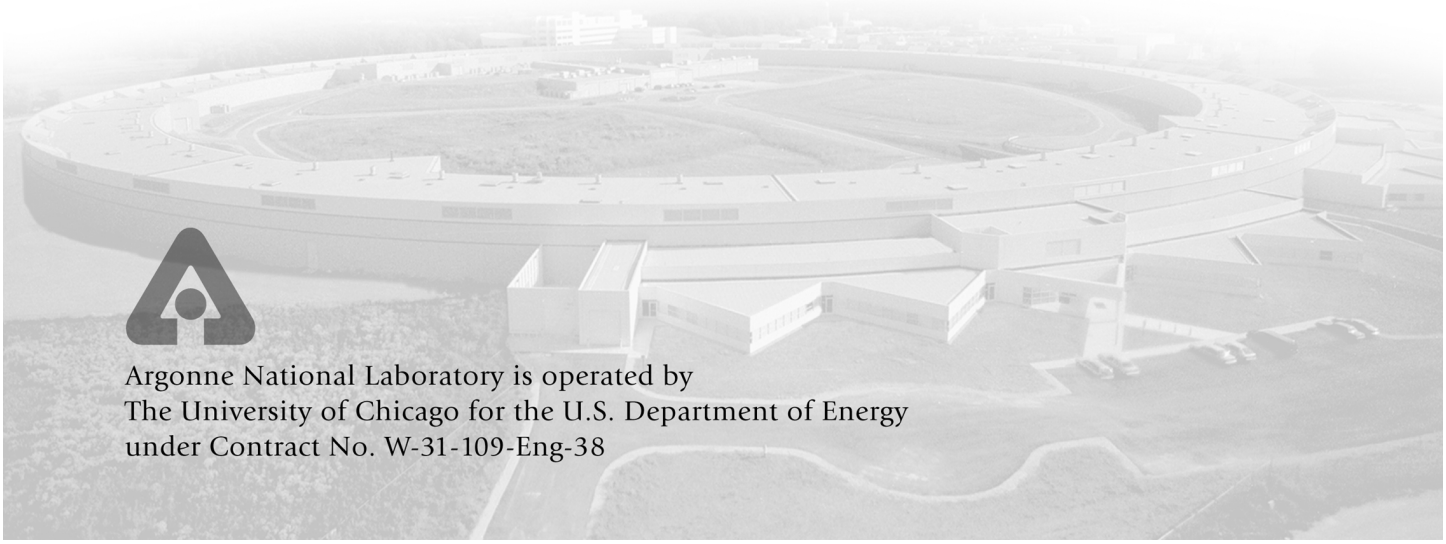
ixs2004

5th International
Conference on

Inelastic X-Ray Scattering

Program/Abstracts Book

September 19-24, 2004
Advanced Photon Source
Argonne National Laboratory
Argonne, Illinois USA



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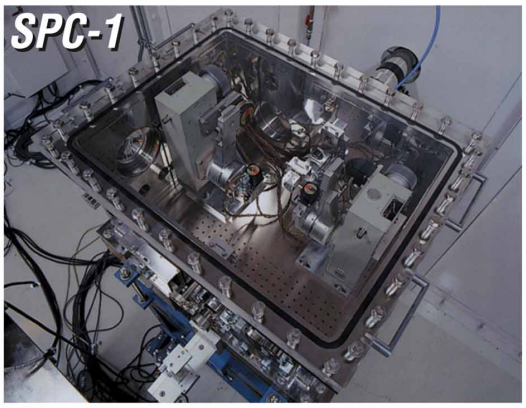

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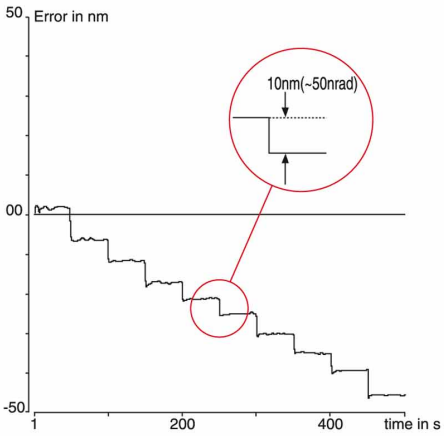
KTG-31 Measurement data



KTG-31 angular increments were measured using a laser interferometer. 10 nm graph displacements correspond to 50 nrad angular increments.

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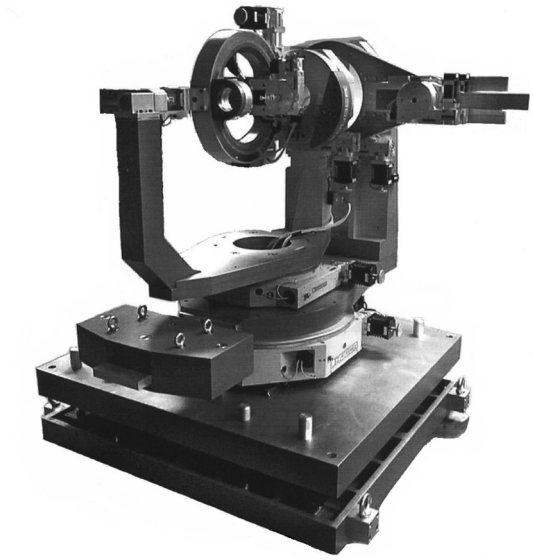

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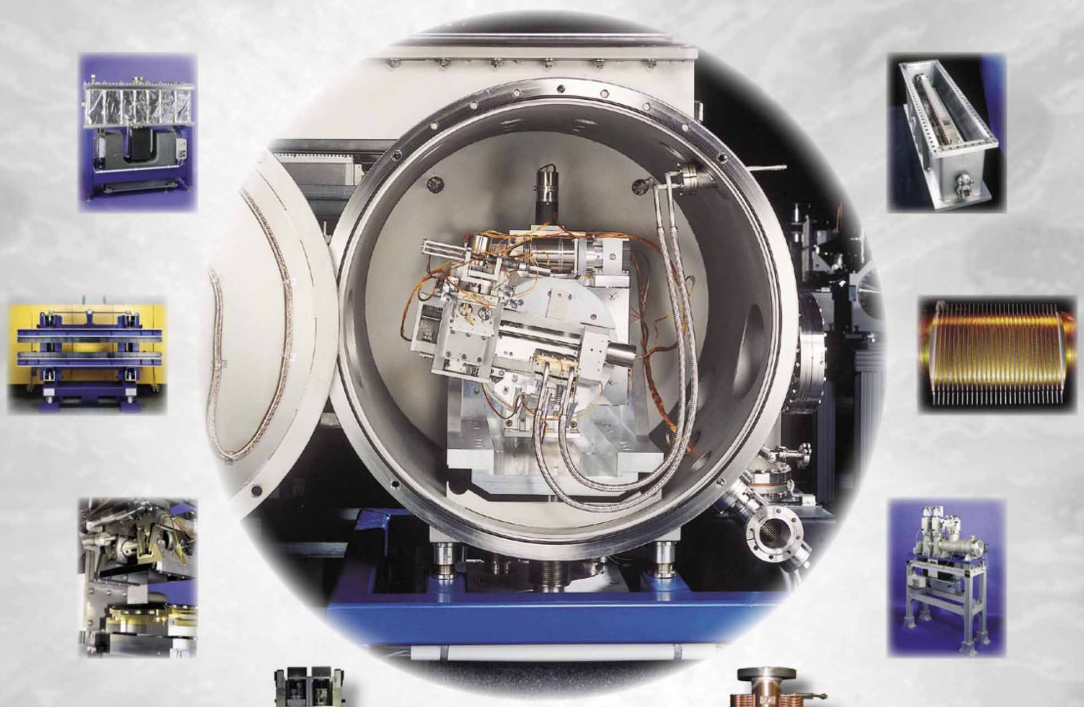

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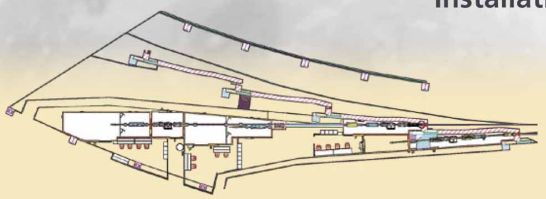

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Comprehensive Program

SUNDAY, SEPTEMBER 19, 2004

7:00 pm **Informal welcome reception**
Argonne Guest House

MONDAY, SEPTEMBER 20, 2004

8:00 am **Registration**

Session 1

Chair: *M. Klein*

8:30 am-8:45 am **Welcome remarks**

8:45 am-9:20 am **Steps in the right direction: IXS on the way between Haikko and Argonne**
Winfried Schuelke, University of Dortmund (emeritus)

9:20 am-9:40 am **Inelastic x-ray scattering in x-ray and neutron sources: DOE perspective**
Pedro Montano, Department of Energy

9:40 am-10:00 am **Coffee break**

Session 2

Chair: *P. Montano*

10:00 am-10:40 am **Theory of correlated electron systems**
G. Kotliar, Rutgers University

10:40 am-11:10 am **Magnetic Compton Scattering as a probe of correlated electron materials**
A. Bansil, Northeastern University

11:10 am-11:40 am **Theory of RIXS in strongly correlated electron systems**
S. Maekawa, Tohoku University

11:40 am-12:10 pm **RIXS Studies of Charge Neutral Excitations in Cuprates**
John Hill, Brookhaven National Laboratory

12:10 pm-1:30 pm **Lunch**

Session 3

Chair: *J. Mizuki*

1:30 pm-2:00 pm **Hole concentration and temperature dependence of Mn 3d orbital state in bilayer manganites: A Magnetic Compton scattering study**
A. Koizumi, University of Hyogo

2:00 pm-2:30 pm **Investigation of phonons in superconductors by IXS**
A. Baron, Spring-8/JASRI, Hyogo

2:30 pm-2:50 pm **RIXS study of hole doped manganites**
K. Ishii, Spring-8/JASRI, Hyogo

2:50 pm-3:10 pm **RIXS in manganites**
S. Grenier, Brookhaven National Laboratory

3:10 pm-3:30 pm **Break**

Session 4

Chair *M. van Veenendaal*

3:30 pm-4:00 pm	**Resonant Inelastic X-Ray Scattering and its MCD** *A. Kotani, RIKEN/Spring-8 and Photon Factory/KEK*
4:00 pm-4:30 pm	**Correlation functions measured in indirect resonant IXS** *J. van den Brink, Leiden University*
4:30 pm-5:00 pm	**Dynamical structure factor of correlated materials** *A. Eguiluz, University of Tennessee*
6:00 pm	**Dinner**

TUESDAY, SEPTEMBER 21, 2004

Session 5

Chair: *D. Price*

9:00 am-9:30 am	**Liquid dynamics in high melting materials** *Harald Sinn, APS, Argonne National Laboratory*
9:30 am-10:00 am	**Fragility of liquids or fragility of glasses?** *Tullio Scopigno, University of Roma, La Sapienza*
10:00 am-10:30 am	**Anomalous vibrational properties of disordered solids** *Walter Schirmacher, Technical University of Munich*
10:30 am-10:50 am	**Break**

Session 6

Chair: *U. Bergmann*

10:50 am-11:20 am	**The local structure of water from ambient to supercritical conditions: New insight from X-Ray Raman scattering** *Philippe Wernet, BESSY*
11:20 am-11:50 am	**Compton scattering on water and aqueous solutions** *Keijo Hamalainen, University of Helsinki*
11:50 am-12:20 pm	**Observation of fast sound in metal-nonmetal transition in liquid Hg** *Masanori Inui, University of Hiroshima*
12:20 pm-2:00 pm	**Lunch**

Session 7

Chair: *A. Chumakov*

2:00 pm-2:30 pm	**Nuclear resonant inelastic x-ray scattering** *Wolfgang Sturhahn, APS, Argonne National Laboratory*
2:30 pm-3:00 pm	**Vibrational density of states of amorphous binary alloy films** *Werner Keune University of Duisburg-Essen*
3:00 pm-3:30 pm	**Molecular rotations studied by nuclear resonant scattering** *Tanja Asthalter, University of Stuttgart*
3:30 pm-4:00 pm	**X-Ray Raman scattering on Si L edge of Si and amorphous SiO** *C. Sternemann, University of Dortmund*
4:00 pm -5:30 pm	**POSTER SESSION**
6:00 pm	**Dinner**

WEDNESDAY, SEPTEMBER 22, 2004

Session 8

Chair: *G. Shenoy*

9:00 am-9:30 am	**Advances in nuclear inelastic scattering** *A. Chumakov, ESRF*
9:30 am-10:00 am	**Vibrational density of states in proteins and its model compounds** *T. Sage, Northeastern University*
10:00 am-10:30 am	**Protein dynamics on different timescales** *F. Parak, Technical University of Munich*
10:30 am-11:00 am	**Break**

Session 9

Chair: *S. Durbin*

11:00 am-11:30 am	**Nuclear resonant vibrational spectroscopy of Fe-S proteins** *S. Cramer, University of California, Davis*
11:30 am-12:00 pm	**IXS studies of phonons in liquid crystalline DNA with different counter-ion atmospheres** *S. H. Chen, MIT*
12:00 pm-12:30 pm	**Dynamics of liquids** *Marie-Louise Saboungi, CNRS-Orleans, France*
12:30 pm-2:00 pm	**Lunch**
2:00 pm	**Excursion to Chicago River, Lake Michigan, and the Millennium Park**
	After dinner guest: *Murray Gibson, Director of the APS*

THURSDAY, SEPTEMBER 23, 2004

Session 10

Chair: *D. Häusermann*

9:00 am-9:30 am	**Electronic properties of transition-metal oxides at extreme conditions** *J.P. Rueff, University of Paris*
9:30 am-10:00 am	**Anisotropy in elastic properties of hcp iron under high pressure** *G. Wortmann, Paderborn University*
10:00 am-10:30 am	**IXS in alkali metals under high pressure: phonons and bulk plasmons** *K. Syassen, MPI Stuttgart*
10:30 am-11:00 am	**Break**

Session 11

Chair: *M. Krisch*

11:00 am-11:30 am	**Resonant scattering in clathrate hydrates** *J. Tse, National Research Council –Ottawa /University of Saskatchewan*
11:30 am-12:00 pm	**Pressure induced phase transitions in FeS via nuclear resonant IXS** *H. Kobayashi, Hyogo University*
12:00 pm-12:30 pm	**Phonon density of states in Kr up to 46 GPa** *J. Zhao, APS, Argonne National Laboratory*
12:30 pm-2:00 pm	**Lunch**

Session 12

Chair: *H. Kawata*

2:00 pm-2:30 pm	**X-Ray Raman Scattering in high pressure research** *P. Eng, University of Chicago/CARS*
2:30 pm-3:00 pm	**IXS at from electronic excitations** *Y. Cai, NSRC-Hsinchu,Taiwan/Spring-8*
3:30 pm-4:00 pm	**Advances in magnetic and high resolution Compton scattering** *Y. Sakurai, JASRI-Spring-8*
4:00 pm-4:30 pm	**Recent results of phonon studies at ESRF** *M. Krisch, ESRF*
4:30 pm-5:30 pm	**POSTER SESSION**
6:00 pm-7:00 pm	**Dinner**

Session 13

Chair: *K. Hamalainen*

7:00 pm-7:30 pm	**High energy photoemission spectroscopy** *C. Dallera, Politecnico di Milano*
7:30 pm-8:00 pm	**Multiple scattering approach to x-ray Raman scattering** *A. Soininen, University of Helsinki*
8:00 pm-8:30 pm	**Reconstruction of Fermi surface from high resolution Compton data** *N. Shiotani, Photon Factory, KEK-IMSS*
8:30 pm-9:00 pm	**Dyson orbitals, quasi-particle effects and Compton Scattering** *B. Barbellini, Northeastern University*

FRIDAY, SEPTEMBER 24, 2004

Session 14

Chair: *G. Srajer*

9:00 am-9:30 am **Electronic environment of $LiFePO_4$ and $FePO_4$ probed with soft x-ray inelastic scattering**
A. Moewes, University of Saskatchewan

9:30 am-10:00 am **High resolution soft X-ray inelastic scattering at the ALS**
Z. Hussain, ALS, Lawrence Berkeley National Laboratory

10:00 am-10:30 am **New light for electronic excitations in 3*d* transition metal systems: High-resolution L_3-edge RIXS**
G. Ghiringhelli, Politecnico de Milano

10:30 am-11:00 am **Break**

Session 15

Chair: *A. Macrander*

11:00 am-11:30 am **Advances in high resolution monochromators**
T. Toellner, APS, Argonne National Laboratory

11:30 pm-12:00 pm **IXS spectroscopy below 10 keV with meV resolution**
Y. Shvydko, Physikalisch-Technische Bundesanstalt (PTB)

12:00 pm-12:30 pm **Advances in crystal analyzers for IXS**
R. Verbeni, ESRF

12:30 pm-2:00 pm **Lunch**

Session 16

Chair: *R. Simmons*

2:00 pm-2:30 pm **Imaging electronic motion with attosecond time resolution**
P. Abbamonte, Brookhaven National Laboratory

2:30 pm-3:00 pm **Compton Scattering: is it still gathering momentum?**
M. Cooper, University of Warwick

3:00 pm-3:30 pm **Future sources for inelastic x-ray scattering**
D. Moncton, MIT

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Invited Talks

Steps in the right direction: IXS on the way between Haikko and Argonne

W. Schuelke
Institute of Physics, University of Dortmund, Germany

An overview of significant contributions in the field of inelastic x-ray scattering (IXS), done within the last three years, is presented. In the Compton regime of charge scattering, papers are highlighted, which open new ways for analyzing bonds in condensed matter and which can help to solve the problems of how electron correlation has properly to be taken into account. Reconstruction of 3D momentum density is more and more placed in the foreground. Magnetic Compton scattering has shown its ability for distinguishing the population of *d*-orbitals of different symmetry upon phase transitions. In the IXS regime of valence electron excitations, experimental tests of calculations using different approaches for electron correlation called special attention. Nonresonant x-ray Raman scattering as a tool to get access to the *K* and *L* edges of low-Z elements found very interesting applications in the structural chemistry, where also the **q**-dependence has been utilized. In the field of resonant inelastic x-ray scattering (RIXS), it is the Mott-gap excitations and their dispersion, especially on orbital-ordered substances, which attracted considerable attention. Ultra-high-resolution IXS has found a wide field of applications both in the analysis of liquids, glasses and in phonon dispersion. The high-pressure applications make this method especially exciting.

Inelastic x-ray scattering in x-ray and neutron sources: DOE perspective

P. Montano
Scientific User Facility Division, Basic Energy Sciences, U.S. Department of Energy, Washington DC, USA

The U.S. Department of Energy operates four synchrotron radiation sources and is constructing a fourth-generation x-ray source at SLAC. Synchrotron radiation has revolutionized our understanding of many physical phenomena. Complex many-body processes in condensed matter physics play a significant role in producing some of the remarkable properties that have been observed in high-temperature superconductors and colossal magnetoresistance. Angle-resolved photoemission using synchrotron radiation sources has provided crucial information needed to understand the many-body effects in highly correlated electronic systems. Techniques that utilize the polarization characteristics of the radiation have been used to gain fundamental understanding of magnetic coupling, orbital and spin contributions, and domain structure. The high brightness provided by third-generation synchrotron radiation sources has facilitated the performance of x-ray inelastic scattering measurements. Resonant inelastic x-ray scattering spectroscopy has provided a powerful tool to directly probe bands in complex materials that are not accessible by regular optical methods. Recently, great progress has been achieved using these techniques in understanding the electronic structure in Mott insulators. Applications of synchrotron radiation techniques to atomic and molecular physics have open new venues of research and provided deeper understanding of atomic and molecular phenomena. X-ray microscopy at third-generation synchrotron source is becoming an extremely important tool in characterizing nanometric structures in materials. There is now a growing interest in studying physical phenomena in the time domain. Research in the nanosecond and picosecond regimes is already possible at third-generation sources. Fourth-generation sources like x-ray free-electron lasers will deliver coherent radiation pulses in the femtosecond time domain. These sources will extend and broaden our technical capabilities to study dynamical phenomena in physics.

Theory of correlated electron systems

G. Kotliar
Dept. Physics and Astronomy, Rutgers University, Piscataway, NJ, USA

The electronic states in strongly correlated materials cannot be described by perturbation theory around free-electron systems. Instead, it requires a framework that describes atomic states and band states on equal footing, in real and momentum space. Dynamical mean field theory (DMFT) is a promising approach to describe correlated materials. We will review the main concepts of the method, how it can be used to describe the electronic structure of correlated materials, and how it can be used in conjunction with experimental probes (transport, photoemission and optical spectroscopy, and inelastic x-ray scattering), to gain new insights into the electronic structure of strongly correlated materials.

Magnetic Compton scattering as a probe of correlated electron materials*

A. Bansil
Physics Dept., Northeastern University, Boston, MA, USA

The magnetic Compton scattering technique is emerging as a powerful new spectroscopic window for understanding the properties of magnetic electrons in complex materials. Here we consider results on three correlated electron systems of current interest: The double-layer manganite $La_{(1.2)}Sr_{(1.8)}Mn_2O_7$, the perovskite manganite $La_{(0.7)}Sr_{(0.3)}MnO_3$ and the magnetite Fe_3O_4. First-principles band theory computations using the conventional local density approximation (LDA), as well as computations going beyond the LDA framework for treating correlation effects, are used to gain insight into recent magnetic Compton scattering measurements. We show how, in the double-layer manganite, the [110] magnetic Compton profile (MCP) contains a distinct signature of the *d* electrons of x^2-y^2 symmetry, allowing us to adduce significant changes in the occupancy of these orbitals as a function of temperature over the range of 5-200K. An itinerant electron contribution is suggested at all temperatures in magnetite; such a contribution also appears in $La_{(1.2)}Sr_{(1.8)}Mn_2O_7$, but seems to be present only at low temperatures in $La_{(0.7)}Sr_{(0.3)}MnO_3$.

*Work done in collaboration with B. Barbiellini, P.E. Mijnarends, S. Kaprzyk, P.A. Montano, Y. Li and J.F. Mitchell

Theory of RIXS in strongly correlated electron systems

S. Maekawa
Institute for Materials Research, Tohoku University, Sendai, Japan

High-temperature superconductivity in cuprates and colossal magnetoresistance in manganites occurs near the Mott insulating states. Therefore, the nature of the Mott gap and its carrier-doping dependence are of crucial importance to understanding the unique properties. Since carrier-doping causes the change of the electronic state in a wide energy range, resonant inelastic x-ray scattering (RIXS) provides an opportunity to study the Mott insulating states and the Mott transition. Here, I would like to present the theory of RIXS, in particular the *K*-edge RIXS, in strongly correlated electron systems. Recent experiments are discussed in the light of the theory.

RIXS Studies of Charge Neutral Excitations in Cuprates

J.P. Hill
Dept. Physics, Brookhaven National Laboratory, Upton, NY, USA

The cuprates are "charge-transfer" insulators, that is the lowest-lying excitations across the insulating gap involve movement of charge from the oxygen site to the copper site. Understanding the electronic properties of the cuprates will require understanding the behavior of such charge-transfer excitations. Resonant inelastic x-ray scattering, in which the incident photon energy is tuned to the copper *K* edge, probes the momentum and energy dependence of such excitations. In this talk, studies on a series of cuprates will be reported. At low energies (2-4 eV), the character of the excitations observed is found to depend strongly on both the dimensionality and connectivity of the CuO_4 sublattices, and the carrier concentration. Contrasts are drawn between one and two-dimensional behavior. For example, in 1D, excitations consistent with holon – antiholon pair creation are observed in a highly-dispersive continuum. Such a continuum is not seen in 2D. At higher energies (~ 6 eV), common features are observed in all cuprates and are associated with a localized molecular orbital excitation. Finally, the prospects for high-resolution (100 meV) work will be discussed.

Work performed at Brookhaven was supported by the US DOE contract no. DE-AC02-98CH10886. The author particularly wants to acknowledge his collaborator, Y-J. Kim in this work.

Hole concentration and temperature dependence of Mn 3*d* orbital state in bilayer manganites: A magnetic Compton scattering study

A. Koizumi,[1] T. Nagao,[1] Y. Kakutani,[1] N. Sakai,[1] T. Arima,[2] K. Hirota,[3] Y. Murakami[2]
[1]*University of Hyogo, Japan*
[2]*Tohoku University, Japan*
[3]*University of Tokyo, Japan*

Perovskite Mn oxides have been actively studied in relation to colossal magnetoresistance (CMR). Particularly, bilayer Mn perovskite $La_{2-2x}Sr_{1+x}Mn_2O_7$ is very attractive, because it shows much larger CMR than the base compound $La_{1-x}Sr_xMnO_3$. In manganites, the importance of the orbital degree of freedom is pointed out, as well as charge and spin. We have studied hole concentration and temperature dependence of magnetic Compton profiles (MCP) in bilayer manganites to directly investigate the Mn 3*d* orbital state from the viewpoint of orbital occupation. The occupation numbers in t_{2g} and two e_g type orbitals (x^2-y^2 and $3z^2$-r^2) of Mn 3*d* state are evaluated from the fitting analysis of MCPs measured on the [001] axis by using theoretical profiles derived from the *ab initio* calculations for an $(MnO_6)^{8-}$ cluster. The population in a $3z^2$-r^2 type orbital decreases with increasing hole doping, while that in a x^2-y^2 type orbital is stabilized at almost constant value. The e_g orbital state varies at T_c, and the change would be involved in the lattice distortion observed above T_c.

Investigation of phonons in superconductors by inelastic x-ray scattering

A.Q.R. Baron
SPring-8/JASRI, Hyogo, JAPAN

We investigate the phonon structure of several superconductors and its relationship to electron-phonon coupling (EPC) using inelastic x-ray scattering (IXS) [1-4]. In this context we rely on the small x-ray beam size, ~100 μm, to investigate similarly small crystals which cannot be investigated using inelastic neutron scattering. The relatively simple, but extreme, case of MgB_2, a conventional Eliashberg-type superconductor, demonstrates the ability of IXS to probe these subjects. In particular, the softening and broadening of the E_{2g} mode through the Kohn anomaly are clearly visible and in good agreement with *ab initio* calculations [1]. In contrast, in carbon doped samples, $Mg(B_{1-x}C_x)_2$, where T_c is reduced, we see hardening of the E_{2g} phonon, and the phonon dispersion comes to resemble that of AlB_2, which is not superconducting. These results provide beautiful confirmation of the present view of superconductivity in this material, including the extremely mode-specific EPC. The high T_c copper-oxide (HTSC) materials are more complicated, but the role of phonons in their superconductivity has received renewed attention recently due to photoemission and neutron work [5]: in particular there is speculation that the softening of the high-energy Cu-O breathing mode in these materials is related to the superconductivity. We observe this softening in optimally doped $La_{2-x}Sr_xCuO_4$ (LSCO, x~0.12) [3] and in optimally doped, de-twinned, $YBa_2Cu_3O_{7-\delta}$ (YBCO) [4], confirming previous neutron work on larger samples. In addition we show that the same softening appears in $HgBa_2CuO_{4+\delta}$ (Hg1201), [2] which has a simpler structure and higher T_c~93K, than the others. The presence of this softening in Hg1201 is important confirmation that it can generally be associated with hole-doped HTSC materials. These results will be discussed in the context of other recent work on HTSCs.

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Resonant inelastic x-ray scattering study of hole-doped manganites

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Resonant inelastic x-ray scattering (RIXS) has been expected to be a new experimental tool to measure electronic excitations of strongly correlated electron systems. In these systems, strong on-site Coulomb interaction separates a partially filled band into the occupied lower Hubbard band and the unoccupied upper Hubbard band, and the system becomes an insulator with a charge gap, known as the Mott gap, which is an important quantity for understanding their properties. A recent development of RIXS using the brilliant x-rays from a third-generation synchrotron and an apparatus with less than 500 meV energy resolution enables us to measure the excitation across the Mott gap with momentum resolution.

We will present recent work on hole-doped manganites focusing on the excitation between the Mott gap in comparison with the insulating $LaMnO_3$. Though interesting physical phenomena, such as high-T_c superconductivity and CMR, occur in the vicinity of metal-insulator transition by hole-doping to the Mott insulator, most of the RIXS work has been concentrated on insulators up to now. We have measured two hole concentrations, $La_{0.6}Sr_{0.4}MnO_3$ and $La_{0.8}Sr_{0.2}MnO_3$. The former has enough holes to be metallic. The latter shows a metal-insulator transition associated with a ferromagnetic transition near 300K, and it was measured across the transition temperature.

Resonant inelastic x-ray scattering in manganites

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We report the observation of temperature-dependent electronic excitations in various manganites utilizing resonant inelastic x-ray scattering (RIXS) at the Mn *K* edge. Excitations were observed between 1.5 and 16 eV with temperature dependence found as high as 10 eV. The change in spectral weight between 1.5 and 5 eV was found to be related to the magnetic order and independent of the conductivity. On the basis of LDA+U and Wannier function calculations, this dependence is associated with intersite d-d excitations. Finally, the connection between the RIXS cross section and the loss function is addressed.

Resonant inelastic x-ray scattering and its magnetic circular dichroism

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Two topics on magnetic circular dichroism in resonant inelastic x-ray scattering (MCD-RIXS) are presented. One is the interference effect in MCD-RIXS, and the other is the application of MCD-RIXS as a tool of high-resolution MCD in XAS (MCD-XAS). When the incident x-ray direction is perpendicular to the magnetization of the sample, we can observe a 100% interference process, where two x-ray transition paths via different intermediate states interfere each other. Detailed theoretical and experimental studies were made for the Gd L_3-$M_{4,5}$ MCD-RIXS with the electric dipole excitation of a Gd L_3 core electron in Gd compounds, and more recently a theoretical study has been made for the behavior of a similar MCD-RIXS with the electric quadrupole excitation for a Sm system.

When the incident x-ray direction is parallel to the magnetization, the MCD-RIXS includes no interference term. In this case, we calculate the L_3 MCD-XAS and the L_3-M_5 MCD-RIXS of $Lu_2Fe_{14}B$, $LuFe_2$ and $CeFe_2$, and show that the excitation spectrum of L_3-M_5 MCD-RIXS is very close to a less broadened version of the L_3 MCD-XAS. Therefore, the L_3-M_5 MCD-RIXS is a powerful tool to detect fine structures of L_3 MCD-XAS beyond the lifetime broadening of the L_3 core hole.

Correlation functions measured in indirect resonant IXS

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The cross section for indirect resonant inelastic x-ray scattering is expressed in terms of an intrinsic dynamic correlation function of the system that is studied with this technique. When the core-hole potential is local, this correlation function turns out to be a linear combination of the dynamic charge and the longitudinal spin density response functions. The relative contributions of these two response functions to the total spectral weight can be tuned by varying the energy of the incoming x-rays.

Dynamical structure factor of correlated materials

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Liquid dynamics in high-melting materials

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The transport properties of high-melting materials are of interest for a variety of applications, including geosciences, nuclear waste confinement and aerospace technology. While traditional methods of measuring transport properties are often extremely difficult due to the high reactivity of the melts, the combination of containerless levitation and inelastic x-ray scattering offers new insights in the microscopic dynamics of these liquids.

Data on the dynamic structure factor several high-temperature liquids including aluminum oxide, mullite, boron and supercooled silicon are presented.

Fragility of liquids or fragility of glasses?

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One of the most intriguing tasks of the physics of glasses is the understanding of how the interactions between the elemental constituents determine the phenomenology of the liquid-glass transition. Approaching this transition from the liquid side, different systems show qualitatively different temperature dependencies of the viscous flow. Accordingly, they have been classified by the useful concept of "kinetic fragility": the more "fragile" is a liquid the faster is the change in its viscosity on approaching the glass transition temperature T_g.

We report here an experimental observation relating the microscopic properties of the glassy phase to the kinetic fragility: we find that the vibrational properties in the glass *away* from T_g are correlated to the viscous flow in the liquid *approaching* T_g. More specifically, we observe that in a number of glass forming systems the steepness of the non ergodicity factor in the T=0 limit stands in a fashion similar to the Angell plot and, therefore, can be used to predict the kinetic fragility of the corresponding liquid. Consequently, we extend the fragility concept to the glassy state and indicate how to predict the fragility uniquely from glass properties far away T_g.

Translated into the language of the Potential Energy Landscape, this finding establishes a correlation between the inter-basin dynamics of the supercooled liquid, and the dynamics proceeding within a single inherent structure visited in the glassy phase.

Anomalous vibrational properties of disordered solids

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The vibrational spectra of disordered solids as revealed by inelastic light, neutron and x-ray-scattering show a spectacular anomalous behaviour if compared to their crystalline counterparts. The vibrational density of states strongly deviates from Debye's ω^2 law ("boson peak"), followed by a decrease according to $\omega^2 e^{-\omega/\omega_0}$. The boson peak anomaly can also be seen in the temperature dependence of the specific heat. Near the boson peak temperature, the thermal conductivity shows a characteristic plateau. It is shown that all these features can be explained by a model in which Debye-like waves encounter different values of the sound velocity at different locations of the material (elastic-constant disorder). This model is solved by a mean-field theory, which is derived by field-theoretical methods. The theory can be generalized to include anharmonic interactions. This yields a mode-coupling theory for the local dynamical susceptibility. From this theory, the temperature dependence of the density of states at elevated temperatures can be calculated. If the disorder is so strong that the system is almost unstable, the theory predicts an anomalous fractal frequency dependence of the dynamical susceptibility and the density of states.

The local structure of water from ambient to supercritical conditions: New insight from x-ray Raman scattering

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The structure of water is of paramount importance, and, although intensely investigated for various thermodynamical conditions during the past decades, it is being debated to date. In contrast to the condensed phase of ordinary hexagonal ice Ih with a well-known ordered crystal structure, the breaking and making of hydrogen bonds on a picosecond time scale in the liquid results in a fluctuating distribution of configurations that is still largely unknown. The hydrogen bonds not only determine water's structure, but they are also responsible for its striking set of anomalous physical and chemical properties. A new approach to the structure of water using x-ray Raman scattering and x-ray absorption spectroscopy at the oxygen *K* edge is presented. Different hydrogen-bonding configurations can be identified through the variation of the local orbital structure with hydrogen bonding by investigating the near-edge region of the spectra (NEXAFS, XANES). The results are interpreted with the aid of experimental model systems, such as bulk ice and the surface of ice, and with calculations based on density functional theory. This allows for a unique determination of local configurations in water at ambient conditions and at high temperatures and pressures up to the supercritical regime and reveals unprecedented insights into the local structure of water.

Compton scattering on water and aqueous solutions

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Compton scattering gives information on the electron momentum density of the target material. Although it has been known for long time that the Compton profile can give unique information on molecular bonding, this technique has not been widely utilized in the study of local molecular structure. We have started a systematic study on water and aqueous solutions concentrating especially on the structure and dynamics of the hydrogen bond under different external conditions. These include temperature, water-to-ice phase transition, and isotope effects, as well as modification of the hydrogen bond network by ionic solutions. A major advance has been made in developing DFT-based computational methods suitable for calculating the Compton profiles for molecular systems using various water cluster models. These include alteration of hydrogen bond length and direction, as well as the length of the internal HO-bond. Our calculations show that the changes in the local molecular structure characteristically modify the Compton profile and that these changes can in deed be detected even with moderate momentum resolution. The key remains to be an extreme statistical accuracy and experimental stability. During the first experiments at ESRF and SPring-8, we have reached the required 0.01% statistical accuracy and verified the feasibility of this technique.

Observation of fast sound in the metal-nonmetal transition in liquid Hg

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Liquid Hg undergoes the metal-nonmetal transition (M-NM) when it is expanded from 13.6 gcm^{-3} at ambient conditions to 9 gcm^{-3} at high temperature and high pressure. The isochore of 9 gcm^{-3} is located near the liquid-vapor critical point (the critical data for Hg: T_c=1751K, p_c=1673 bar, d_c=5.8 gcm^{-3}). The correlation between fluctuations near the critical point and the M-NM transition has extensively been argued to date. To investigate collective and single particle motions in expanded fluid Hg, since 2001 we have undertaken inelastic x-ray scattering experiments and obtained the dynamic structure factor, S(**Q**,E), of fluid Hg. We analyzed S(**Q**,E) within the framework of generalized hydrodynamics and found that the excitation energies of collective modes disperse three times as fast as the hydrodynamic sound velocity in the M-NM transition region at 9 gcm^{-3}. The present result suggests the existence of fast sound in expanded fluid Hg accompanying the M-NM transition and means that fluctuations intrinsic to the M-NM transition are induced on the atomic length scale and subpicosecond time scale.

Nuclear resonant inelastic x-ray scattering

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In recent years, nuclear resonant scattering techniques that use synchrotron radiation have provided new opportunities for the study of vibrational and magnetic properties of condensed matter. In particular, the determination of the vibrational density of states with nuclear resonant inelastic x-ray scattering (NRIXS) and the study of magnetic properties with synchrotron Mössbauer spectroscopy (SMS) provided new and unique results. In this presentation, the basic features of NRIXS will be explained with emphasis on their unique applications in various areas of research. The high brilliance of third-generation synchrotron radiation sources is essential to nuclear resonant scattering techniques because monochromatization to meV levels can be achieved with high spectral flux. The applications of NRIXS and SMS also greatly benefit from focusing the x-rays to spot sizes below 10 microns. The small beam sizes available and the minute amounts of material required make these novel nuclear resonant scattering techniques ideally suited for high-pressure measurements using diamond anvil cells, studies of biological materials, and investigations of magnetic nanostructures.

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Vibrational density of states in amorphous binary alloy films

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The microscopic origin of the so-called "boson peak," i.e., the anomalous excess contribution to the low-energy vibrational density of states (VDOS), g(E), in glasses and disordered systems, is a matter of continuing debate [1]. ^{57}Fe and ^{119}Sn nuclear resonant inelastic x-ray scattering (NRIXS) of synchrotron radiation at room temperature were used to measure directly the ^{57}Fe-projected and ^{119}Sn-projected partial VDOS of vapor-quenched amorphous (a-) $M_{(1-x)}{}^{57}Fe_{(x)}$ [M = Tb, Y, Mg, or ^{119}Sn] thin film alloys over a wide concentration range. A plot of $g(E)/E^2$ proves the existence of non-Debye-like excess vibrational excitations (boson peak) below ~ 10 meV in all systems studied here. While the energy of the boson peak was found to depend on atom M and to be only weakly dependent on (x), the amplitude of the boson peak was observed to be about proportional to (1-x) with a slope depending on the type of atom M. It is important to note that a boson peak in the amorphous $^{119}Sn_{(1-x)}{}^{57}Fe_{(x)}$ system was observed in both, the ^{57}Fe- and the ^{119}Sn-projected VDOS. Our results will be discussed within the framework of recent theories.

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Molecular rotations studied by nuclear resonant scattering

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Nuclear resonant scattering of synchrotron radiation yields selective, background-free information about the slow and fast dynamics of Mössbauer nuclei. Whereas time spectra in QNFS (quasielastic nuclear forward scattering) are influenced both by translational and rotational motion, using SRPAC (synchrotron-radiation-based perturbed angular correlation) only the rotational motion of the resonant nuclei is observed. We present combined results using QNFS and SRPAC on two different types of systems:

1. Highly substituted ferrocenes, such as octamethyl ferrocene (OMF) and octamethyl-ethinyl ferrocene (OMFA), have been proven to undergo order-disorder transitions to high-temperature rotator phases with a negligible Lamb-Mössbauer factor [1]. The transitions exhibit a large thermal hysteresis and, in the case of OMFA, strong deviations from simple activated behaviour on cooling. Possible correlations between structural and dynamical properties are discussed.

2. The dynamics of ferrocene in unidimensional channels of AlPO4-5 was investigated both in oriented [2] and in unoriented samples. We present the first evidence of a temperature-dependent crossover from anisotropic to isotropic rotation and discuss the results in the light of various theoretical models.

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X-ray Raman scattering at the Si *L* edge of Si and amorphous SiO

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We present measurements of the Si *L* edge of polycrystalline Si and amorphous SiO using x-ray Raman scattering (XRS). The experiment has been performed at the inelastic x-ray scattering beamline ID16 of ESRF in backscattering geometry at 9877 eV analyzer energy for scattering angles of 26° and 150°, corresponding to a momentum transfer of 2.28 $Å^{-1}$ and 9.77 $Å^{-1}$, respectively. This way we make use of the momentum transfer dependence of XRS. Additional monopole excitation channels become accessible for the high momentum transfer regime, where the dipole approximation is no longer valid. The Si *L*-edge spectra show clear momentum-transfer dependence with respect to their total shape and will be compared to calculations using a Bethe-Salpeter equation-based approach including core-hole and lifetime effects. In contrast to the Si spectra, the Si *L* edge of amorphous SiO exhibits distinct fine structure along with pronounced momentum-transfer dependence. These spectra will be discussed in terms of the interface-clusters mixture model for the structure of amorphous SiO on the basis of a disproportionation of SiO into Si and SiO_2 implying clusters of Si and SiO_2 surrounded by sub-oxidic interfaces.

Advances in nuclear inelastic scattering

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We review theoretical and experimental advances in nuclear inelastic scattering at the European Synchrotron Radiation Facility. Namely, we report on combined nuclear-molecular resonance inelastic scattering [1] and on universal dynamics of glasses discovered using nuclear inelastic scattering [2].

In molecular crystals, vibrational modes can be divided to lattice modes and molecular resonances. We found that the energy dependence of nuclear inelastic scattering around a molecular resonance is an exact copy of that around the main nuclear resonance [1]. In case of phase transitions, this effect can help to study lattice dynamics separately for each of coexisting phases.

Vibrational dynamics of glasses is one of the last puzzles in solid-state physics. A focusing point of numerous studies is the "boson" peak, i.e., an excess of the low-energy density of states relative to the Debye model. Using resonant probe molecules, we showed that the boson peak originates mainly from collective vibrational modes. At energies above the boson peak, we found a universal energy dependence of the density of states [2].

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Vibrational dynamics of iron in biological molecules

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High-resolution x-ray measurements near a nuclear resonance enable determination of the complete vibrational spectrum of a probe nucleus. This provides a highly selective probe for the vibrational dynamics of ^{57}Fe at protein active sites. Data on the frequency, the amplitude, and in some cases, the direction of iron vibrations provide a uniquely detailed, quantitative benchmark for modern quantum chemical normal mode predictions, with which they can be directly compared on an absolute scale. Measurements on oriented single crystals of iron porphyrins identify low-frequency vibrations that we identify with the long-sought heme "doming" mode, similar to the motion that takes place on oxygen binding to hemoglobin and other heme proteins. Moreover, the experimental data provide a direct estimate of the force constant for Fe displacement normal to the heme plane, independent of a specific normal mode interpretation, and suggest that this Fe motion is an important element in protein control of biological reactions. The experimentally determined energetics do not depend on a specific normal mode interpretation. In the protein environment, coupling with global vibrations can reduce the expected Fe signal from these reactive modes.

Protein dynamics on different timescales

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For the function of myoglobin, internal motions on different time scales are necessary. Mössbauer effect with synchrotron radiation allows one to determine fast intramolecular vibrations (1 fs to 0.6 ps) present from cryogenic to room temperatures [1]. They are comparable to the optical modes in solid-state physics. Combining the results of neutron structure analysis and incoherent neutron scattering allows one to separate three types of hydrogen mean square displacements at room temperature: backbone like (slower than 100 ps), methyl like (partly slower partly faster than 100 ps) and lysine like (faster than 100 ps) [2]. Mössbauer spectroscopy on the heme iron shows two regimes. Below 180K the mean square displacements increase nearly linear with temperature. The strong increase of $<x^2>$ above 180K is accompanied by a change of the shape of the Mössbauer spectra indicating diffusion-like motions in a time range between 6 and 1 ns [3,4].

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Nuclear resonant vibrational spectroscopy of Fe-S proteins

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Iron-S clusters are ubiquitous in living systems. They play important roles in electron transfer, protein structure, metal sensing, catalysis, and perhaps even in the origin of life. We are using nuclear resonant vibrational spectroscopy (NRVS) with ^{57}Fe to probe the Fe partial vibrational densities of states in protein Fe-S clusters and small model systems. One-, 2-, 4-, and 6-Fe clusters have already been interpreted by normal mode analysis using a modified Urey-Bradley force field. We also have preliminary results on the $MoFe_7S_9$ (FeMo-co) and Fe_8 P clusters in the enzyme nitrogenase, which catalyzes the reduction of dinitrogen to ammonia.

The NRVS data will be compared with results from Raman, IR, and femtosecond pump-probe spectroscopy. The improvements needed to make metalloprotein experiments easier will be highlighted, along with other nuclear isotopes that would be attractive for biochemical studies.

Inelastic x-ray scattering studies of phonons in liquid crystalline DNA with different counter-ion atmospheres

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Inelastic x-ray scattering spectroscopy is used to measure spectra of the collective density oscillations propagating along the axis of a rod-like supramolecular system made of a shear-aligned columnar hexagonal liquid crystalline phase of DNA dispersed in water with different counter-ion atmospheres. The samples are made of 40 wt% calf-thymus Na-DNA in water. The dynamical structure factor is extracted from the spectrum using a generalized three effective eigenmode (GTEE) theory. The phonon dispersion relations are constructed for different samples. Without the addition of counter-ions, the phonon dispersion relation shows an oscillatory behavior and extends to very large Q-values corresponding to the second Brillouin zone in a crystalline system, while in the samples with divalent and trivalent counter-ions, the phonons are dampened out at intermediate Q-range. The damping of phonons with different counter-ion atmospheres at small Q-values is also compared.

Dynamics of liquids

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Inelastic scattering experiments provide information about the dynamics of liquids on the atomic scale. In classical liquids, atomic motions are best understood in terms of particle configurations. Collective vibrational motions take place whenever atoms within a configuration oscillate for times longer than their characteristic periods, leading to dynamic structure factors S(**Q**,E) that show well-defined peaks at finite frequencies. In contrast, stochastic motions, such as those involved in long-range mass diffusion, can be thought of as taking place once the configurations become unstable, leading to local rearrangements that restore local equilibrium. These give rise to quasi-elastic scattering centered at zero frequency. In the case of neutron scattering with mainly incoherently scattering isotopes, these have a width, at low wave vectors, related to the macroscopic diffusive coefficient and, at high wave vectors, to the short-time behavior of a free gas. A clear transition is seen to take place at wave vectors around **Q**p, the main peak in the static structure factor. In the case of x-ray scattering or neutron scattering with mainly coherently scattering isotopes, the quasi-elastic scattering contains information about the dynamic correlations between a diffusing particle and its neighbors. The linewidth of this spectral component still resists a fully quantitative understanding. The inelastic part of the dynamic structure factor contains details pertaining to collective density fluctuations that may, in some cases, show well-defined peaks that reveal the presence of collective particle oscillations. In this talk I will discuss these phenomena in relation to results of inelastic scattering measurements and computer simulations on liquid metals, molten salts, molecular liquids, polymer and polymer electrolytes melts and aqueous solutions [1-5].

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Electronic properties of transition-metal oxides at extreme conditions

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We have applied inelastic x-ray scattering (IXS) to the study of transition-metal oxide electronic properties under very high-pressure conditions. Besides Mössbauer spectroscopy or x-ray magnetic dichroism, IXS, particularly in the fluorescence regime (XES), appears as a powerful probe of the transition-metal magnetism. The XES is well-suited to high-pressure studies thanks to the intense fluorescence yield in the hard x-ray energy range, especially when combined with a bright and focused x-ray beam provided by third-generation synchrotron sources. More specifically, the $K\beta$ emission line turns out to be extremely sensitive to the transition-metal spin state. Pressure-induced spin-state transitions and their implications on transport properties or ordering process will be discussed in a series of simple metal oxides. Complementary information about the electronic properties at extreme conditions may be gained by measuring the IXS spectra at the metal *K*-edge resonance. Thanks to the resonant process, low-lying excited states, such as gap or charge-transfer excitations, may be specifically enhanced. We will see how theoretical advances help us relate the IXS data with the transition-metal oxides fundamental parameters, including the d-d Coulomb interaction, hybridization strength or charge-transfer energy.

Anisotropy in elastic properties of hcp iron under high pressure

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Recent applications of high-pressure phonon spectroscopy with ^{57}Fe NIS will be presented with emphasis on the high-pressure phase of iron, hcp Fe, where in continuation of previous NIS studies [1,2], the phonon density of states (DOS) of textured hcp-Fe samples was studied up to 130 GPa. From NIS spectra measured parallel and almost perpendicular to the texture axis (the hcp c-axis), it is possible by the new technique of difference spectra [3,4] to extract the DOS of hcp-Fe as seen parallel and perpendicular to the c-axis. This allows for a mode-specific analysis of the phonon spectra, for instance, an identification of the two optical modes and provides the first experimental proof of an anisotropy in the sound velocities with respect to the c-axis [5].

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Inelastic x-ray scattering in alkali metals under pressure: phonons and plasmons

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We report results of high-pressure IXS experiments on phonons and plasmons in cesium and sodium, respectively. The IXS investigation of phonons in the bcc and fcc phases of Cs was partly motivated by recent theoretical predictions of small- or negative-mode Grüneisen parameters in fcc-Cs and related anomalies in thermodynamic properties. Our experimental results clearly show anomalous pressure dependences of zone-boundary LA phonon frequencies. The experimental data are compared with results of first principles frozen-phonon calculations.

Collective electronic excitations were studied by IXS in Na, the prototype of a nearly free-electron metal. The conduction electron density is the fundamental parameter in the collective-electron physics of metals. In the case of Na, the electron density can be nearly tripled in the pressure range up to 45 GPa, which was investigated here. In addition, pressure also affects electron correlations as well as the electronic band structure. Thus, high-pressure IXS studies provide valuable input to recent theoretical advances in describing the excitations of interacting electrons in metals. The main observations of the plasmon IXS experiments on Na are, first, that the difference between the free-electron behavior and the observed plasmon energies increases dramatically with increasing density. Second, the plasmon linewidth increases too, signaling a reduction in the plasmon lifetime under pressure. The results will be discussed in comparison with similar experiments on K and Rb.

Resonant scattering in clathrate hydrates

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The concept of phonon glass and electronic crystal (PGEC) is a prevailing paradigm for the engineering of materials with high thermopower. The basic premise of this concept is the observation that crystalline materials with localized vibrations may possess unusually low thermal conductivity that helps to enhance the thermoelectric performance. The first observation of this interesting phenomenon was on clathrates of ice, where it was shown that their thermal conductivity behaves like a glass. A “resonant scattering” model was proposed to account for the dissipation of heat transport in this system. To investigate the validity of this model, inelastic x-ray scattering experiments using synchrotron x-ray were performed on the clathrates. Using x-ray inelastic scattering on powder samples of xenon and methane hydrates, it is demonstrated crossing between the localized vibrations with the lattice acoustic branches is avoided. Employing the site-specific nuclear resonance inelastic scattering technique, unexpectedly large anharmonic effects on the vibration of enclathrated kryption were observed. The implication of the experimental measurements on the thermal conductivity of the clathrates will be discussed.

Pressure-induced phase transitions in iron sulfide studied by nuclear resonant inelastic scattering

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Knowledge of lattice dynamics under pressure is essential for understanding pressure-induced phase transitions. Iron sulfide undergoes two successive first-order phase transitions at 3.5 and 6.5 GPa corresponding to the semiconductor-metal and metal-semiconductor transitions, respectively. Here we show the partial phonon densities of states of iron sulfide measured by ^{57}Fe nuclear resonant inelastic x-ray scattering and calculate the total phonon densities of states under pressure. The thermodynamic parameters are estimated by integration of these extracted partial phonon densities of states with various energy weights. An abrupt change in the mean force constant is observed only around 6.5 GPa, which is closely related to the electron configuration change of the Fe^{2+} ion from high-spin to low-spin states. In the metallic state, comparison of the observed and estimated compressibilities makes it clear that there is a large pure electronic contribution in the observed compressibility.

Phonon density of states of krypton up to 46 gigapascals

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The phonon density of states (DOS) in solid krypton under high pressure (up to 46 GPa) has been measured for the first time by means of nuclear resonant inelastic x-ray scattering (NRIXS). Thermodynamic and elastic parameters of krypton are derived from the measured DOS and compared with the calculation by the density functional theory.

X-ray Raman scattering in high-pressure research

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K-edge absorption spectroscopy of first- and second-row elements has been limited to soft x-rays and low-energy electrons to date. Due to the high attenuation factors of these probes, such measurements are typically performed in low-absorbing environments—samples are contained either in vacuum or at atmospheric pressure with extremely short path lengths, with only the sample's surface region probed. However, through the use of the high-energy inelastic x-ray scattering technique, not only is the bulk accessible, but samples can be studied in highly absorbing environments, such as liquid and high-pressure diamond anvil cells. This allows information about chemical bonding to be determined under extreme conditions. We have developed an instrument optimized for inelastic x-ray scattering measurements of samples at high pressure in a diamond anvil cell. To overcome the difficulties of small sample size (typically 100 x 20 microns), high background from the pressure medium, the small inelastic cross section, and the need to probe multiple bond directions, we have combined strong focusing with a multielement analyzer and a multiaxis diffractometer. This combination has allowed us to collect *K*-edge spectra of compounds containing boron, carbon, nitrogen and oxygen at pressures up to 30 GPa.

Inelastic x-ray scattering from electronic excitations

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Inelastic x-ray scattering (IXS) is a powerful experimental technique that probes directly the dynamical behavior of a variety of condensed matter systems and offers in particular unique strengths in frontier research in correlated electron systems. As part of the Taiwan x-ray facility at SPring-8, the Inelastic X-ray Scattering Beamline (BL12XU) is designed for both resonant and nonresonant experiments on electronic excitations with variable energy resolution from 10-1000 meV. So far, a total energy resolution of 70 meV at 9.886 keV has been achieved for nonresonant experiments. For resonant experiments, the current setup covers the *K* absorption edges of the late transition metals (Co, Ni and Cu) with a total energy resolution of about 0.4 eV. This has opened up the possibility of studying a variety of electronic excitations in materials of current interest. In this presentation, the current scientific and instrumental activities at BL12XU will be discussed and illustrated with the following examples:

1. Near-edge Raman scattering of oxygen in high-pressure low-temperature H_2O
2. Resonant inelastic x-ray scattering of low-dimensional cuprate systems

Advances in magnetic and high-resolution Compton scattering

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We will report the recent progress of the "High Energy Inelastic Scattering" (BL08W) beamline and the middle-term perspectives on the momentum density study by magnetic and high-resolution Compton scattering.

The magnetic Compton scattering spectrometer has achieved high sensitivity to magnetic effects as small as 0.01%, which is about two hundredth of the magnetic effect for Fe. The Cauchois-type high-resolution spectrometer has much improved its data-taking efficiency by successfully installing the x-ray image intensifier as a position-sensitive detector. These advances have made the Compton scattering technique a useful tool for materials science.

Currently, many research subjects are running with the spectrometers. Among them, we will present the subjects of metal hydrides and magnetic multilayers.

Recent results of phonon studies at the ESRF

M. Krisch
European Synchrotron Radiation Facility, Grenoble, France

The present state of the art of phonon studies by inelastic x-ray scattering (IXS) with meV energy resolution at the ESRF shall be illustrated discussing several recent experiments. These comprise high-pressure studies, phonon dispersion in correlated electron systems and novel applications of the IXS technique.

High-energy photoemission spectroscopy

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Hard x-ray photoemission spectroscopy (HaXPES) reaches a bulk sensitivity of several tens of atomic layers. The very high photon fluxes at modern synchrotrons and the strong interest in bulk sensitive spectroscopies are now boosting the development of HaXPES, first proposed by Lindau et al. [1].

We performed a quantitative evaluation of the escape depth reached with hard x-rays. Benchmark samples (buried AlAs layer in GaAs) demonstrated that a probing depth of 60 Å is reached at a kinetic energy of 6 keV, The spectral shape variation with energy makes HaXPES a precious non-destructive depth-profiling tool [2].

We applied the technique also to layered samples for microelectronic, where "high-κ" dielectric oxides (Al_2O_3, HfO_2) replace the SiO_2 layer. High-κ oxides can keep a high gate capacitance without the need of excessively reducing the oxide thickness. We could determine the presence of SiO_2 at the high-κ/Si interface, which affects the device performances. HaXPES appears to be a powerful tool to characterize materials on the depth scale interesting for nanotechnologies. Its potentialities and limits will be discussed.

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Multiple-scattering approach to x-ray Raman scattering

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Real-space multiple-scattering (RSMS) approach calculations have been used extensively to model x-ray absorption near-edge structure (XANES) and extended x-ray absorption fine structure (EXAFS) [1]. *Ab initio* self-consistent RSMS method naturally includes multiple scattering of the photoelectron from neighboring atoms and is applicable to aperiodic or periodic systems alike. The method also includes final state self-energy effects and an approximate treatment of the photoelectron-core hole interaction. Here we present an implementation of the RSMS approach for x-ray Raman scattering (XRS). The momentum transfer dependence of the XRS near-edge spectra is found to be in agreement with previous calculations. We also demonstrate how the RSMS approach can be used to calculate the fine structure in XRS for an extended energy range. In the high-momentum transfer limit, the RSMS method can be used to calculate effects beyond the impulse approximation for the core-electron contribution. We demonstrate some of the strengths of the RSMS approach by comparison with experiments for selected examples.

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Reconstruction of Fermi surface from high-resolution Compton data

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We present our recent results on the Fermi surfaces of a nearly equiatomic TiNi, which is a well-known shape memory alloy and a Cu-Al disordered alloy. We address the nesting features of the Fermi surfaces of these alloys. In order to do quantitative callipering of small surfaces, we point out an obvious fact that the experimental resolution should be kept better than 0.10 a.u. A comment is made on two methods currently used to obtain the occupation number density from high-resolution Compton scattering data.

Dyson orbitals, quasi-particle effects and Compton scattering*

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The Dyson orbitals provide a rigorous description of ionization and Compton scattering processes [1]. These orbitals can be calculated via the Dyson's quasi-particle equation where many-body effects are included through the self-energy operator. Although accurate approaches to compute the self-energy have been developed, these are often computationally demanding and not particularly transparent physically. Therefore, more intuitive schemes for treating complex materials are useful. We have recently proposed [2] a simple self-energy approximation based on the exchange-correlation hole, which is appropriate for atomic, as well as solid-state systems. Illustrative applications indicate that our scheme should provide a reasonable description of excitation energies in metals and semiconductors with an accuracy roughly comparable to that of the GW method. In transition metal oxides, the electronic density of state (DOS) is found to be quite different from the DOS based on the local density approximation (LDA) in that the O 2*p* states are pushed nearer the Fermi energy. Our self-energy approximation would also provide a relatively straightforward approach for treating Compton scattering profiles beyond the standard LDA framework.

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*Work done in collaboration with A. Bansil

Electronic environment of $LiFePO_4$ and $FePO_4$ probed with soft x-ray inelastic scattering

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Density of states calculations for $LiFePO_4$ and $FePO_4$ predict that $LiFePO_4$ should be half metallic. Normally the half-metallic nature of $LiFePO_4$ would be investigated using x-ray magnetic circular dichroism (XMCD) techniques in order to preferentially excite the spin-up or spin-down electrons in turn. However, $LiFePO_4$ is also antiferromagnetic. This renders the application of XMCD techniques useless for this system. We illuminated powdered samples of $LiFePO_4$ and $FePO_4$ with soft x-rays to obtain XAS and RIXS data, which we compared against theory. We show that the inelastic features present in the Fe RIXS spectra, due to O-Fe charge transfer and Fe 3*d* inner-shell excitations, are predicted with great accuracy by LSDA-based theory. Experimental spectra also show strong elastic features due to a magnon-induced photoexcitation-electron trap of the type seen in CrO_2, another half-metallic system.

High-resolution soft x-ray inelastic scattering at the ALS

Z. Hussain
Lawrence Berkeley National Laboratory, Berkeley, CA, USA

Soft x-ray scattering (photon-in photon-out) with high resolution provides new scientific opportunities for the study of low-energy excitations in complex, strongly correlated systems. The use of resonant inelastic scattering near the *L/M* absorption edges of 3*d* metals allows exploring directly with high sensitivity unoccupied and occupied *d* electron bands over a good part of the Brillouin zone. In this talk, I will provide scientific motivations and the progress of this effort at the Advanced Light Source.

New light for electronic excitations in 3*d* transition metal systems: High-resolution L_3-edge RIXS

G. Ghiringhelli
INFM, Politecnico di Milano, Italy

Resonant inelastic x-ray scattering (RIXS) performed at the L_3 edge of 3*d* transition metal compounds is an ideal tool in the selective study of electronic excitations. The second-order resonant process involves directly the 3*d* shell, which determines the properties of intriguing materials, such as cuprates, manganites, nickelates. Until recently, the main obstacle to RIXS in the soft x-ray range had been technological rather than conceptual: the measured spectra had insufficient quality and energy resolution to be really informative regarding the electronic excitations of those oxides. Thanks to some recent technical upgrades in the source, in the optics and in the detection, our apparatus for RIXS (called AXES) is now capable of unprecedented quality spectra. The first data on cuprates [see Phys. Rev. Lett. **92**, 117406 (2004)], manganites, and NiO can be directly interpreted in terms of crystal field and charge transfer excitations. The combined resolving power is now better than 2000, giving access to rich and detailed information on the neutral excitations from 200 meV to a few eV. In particular, we have detected the influence of the local coordination (symmetry, nearest neighbour distances, unit cell distortion) on the crystal field excitations.

Advances in high-resolution monochromators

T.S. Toellner
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High-energy-resolution spectroscopies that use hard x-rays, like nuclear resonant scattering and inelastic x-ray scattering, have motivated advancements in the design of multicrystal, high-resolution monochromators (HRM) in the 5-30 keV energy range. Recent developments in the use of cryogenically cooled crystals have resulted in enhanced performance of HRM. This is due both to mitigation of thermally induced inefficiencies and to increased Debye-Waller factors for high-indexed crystal reflections. Recent results of a 1.2 meV, six-reflection, cryogenically cooled HRM working at 21.6 keV will be presented. Prospects for inelastic x-ray scattering with sub-meV resolution will be discussed.

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

IXS spectroscopy below 10 keV with meV resolution

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A concept of a new spectrometer for inelastic x-rays scattering (IXS) with meV and sub-meV resolution will be presented [1]. The main distinguishing features of the spectrometer are:

1. Spectral properties tend to become better with decreasing photon energy. Most optimal is using x-rays in the low-energy spectral range from 5 to 10 keV.
2. Applicable even at low-energy synchrotron radiation facilities (including X-FELs).
3. Higher count-rates, since undulators produce many more photons in the low-energy range (also at high-energy facilities).
4. Variable energy bandpass from about 5 to about 0.2 meV at a fixed photon energy.
5. Peak throughput is practically independent of the energy bandpass.
6. Using low-energy photons means better momentum transfer resolution for the same angular acceptance.
7. Spectral function with steep wings.
8. Proximity to *K* absorption edges of the important transition metals.

Principles, example designs, technical challenges of the spectrometer, as well as the present status of the experimental effort will be discussed.

[1] Y. Shvyd'ko, *X-Ray Optics: High-Energy-Resolution Applications* (Springer Series in Optical Sciences, Vol. 98, 2004)

Advances in crystal analyzers for IXS

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European Synchrotron Radiation Facility, Grenoble, France

The realization of spherical crystal analyzers for inelastic x-ray scattering experiments (IXS) is an ongoing project at ESRF since 1992. These analyzers are meanly used for IXS experiments that need very high energy resolution (VHER) (1 - 10 meV) or high energy resolution (HER) (0.1 - 2 eV). In these years, we have developed a reliable technique to routinely produce spherical analyzers of silicon with very high and high energy resolution, very good focus and efficiency. In this presentation, I will report the state of the art of the analyzer project and the main improvements made during the last years as, for example, the introduction of the anodic-bonding technique.

Imaging electronic motion with attosecond time resolution

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Brookhaven National Laboratory, Upton, NY, USA

"Attoscience" is considered the frontier of ultrafast spectroscopy and has motivated the recent development of subfemtosecond lasers based on high harmonic generation. These techniuqes have promised a new era of ultrafast science in which many-electron dynamics will be probed in real time [1-5]. In this talk, I will present an analytic technique for integrating causality with data from inelastic x-ray scattering experiments. This allows the loss function to be inverted and electron dynamics to be imaged in real time. I will show the density response due to a point perturbation in liquid water with resolutions of 41.3 attoseconds and 1.27 angstrom. This result will be used to determine the structure of the screening cloud around a photoexcited molecule in solution and the density wake of a 9 MeV gold ion. I will draw an analogy with pump-probe techniques and argue that inelastic x-ray scattering may be applied more generally to the study of attosecond phenomena.

[1] A. Zewail, Nobel Address, 1999
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[4] M. Drescher, Nature **419**, 803 (2002)
[5] A. Baltuska, Nature **421**, 611 (2003)

Compton scattering. Is it still gathering momentum?

M.J. Cooper
University of Warwick, UK

Progress in inelastic scattering, especially in Compton studies of electron momentum density, as illustrated by this meeting, will be set into the context of a decade of IXS conferences, four decades of Sagamore meetings and, arguably, almost a century of Compton scattering. What new insights are the current improvements in resolution and statistical accuracy of this synchrotron era actually providing? What, if anything is "just around the corner" and where should our attention now be focused?

Future sources for inelastic x-ray scattering

D.E. Moncton
Massachusetts Institute of Technology, Cambridge, MA, USA

Fourth-generation x-ray sources have the potential to revolutionize inelastic x-ray scattering (IXS). As demonstrated with 3rd-generation synchrotron sources, IXS is a very powerful method for studying the dynamics of condensed matter. However, when one approaches millivolt resolution levels possible with novel modern monochromator and analyzer optics, the photon flux available today decreases proportionally to levels challenging for phonon studies and generally too weak for studying electronic excitations. A transform-limited pulse from a seeded FEL source could achieve millivolt bandwidths with picosecond pulse duration. The time-average flux could be 4 to 5 orders of magnitude higher than that available today. Furthermore, the transform-limited character of the source will permit a natural integration of energy-domain and time-domain methods.

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Poster Abstracts

Compton profile study of holmium and terbium

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We present the first experimental Compton profiles of two rare-earth metals, namely holmium and terbium. Measurements have been made using 661.65 keV gamma rays emitted by 20 Ci ^{137}Cs source. The incident beam scattered inelastically on the sample through 160° (± 0.7°) was detected by a high-purity Ge detector. The overall momentum resolution of the spectrometer was 0.40 a.u. In the absence of band structure calculations, theoretical computations have been carried out using renormalized-free-atom (RFA) and free-electron models. Duly corrected experimental profiles are compared with the RFA model and free-electron Compton profiles. It is seen that the RFA results are in better agreement with both the experiments. The data are interpreted in terms of s-p hybridization in the valence state of the rare earths. The calculated cohesive energy of holmium and terbium compares well with other band structure and experimental investigations.

Compton-scattering experiments with 662 keV gamma radiation

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A gamma-ray Compton spectrometer, which uses a 20 Ci ^{137}Cs (662 keV) cylindrical source and an intrinsic Ge detector, has been designed and built. The total resolution of the spectrometer in momentum scale is 0.40 a.u., which is significantly higher than the conventional ^{241}Am Compton spectrometers. The experimental design of the present spectrometer differs in several aspects from the existing high-intensity (85-100 Ci) ^{137}Cs-based Compton spectrometers. We have developed, for the first time, a methodology for correction of additional background in such high-energy spectrometers due to bremsstrahlung contribution owing to photo and Compton electrons. The performance of the machine is assessed using the isotropic Compton profile of Al and directional profiles of Ta. The anisotropy in the momentum densities in Ta are compared with available APW band structure calculations and are interpreted in terms of Fermi-surface topology.

Magnetic Compton scattering study of Ir-doped $CeFe_2$ at 70K

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[3]Low Temperature Physics Group, Centre for Advanced Technology, Indore, India
[4]Material Science Division, Himeji Institute of Technology, Hyogo, Japan

The contribution of cerium and iron to the total spin moment in $Ce(Fe_{0.97}Ir_{0.03})_2$ compound at 70K (well below its T_N) has been studied using magnetic Compton scattering. The measurements on a polycrystalline sample were carried out on the high-energy inelastic scattering beam line at SPring8, Japan, with 175 keV elliptically polarized synchrotron radiation. The data give a direct indication of recovery of FM behaviour of $CeFe_2$ in $Ce(Fe_{0.97}Ir_{0.03})_2$ on application of sufficiently strong magnetic field (2 T). The data of doped sample in induced FM phase are analyzed in terms of induced spin-moment contributions from different magnetic electrons at 1.5 T and 2.0 T external magnetic fields.

Inelastic x-ray scattering study of super-cooled liquid and hot solid silicon

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[2]CNRS,University of Orleans, Orleans, France

We present high-resolution inelastic x-ray scattering measurements of the dynamical structure factor of silicon at the same temperature (T=1300°C) for super-cooled liquid and hot solid phases.

Lattice dynamics and elastic properties of high-pressure structures of methane hydrate

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[5]*European Synchrotron Radiation Facility, Grenoble, France*

In situ high-pressure inelastic x-ray scattering experiments of the high-pressure structures MH-II and MH-III are described. The elastic properties of these structures have been obtained from the measured phonon dispersion curves using high-energy-resolution inelastic x-ray scattering. The orientationally averaged sound velocities and orientationally averaged elastic constants were derived from the experimental data. They were found to strongly reflect the transition from a cage clathrate (MH-II) to a dense filled ice structure (MH-III).

Hydrogen bonding in supercritical water: Compton scattering study

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Water in the supercritical (sc) domain exhibits remarkably different properties compared to water at ambient pressure and temperature. In particular, sc-water can be used as a very efficient solvent for chemical processes, such as oxidation reactions for ultimate treatment of hazardous organic wastes.

The peculiar properties of sc-water are attributed to the change of intermolecular structure and, in particular, change in hydrogen bond network. X-ray and neutron-scattering investigations of the intermolecular structure showed that the tetrahedral arrangement of water molecules collapses in the sc state.

Compton scattering is a direct probe of the ground-state electronic momentum density and thus is very sensitive to intermolecular interaction and chemical bonding. The purpose of our study is to evaluate the variation of the intermolecular attraction in sc-water over a wide range of the phase diagram by tuning water density from 1 g/cm^3 to a low density of 0.3 g/cm^3 and quantify variations in the charge transfer involved in the hydrogen bond at different conditions of pressure and temperature. Preliminary results will be shown.

Design of the HERIX spectrometer

B. Brajuskovic, D. Shu, H. Sinn
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A new spectrometer for high-resolution inelastic x-ray scattering will be built at sector 30 of the Advanced Photon Source. The spectrometer is optimized for an energy resolution of 1 - 2 meV at x-ray energies of 20-26 keV and will enable novel experiments in the areas of dynamics in liquids, glasses, and single crystals under extreme conditions. A nine-meter-long arm, which carries nine crystal analyzers, detectors, and a vacuum vessel, can be rotated in the horizontal scattering plane to a maximum scattering angle of 30 degrees. To allow maximum space for specialized sample environments, pivoting around the sample is achieved by a coordinated motion of three linear stages outside the center of rotation. The design of the vacuum vessel and the arm was optimized by finite element analysis.

Vibration modes in lithium ammonia complexes

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We have studied the vibration modes of lithium ammonia complexes using inelastic x-ray scattering with a resolution of about 2 meV. We compare these results with the theoretical calculations of the modes for an isolated complex.

IXS at NSLSII

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The National Synchrotron Light Source (NSLS) at Brookhaven National Laboratory submitted a proposal to the U.S. DOE to build a new, high-brightness synchrotron radiation source to replace the aging NSLS. The new source is perfectly suited for IXS in the energy range 300 eV – 25 keV. One end station will be dedicated to IXS in the soft x-ray range (300-1000 eV), and two for hard x-ray IXS in the energy range 5-25 keV with energy resolution of 5 and 50 meV, respectively. Different design options for the beamlines will be discussed, and various areas of research presented.

Spherically bent Si analyzer crystals for resonant inelastic x-ray scattering (RIXS) with an intrinsic resolution of 150 meV

E. Collart, A. Shukla, F. Gelebart, M. Morand, J.-L. Pelouard, N. Bardou
University of Paris, France

High-resolution RIXS is a promising technique for investigating the electronic structure of strongly correlated materials.

The spherical analyzer is the most important element of a Rowland circle spectrometer, and its intrinsic energy resolution is a key factor for the overall experiment resolution. In order to be able to measure excitations with an energy below 1 eV, the overall energy resolution (FWHM) needs to be of the order of ~ 200-300 meV at the most. Both the RIXS process and the spectrometer geometry impose certain constraints on the possibility of obtaining this resolution.

By perfecting each aspect of the fabrication and by using the “anodic bonding” technique to bind the Si wafer to a spherical glass substrate, silicon bent analyzers can provide the required energy resolution. We have succeeded in producing such analyzers for several *K* edges of 3*d* transition metals, enormously improving the energy resolution with respect to “standard” spherically bent analyzers.

Crystal-field excitations in transition metal oxides

E. Collart, A. Shukla, J.-P. Rueff, P. Leininger, H. Ishii, I. Jarrige, Y. Cai
University of Paris, France

We have undertaken a systematic study to identify low-energy excitations in transition metal oxides CuO, NiO and CoO using high-resolution RIXS at the metal *K* edge. These materials have been studied in the past with medium-energy resolution, and features measured at energy losses in the 5-10 eV range have been identified generically as "charge-transfer" excitations. By improving experimental resolution (~ 300 meV FWHM), we have measured sharp features in the charge-transfer gap corresponding to excitations of the crystal field or "d-d" excitations. These are forbidden by dipole selection rules and hence invisible by optical spectroscopy, making RIXS a unique probe for their investigation. We discuss their dependence on crystal orientation with respect to the polarization of the incoming photon, the transferred momentum and the incident energy.

Magnetic Compton scattering study of ferromagnetic Sr_2FeMoO_6

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The spin-polarized electron momentum distribution (magnetic Compton profile, MCP) of ferromagnetic Sr_2FeMoO_6 has been measured using the magnetic Compton scattering technique at 10K and 300K along the [100] and [110] principal directions. The experimental results have been compared with results from electronic structure calculations performed using the full potential linearized augmented plane-wave (FLAPW) method. The calculated results clearly show that only down-spin states contribute to the EF intensity (half metallic character). The experimental observations clearly show evidence for the existence of negative spin polarization that arises from down-spin bands. We have observed the change in the MCP, which arises from the band spin fluctuation, between the low temperature 10K and high temperature 300K.

The Cornell Energy Recovery Linac: Prospects for inelastic x-ray scattering

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X-ray and accelerator scientists at Cornell want to build an energy-recovery linac (ERL) x-ray source over the next 10 years. The ERL is a true 4th-generation source that is neither an XFEL nor an "ultimate storage ring." This almost diffraction-limited, hard x-ray source uses a laser-driven photocathode to produce an exceeding bright electron beam with extremely flexible bunch structure and superconducting linac-storing particle beam energy instead of charge.

Design and construction of an apparatus for rapid measurement of q-dependent nonresonant IXS

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We report on the design and construction of a multicrystal analyzer for simultaneous measurement of nonresonant IXS at many different momentum transfers. When completed, the instrument will have 21 spherically bent Si (111) analyzers spaced at 8 degree intervals in the vertical scattering plane and each focusing on a different photon-counting detector. When operated at 9890 eV for near backscattering from the (555) reflection, this will provide simultaneous measurement of momentum transfers from approximately 0.5 to 10 inverse Angstroms. The instrument will be located at sector 20 of the APS and will eventually be available for general users. Use of the Si (311) monochromater already available at the 20-ID undulator beamline should result in a final energy resolution of approximately 0.5 eV.

Phonon DOS in oriented SnO by nuclear inelastic scattering

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Nuclear inelastic scattering (NIS) of synchrotron radiation (SR) is a unique tool to study the partial phonon density of states (DOS) of Mössbauer isotopes in various compounds. Here we report on a high-pressure study of the partial phonon DOS of ^{119}Sn in SnO up to 6 GPa measured parallel and almost perpendicular to the texture axis in oriented SnO absorber. Tetragonal SnO has a graphite-like structure, and it is very easy to prepare from small SnO crystallites a strongly oriented absorber with the c-axis perpendicular to the absorber plane. With the new technique of difference spectra [1,2], it is possible to obtain projected partial phonon DOS of Sn in SnO as seen parallel and perpendicular to the c-axis. Applying pressure up to 6 GPa leads to a weakening of the pronounced difference of the projected DOS in the two different directions. In addition, a hardening of a soft phonon mode with pressure is observed. This behaviour is explained by the graphite-like structure of SnO with weak van der Waals forces between the plains and strong covalent binding within the plains.

[1] H. Giefers et al., High Pressure Research **22**, 501 (2002).
[2] G. Wortmann et al., Hyp. Interact. **144/145**, 103 (2002).

Resonant inelastic x-ray scattering (RIXS) at the Mn *K* absorption pre-edge - application in biocatalysis

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A study of the Mn 3*d* orbitals in oxides and the oxygen-evolving complex (OEC) of photosystem II (PS II) using resonant inelastic x-ray scattering (RIXS) is presented. The RIXS data yield three-dimensional plots that can be interpreted along the incident (absorption) energy and along the energy-transfer axis. The energy-transfer dimension enhances the separation of the pre-edge (predominantly 1*s* to 3*d* transitions) from the main *K* edge, and a detailed analysis is thus possible. The 1*s*2*p* RIXS final-state electron configuration along the energy-transfer axis is identical to conventional *L*-edge absorption spectroscopy, and the RIXS spectra are therefore sensitive to the Mn spin state. This technique thus yields detailed information on the electronic structure that is not accessible in conventional *K*-edge absorption spectroscopy. The line splittings can be understood within a ligand-field multiplet model, showing that (3*d*,3*d*) and (2*p*,3*d*) two-electron interactions have to be considered to describe the spectral shapes in all systems.

Hydrogen bonding in water studied by x-ray Compton scattering

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We study hydrogen bonding and coordination properties of water molecules using x-ray Compton scattering (inelastic x-ray scattering at high energy and momentum transfers) [1]. In x-ray Compton scattering, the scattering cross section is, within the impulse approximation, proportional to the so-called Compton profile, i.e., a plane integral of the momentum density of the system. In this work, the momentum density is calculated using the density-functional theory (GGA functionals, Gaussian-type basis functions). From our model calculations using clusters of water molecules, we obtain the fingerprint of the hydrogen bond in the Compton profile. The main effect in the Compton profile upon the hydrogen bond formation follows from the exchange interaction between the overlapping orbitals of the neighboring molecules. The effect of intramolecular polarization is weak, whereas charge transfer modifies the profile. The calculations suggest that x-ray Compton scattering is potentially an important complementary method to study the nature of the hydrogen bond.

[1] M. Hakala, S. Huotari, K. Hämäläinen, S. Manninen, Ph. Wernet, A. Nilsson, and L.G.M. Pettersson, Phys. Rev. B (in press).

A novel application of inelastic x-ray scattering to probe quantum magnetism

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We have recently employed inelastic x-ray scattering near *K* edges of transition metal oxides that exhibit strong magnetism. Our results on a variety of systems, such as $Nd_{2-x}Ce_xCuO_4$, $SrCuO_2$ and $Sr_{14}Cu_{24}O_{41}$, suggest that electron-hole pair dispersion is related to the details of magnetism. A clear correlation is established by a novel analysis technique applied to these data. We argue that in all these materials one can extract a high-q effective pair velocity: $Nd_{2-x}Ce_xCuO_4$ serves as a material that exhibits an indirect Mott gap and quantum magnetic critical point, $SrCuO_2$ exhibits spin-charge separation, and $Sr_{14}Cu_{24}O_{41}$ exhibits quantum ladder behavior. We show that this renormalized pair velocity we extract from x-ray data is directly correlated with unusual quantum magnetism exhibited by these materials.

Selective XANES spectroscopy from RIXS contour maps

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State-selective XANES spectroscopy is a powerful tool in studies of electronic and structural properties of materials. "Genuine" selective XANES can be deduced by measuring emission spectra with high resolution over wide-energy ranges both in excitation and emission, and analyzing the data in terms of a formula derived from the Kramers-Heisenberg equation. Selective XANES spectroscopy can be achieved by the combination of a third-generation synchrotron source and a spectrometer with large-acceptance;high-resolution analyzer [1]. As examples, we will present spin-selective XANES spectra of Mn oxides by using $MnK\beta_{1,3}$ and $K\beta'$, which are considerably different from those by conventional method, but are consistent with an anticipation from Hund's rule. The overall spectral shapes agree well with theoretical calculations. We will also show site-selective XANES of Ga chlorides, which is the first example that weak outer shell emissions ($GaK\beta_2$) are utilized for selective-XANES measurements. Through these studies, the possibility of selective XANES spectroscopy from RIXS contour maps will be discussed.

[1] H. Hayashi et al., J. Electron Spectrosc. Relat. Phenom. **136**, 191 (2004).

Fermi-surface mapping on complex materials using the 90 keV new Compton spectrometer at ESRF

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A new Compton spectrometer has been constructed at ID15B, ESRF. This spectrometer provides a higher count rate with a better momentum resolution using 90 keV high-energy x-rays, compared with the 60 and 30 keV spectrometers, currently operating. We show that it is possible to routinely carry out a 2D Fermi-surface reconstruction experiment on complex materials, which include heavy elements, in a reasonable beam time (- one week).

Inelastic x-ray scattering for high-pressure research at HPCAT, APS

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As part of a third-generation synchrotron radiation beamline dedicated to high-pressure physics research, 16-IDD of HPCAT at the Advanced Photon Source is being commissioned to carry out x-ray spectroscopy studies of samples under high pressures. This focus allows us to optimize our instruments to conduct experiments with diamond anvil cells. We present some of the results from *K*-edge studies of light elements, plasmons, x-ray emission spectroscopy, resonant inelastic x-ray scattering, and nuclear resonant scattering.

HPCAT is a collaboration among the Carnegie Institution, Lawrence Livermore National Laboratory, the University of Hawaii, the University of Nevada Las Vegas, and the Carnegie/DOE Alliance Center (CDAC).

High-resolution Compton-scattering studies

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Inelastic x-ray scattering as a probe for electronic structure of matter has reached a level where, for example, the Compton profiles of low-Z elements can be measured with a momentum resolution of the order of 0.02 atomic units of momentum (a.u.). Some of the previous Compton-scattering experiments [1], where incident photon energies of about 10 keV were used, showed that, while experimental geometry should have allowed the resolution of 0.02 a.u., the anticipated Fermi-surface-related structure was unexpectedly still not resolved due to final state effects [2]. This problem can only be overcome by using photons with higher energies. At the beamline ID16 of the European Synchrotron Radiation Facility (Grenoble, France), studies have been performed using up to 18 keV radiation to reduce the final-state effects in momentum resolution to a level of 0.03 a.u., while the experimental geometry allows a resolution better than 0.02 a.u.

[1] S. Huotari et al., Phys. Rev. B **62**, 7956-7963 (2000).
[2] J.A. Soininen et al., Phys. Rev. B **64**, 125116 (2001).

Correlation-induced double-plasmon excitation in Al and Na

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Although the dynamic structure factor S(**q**,ω) of simple metals has been discussed extensively in terms of electron-electron correlation and electron-ion interaction, the separation of these two contributors in the analysis of S(**q**,ω) has not been straightforward. In this study, a new type of structure in the S(**q**,ω) of simple metals was found. This structure is believed to originate solely from dynamic correlation effects in the homogeneous electron gas and is not largely affected by electron-ion interaction.

The nonresonant inelastic x-ray scattering experiments were performed at the ESRF beamline ID16. The photon energy-loss spectra of both aluminum and sodium were measured in the momentum-transfer range of 0.7 $\mathbf{q}_c$ – 1.5 $\mathbf{q}_c$, i.e., across the plasmon cut-off. For the first time, peak-like structures were found in the high-energy-loss tail of the dynamic structure factor of both metals. According to their shape, the q-dependence of their peak energies, as well as their intensities, these structures can be attributed to intrinsic plasmon-plasmon excitations, as proposed theoretically by Sturm and Gusarov [1]. Thus a new type of feature in S(**q**,ω) has been observed, and this may offer possibilities to probe effects that are second order in the dynamically screened Coulomb interaction.

[1] K. Sturm and A. Gusarov, Phys. Rev. B **62**, 16474 (2000)

Resonant inelastic x-ray scattering study of Co oxides

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Resonant inelastic x-ray scattering has been used to study charge-transfer excitations in CoO and $Na_{0.7}CoO_2$, the parent compound of the newly discovered superconductor $Na_{0.35}CoO_2 \bullet 1.3H_2O$. Three charge-transfer excitation features have been identified at energy transfers of 5.3, 7.1 and 10.7 eV, respectively. The first two features correspond well in energy to similar features observed in CoO and are assigned as transition from ground state to $3d^{n+1}\underline{L}$ with $\underline{L}$ being a hole state at the oxygen site. The higher energy feature at 10.7 eV, on the other hand, can be assigned as double charge-transfer excitation to $3d^{n+2}\underline{L}^2$, in which two holes at the oxygen site are involved. This double charge-transfer excitation can be expected when the system is in a low-spin ground state, consistent with recent high-energy photoemission experiments. Details of the study will be presented.

$(Mg,Fe)SiO_3$ perovskite to 120 GPa using synchrotron Mössbauer spectroscopy

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Iron-bearing magnesium silicate perovskite, coexisting with small amounts of (Mg,Fe)O ferropericlase and $CaSiO_3$ perovskite, is suggested to be the most abundant phase in Earth's lower mantle. Therefore, knowledge of the behavior of iron in perovskite under pressure conditions of the lower mantle is necessary for our understanding of this region within Earth. The electronic environment of the Fe atoms in two silicate perovskite samples, $Fe_{0.05}Mg_{0.95}SiO_3$ (Pv05) and $Fe_{0.1}Mg_{0.9}SiO_3$ (Pv10), have been measured to 120 GPa and 75 GPa, respectively, at room temperature using diamond anvil cells and nuclear forward scattering, also termed synchrotron Mössbauer spectroscopy (SMS). Such investigations of extremely small and dilute ^{57}Fe-bearing samples have become possible through the development of SMS. Our results are explained in the framework of the "three-doublet" model, which assumes two Fe^{2+}-like sites and one Fe^{3+}-like site that are well distinguishable by the hyperfine fields at the location of the Fe nuclei (e.g., McCammon et al. 1992; Fei et al. 1994). Our results show that, at pressures extending into the lower most mantle, the fraction of Fe^{3+} remains essentially unchanged, indicating that pressure alone does not alter the valence states of iron in $(Mg,Fe)SiO_3$ perovskite. Around 70 GPa, a change in the volume dependence of the isomer shift could be indicative of the endpoint of a continuous transition of the Fe^{3+} from a high-spin to a low-spin state.

The study of momentum density distribution in MgB_2

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Compton profiles of MgB_2 using the *ab initio* HF-LCAO method have been calculated. The profiles have been calculated at 15K, 55K and 293K, while taking the thermal expansion of real-space lattice into account. The findings are compared with the published experimental data of Nygard et al. Theoretical results are in good agreement with the high-resolution measurements. It is also observed that the agreement further improves when the core contribution is also calculated employing the *ab initio* method.

Electron correlation effects on Compton profiles of Cu in the GW approximation

Y. Kubo

The occupation number densities N(k)s of Cu are evaluated from a first-principle calculation of the spectral function within the GW approximation. The dielectric matrix needed for the dynamically screened potential is calculated within the random-phase approximation. The dynamical screening effects are important for bandwidth narrowing. The Compton profiles (CPs) of Cu are calculated using the N(k)s. The bandwidth narrowing leads to an excellent agreement between theoretical and experimental results.

The dynamical structure factor of NiO and CoO

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We have used nonresonant inelastic x-ray scattering and *ab initio* dynamical electronic response calculations to study electron dynamics in the highly correlated mono-oxides NiO and CoO. Absolute IXS measurements were made as a function of magnitude and orientation of the momentum transfer, **q**, on the UNICAT beamline at the APS and C-Line at CHESS with energy resolution ranging from 0.3 – 1.1 eV. Dynamical response calculations were performed within LDA + U including crystal local field effects. Comparisons of absolute $S(\mathbf{q},\omega)$ measurements with theory showed that both the gap energy and the structure of the electronic response above the gap are described by U ~ 8 eV within RPA for low **q**-values and that non-RPA many-body excitonic effects appear at larger momentum transfers for NiO and CoO. The combined use of IXS and dynamical response calculations to perform unoccupied-state spectroscopy will be discussed. The measured excitonic spectra for NiO and CoO will be compared and discussed in connection with published resonant emission x-ray spectroscopy and reflection electron energy loss data.

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Quantitative vibrational dynamics of iron in model compounds

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We use quantitative experimental (nuclear resonance vibrational spectroscopy - NRVS) and theoretical (density functional theory - DFT) approaches to characterize the vibrational dynamics of the ^{57}Fe atom in a series of porphyrins designed to mimic the active site of heme proteins. NRVS yields the frequencies, amplitudes, and directions of the Fe vibrations and thus provides a quantitative test of DFT-based normal mode predictions. With the exception of the predicted Fe-NO bond length and frequency for Fe(TPP)(NO), quantitative comparison of calculated and measured Fe dynamics on an absolute scale reveals good agreement for the nitrosyl porphyrins. This suggests that DFT can be a reliable guide to the character of observed Fe vibrational modes, including a series of modes involving Fe motion in the plane of the heme, Fe-ligand modes, and reactive modes. In contrast to expectations from a simple three-body oscillator, mode energy remains localized on the FeNO group for only two modes. Bending of the FeNO unit contributes to several in-plane modes, but no primary FeNO bending mode is identified for Fe(TPP)(NO). Vibrations associated with hindered NO rotation and heme doming are predicted at low frequencies. We compare these results with experimental data and computational predictions for model compounds involving CO.

Doping evolution of Mott-gap excitations in two-dimensional cuprates

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Momentum-dependent charge excitation of 2-D cuprates with various doping levels ($La_{2-x}Sr_xCuO_4$ and $Nd_{2-x}Ce_xCuO_4$) is measured using high-resolution inelastic x-ray scattering. Although a low-energy continuum is built up with doping, a remnant excitation gap behavior continues to exist even in a highly doped metallic phase. The excitation of the Mott gap becomes less dispersive with the increase of doping level. Results also suggest a dramatic reduction of pair velocity upon doping.

Temperature-dependent magnetic Compton scattering from magnetite

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We have used the magnetic Compton scattering (MCS) technique to investigate the spin density in magnetite Fe_3O_4. The magnetic Compton profiles (MCP) were measured using the elliptical multipole wiggler (EMW) installed at beamline 11-ID-B of the Advanced Photon Source (APS). The experiments were carried out at various temperatures and along different crystallographic directions in the presence of two different magnetic fields. Spin moments were calculated, and their variations measured as function of temperature along three different crystallographic directions. The lineshapes of the MCPs were analyzed in terms of first-principles computations on the cubic spinel structure. Further insight was obtained via a simple approach using atomic d-orbitals and a free-electron gas model. The MCPs show features at all temperatures, which can be attributed to itinerant electrons. The spin moments show correlation with conductivity around the Verwey transition temperature. We also observed a significant anisotropy in spin values around the Verwey transition.

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Inelastic x-ray scattering studies of phonons in liquid crystalline DNA with different counter-ion atmospheres

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Using inelastic x-ray scattering, we studied 40 wt% calf-thymus Na-DNA in water with different counter-ion atmospheres. The samples are prepared in columnar hexagonal liquid crystalline phase. The generalized three effective eigenmode (GTEE) theory is successfully applied to analyze the IXS spectra to extract the dynamical structure factor. The phonon dispersion relations are constructed for different samples. Without the addition of counter-ions, the phonon dispersion relation shows an oscillatory behavior and extends to a very large-**Q** values corresponding to the second Brillouin zone in a crystalline system, while in the samples with divalent and trivalent counter-ions, the phonons are dampened out at intermediate-**Q** range. The direct analysis of the phonon damping at low-**Q** values also indicates the stronger damping effects caused by condensation of counter-ions on the DNA surface.

Resonant inelastic x-ray scattering study of $HgBa_2CuO_{4+\delta}$

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Charge transfer excitations in optimally doped $HgBa_2CuO_{4+\delta}$ up to 8 eV were studied for the first time by resonant inelastic x-ray scattering. We performed a detailed measurement at different high symmetry points in the Brillouin zone. A strong incident energy dependence was observed and carefully utilized to resolve a multiplet structure. We proposed that contributions from various O-2*p* bands could account for the multi-excitation spectrum. Our high-resolution measurements may also help resolve some controversy regarding the dispersion and thus the nature of charge excitations and lead to a better understanding of the electronic structure of strongly correlated cuprates.

Anisotropic niobium-oxygen covalent bonds in single-crystal ferroelectric potassium niobate studied by resonant x-ray scattering

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Resonant x-ray scattering has been used to study the ferroelectric orbital ordering in a model ferroelectric potassium niobate. To probe the hybridized niobium-oxygen states, the absorption and scattering measurements were performed by scanning the incident x-ray energy through the *K* edge of niobium. Qualitatively similar polarization-dependent anisotropy of the real part of x-ray anomalous dispersion was observed in both x-ray absorption and resonant scattering measurements. In the latter case, the anisotropy exhibited dependence on the scattering momentum, **Q**, shifting downward in energy as **Q** increased from (0, 0, 8) to (0, 0, 10) to (0, 0, 12). In the geometry we used in the experiment, this shift was due to the increasing relative strength of the quadrupolar transition into the *d* states that are lower in energy than *p* states. The matrix element for the quadrupolar transition into the *d* states is dependent on **Q**, while that for the dipolar transition into the *p* state is not. This measurement demonstrates the possibility of probing the orbital character of the conduction band involved in directional bonds by assessing the scattering momentum dependence of resonant x-ray scattering.

The electronic bonding change in compressed BN

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Recent advances in high-pressure *K*-edge spectroscopy using inelastic x-ray scattering have allowed us to probe the bonding changes in BN *in situ* at high pressure for the first time. Using IXS, we observed the conversion process of boron and nitrogen sp^2 and *p*-bonding to sp^3 and the directional nature of the sp^3 bonding. In combination with *in situ* x-ray diffraction, this study provides new insights into the transformation mechanism of BN from an ordinary soft graphitic structure to a superhard material.

Doping dependence of the bond-stretching phonon mode in $La_{2-X}Sr_XCuO_4$

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We have investigated systematically the doping dependence of the Cu-O bond-stretching optical phonons in the <1 0 0> direction of $La_{2-X}Sr_XCuO_4$ by inelastic x-ray scattering. Since the softening of this phonon mode is commonly observed among superconducting oxides and also non-superconducting oxides, the relation of the softening of this mode with the high-T_c superconductivity is not understood. We will show in the presentation that anomalous enhancement of the softening is observed in the superconducting region of the doping concentration. The degree of the anomalous enhancement has a one-to-one correspondence with the T_c value in the phase diagram. This observation is discussed in terms of the coupling between the phonon and the charge fluctuation on the doped CuO_2 planes.

Origin of ^{40}Zr to ^{92}U x-ray satellite spectra in the $L\alpha_1$ region

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The x-ray satellite spectra arising due to the $2p_{3/2}^{-1}3x^{-1}$-$3x^{-1}3d^{-1}$ ($x \equiv$ s, p, d) transition array, in elements with Z = 40 to 92, have been calculated. While the energies of various transitions of the array have been determined by using available Hartree-Fock-Slater data on $1s^{-1}$-$2p^{-1}3x^{-1}$ and $2p_{3/2}^{-1}$-$3x^{-1}$,$3x'^{-1}$ Auger transition energies, their relative intensities have been estimated by considering cross sections of singly ionized $2x^{-1}$ ($x \equiv$ s, p) states and then of subsequent Coster-Kronig and shake off processes. The calculated spectra have been compared with the measured satellite energies in $L\alpha_1$ spectra. Their intense peaks have been identified as the observed satellite lines. The one-to-one correspondence between the peaks in calculated spectra and the satellites in measured spectra has been established on the basis of the agreement between the separations in the peak energies and those in the measured satellite energies. It has been established that six satellites observed in the $L\alpha_1$ region of the x-ray spectra of various elements and named α_3, α_4, α_5, α', α^{ix} and α^{x} in order of increasing energy are mainly emitted by $2p_{3/2}^{-1}3d^{-1}$-$3d^{-2}$ transitions. On the basis of agreement between computed spectra and measured satellites, It is observed that the satellite α_3 in ^{40}Zr to ^{48}Cd and α' in ^{74}W to ^{92}U is emitted by the superposition of the most intense transition $^3F_4$-$^3F_4$, contributing in order of decreasing intensity. It has been well established that the transition $^1F_3$-$^1G_4$ is the main source of the emission of the satellite α_4 in the spectra of elements with Z = 40-48. The same transition $^1F_3$-$^1G_4$ and other two transitions namely $^1P_1$-$^1D_2$ and $^1F_3$-$^1D_2$ have been proved to be the main origin of the satellite, α^{ix}, reported in the range Z = 74-92. Further, the line α_5 in the spectra of elements with Z = 40 - 48 has been assigned to mainly the $^3D_3$-$^3F_4$, $^3D_2$-$^3F_3$, $^1P_1$-$^1D_2$ and $^1F_3$-$^1D_2$ transitions. Finally, the satellite α^{x}, reported in the spectra of elements with Z = 74-92, has been associated with the transition $^3D_3$-$^3F_4$.The possible contributions of other transitions of the $2p_{3/2}^{-1}3x^{-1}$-$3x^{-1}3d^{-1}$ ($x \equiv$ s, p, d) array having appreciable intensities, have also been discussed.

Holon-Doublon resonance in 1-D cuprate Mott systems

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We investigated the charge dynamics in quasi-one-dimensional cuprate Mott systems $SrCuO_2$ and Sr_2CuO_3 using a momentum-resolved inelastic x-ray scattering technique under various geometries and polarizations. The excitation over the Mott gap edge is found to be highly dispersive compared to both quasi-zero and quasi-two-dimensional systems. The electron-hole pair turns out to move quite "freely" with a light effective mass and with a long lifetime of about a femtosecond. These results are consistent with spinless charge motion.

Highly efficient medium-energy-resolution spectrometer for inelastic x-ray scattering

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A nine-element analyzer system for inelastic x-ray scattering has been designed and built. Each individual analyzer crystal is carefully developed and aligned with an inverse joy-stick goniometer. Each analyzer crystal was bent spherically 4" size with a radius of 1 meter or 0.85 meter with silicon or germanium wafers, respectively. All have perfect uniform focus. The energy of the scattered photons is measured with a conventional double-circle goniometer mounted on a translation stage, which allows the maintenance of the sample, analyzers and detector, also mounted on a separate translation stage, on a Rowland-circle. The total energy resolution is around 0.2 to 0.5 eV at backscattering. Measurements of NRRS on graphite, Mn Kβ fine structure and Mn spin-polarized XAS were carried out.

Perspectives for inelastic x-ray scattering at the PETRA-III synchrotron radiation source

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PETRA-III will be a new third-generation synchrotron radiation source to become operational in 2009 at DESY (Hamburg). Due to its low emittance of 1 nmrad, many experimental techniques will benefit from the outstanding brilliance of this machine.

A unique feature of inelastic x-ray scattering at PETRA III will be the combination of this spectroscopy with microfocusing techniques. Experiments on smallest amounts of material like thin films, single crystallites within a polycrystalline material and tiny grains of materials in diamond-anvil cells under extreme conditions of pressure and temperature will be possible. Metastable and nonequilibrium phases, which can only be produced in small quantities like tiny crystals or thin films, become accessible.

The small beam sizes available at PETRA III allow for a very efficient implementation of spectrometers with sub-meV resolution. This will help to clearly identify low-energy collective excitations that are often observed in disordered materials and in the vicinity of phase transformations. KB mirror optics will be used for the generation of submicron focal spots for the investigation of extremely small amounts of material. The instrument planned at PETRA III will be installed at a 20-m-long undulator. It consists of a vertical spectrometer for the investigation of excitations in single crystals with 2-3 meV energy resolution and a horizontal spectrometer for the study of dynamical properties of disordered materials with sub-meV energy resolution.

Study of insulator to metal transition in Rb_4C_{60} by Compton scattering, under pressure

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The LDA band structure calculations on the bct Rb_4C_{60} claim a metallic behaviour for this material, but they are strongly at odds with the NMR and photoemission results finding an insulator ground state. The Jahn-Teller distortion of the molecule in the molecular solid, which is not taken into account by calculations—and has not yet been experimentally observed—is invoked to be responsible for the Mott insulating phase in A_4C_{60}. Compton Scattering can be used to measure the ground-state electronic density in solids and to check the results of wave functions calculated by the LDA method. Our aim was to understand the Rb_4C_{60} electronic density change leading to the insulator-metal transition at 0.8 GPa. The pressure effect is experimentally studied on Compton profiles and compared with the corresponding calculated results, obtained from new *ab initio* energy-band structure calculations. Our results allowed us to quantitatively discriminate between contraction of the unit-cell and contraction of the C_{60} molecule itself. As a result, we pointed out an unexpected C_{60} molecule volume contraction leading to a major effect on the electronic density.

Magnetic Compton profiles of Pd/Fe and Pd/Co multilayers

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Anisotropies of magnetic Compton profiles are measured on Pd/Fe and Pd/Co multilayers. The anisotropies are prominent in the Pd/Co multilayers that have perpendicular anisotropies. On the contrary, the anisotropies are small in the Pd/Fe multilayers that have high permeability. These facts suggest that the anisotropy of wave function dominates magnetic properties, such as anisotropy and permeability.

A RIXS study of valence excitations in CuO

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Shakeup satallites are found in the synchrotron-radiation-based RIXS spectra of CuO single crystals, excited near the Cu *K* edge. Based on a third-order perturbation treatment, the satellites are attributed to charge-transfer transitions between a binding b_{1g} ground state and antibinding states of a_{1g},b_{2g},b_{1g} and e_g symmetry, induced by the Coulomb interaction of the 1s hole with the Cu 3*d* system. Only by use of third-order perturbation treatment, the rather complicated dependence of the satellite's energy-loss position on the incident photon energy could be modelled, where two different transitions of the Cu 1*s* electron into 3*d*9 4*p* states must be conceded to constitute the RIXS process. These transitions were investigated in greater detail by means of resonantly excited 1*s*2*p* ($K\alpha$) emission, especially with respect to their dependence on the incident polarization.

High-resolution Compton scattering study of $Nb_{50}Mo_{50}$

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The Nb-Mo system is very interesting because Nb and Mo both possess partially filled 4*d* shells and very similar band structures, indicating the alloy to be in the weak scattering regime. In this paper we present high-resolution directional Compton profiles of $Nb_{50}Mo_{50}$ along the [100], [110], [111], [112] and [221] directions. The measurements were made using a high-resolution Compton spectrometer with 55.82 keV x-rays located at the European Synchrotron Radiation Facility (ESRF), France. The results are compared and contrasted with corresponding KKR-CPA calculations. The anisotropy in momentum densities is interpreted in terms of Fermi surface topologies. It is seen that KKR-CPA calculations substantially reproduce fine structures in the anisotropy of the electron momentum distribution.

Probabilities for radiative vacancy transfer from L_i subshells to *M* and *N* shells for some heavy elements

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The probabilities [$\eta_{L_i}J(R)$] for transfer of vacancies to the *M* and *N* shells following radiative decay of L_i (i = 1,2,3) subshell vacancies for elements with 77 < Z < 83 have been deduced using theoretical photoionization cross sections and the measured fluorescence cross sections for the L_i subshell x-rays following ionization by the 59.54 keV gamma-rays $\beta_{L_1}<E_{inc}<\beta_k$ and for the L_3 subshell x-rays following ionization by the *K* x-rays of a suitable secondary target ($\beta_{L_3}<E_{k\alpha}<\beta_{L_2}$,$\beta_{L_1/L_2}<E_{k\beta}<\beta_K$); where β_{K/L_i} is the *K* shell/L_i subshell ionization threshold of the target element. The error in the measured values is estimated to be 6-8%. The measured probabilities $\eta_{L_2}J(R)$ and $\eta_{L_3}J(R)$ [J = M, N] are in good agreement with the calculated ones. The present values of $\eta_{L_1}J(R)$ [J = M, N] are 15-30% higher than those calculated using the theoretical Dirac-Fock model-based radiative transition rates and relativistic Dirac-Hartree-Slater model-based nonradiative transition probabilities for all the elements under investigation, except for Pt where these are higher by 55-60% than the calculated ones. The exceptionally high value of the deduced $\eta_{L_1}J(R)$ indicates that the predicted jump in the calculated value due to onset of L_1-L_3M_4 CK transition at Z=78 is not observed. Further, the deduced $\eta_{L_1}J(R)$ values exhibit a decrease ~ 14% at Z=79, which is likely to be due to onset of the L_1-L_3M_4 CK transition predicted at Z=78.

X-ray Raman spectroscopy studies of C_{60} fullerenes and multi-wall carbon nanotubes‡

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The electronic structures of C_{60} fullerenes and multiwall carbon nanotubes (MCNT) were probed by x-ray Raman scattering spectroscopy. The measurements were performed at HPCAT ID-D of the Advanced Photon Source. Spectra of the C_{60} fullerenes and MCNTs at ambient pressure reveal similarities between the carbon *K*-edge spectra and the spectrum of graphite [1,2]. The distinction between the *K*-edge spectra is that the C_{60}'s have three narrow π*-bands below 292 eV and two broad σ*-bands above 292 eV, whereas MCNTs have one narrow π*-band and two broad σ*-bands. The π*- and σ*-bands in the Raman spectra of both materials are of similar intensities. Measurements at several scattering angles show an angle-independent x-ray Raman scattering process in both C_{60}'s and MCNTs. Preliminary high-pressure experiments below 5 GPa show that with pressure the π*-band intensity clearly decreases relative to the σ*-bands in both C_{60}'s and MCNTs. The ambient and high-pressure results will be discussed in detail.

[1] J.P. Rueff, et al., J. Phys.: Condens. Matter **14**, 11635 (2002).
[2] W. Mao, et al., Science **302**, 425 (2003).

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1*s*-2*p* Resonant x-ray emission in $La_{(2-x)}Sr_xCuO_4$

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We have measured 1*s*-2*p* resonant x-ray emission spectra in undoped and under-doped $La_{(2-x)}Sr_xCuO_4$ around the copper *K* edge. We observe fine structure that is dependent on the orientation of the polarization with respect to the *a*-*b* plane of the samples and to the doping in the samples. The fine structure is also very sensitively dependent on the incident energy and thus the intermediate state of the RXES process, permitting us to distinguish between the dipolar 1*s*-4*p* pi and sigma transitions, as well as quadrupolar 1*s*-3*d* transitions. Measurements are compared with calculations based on the Anderson impurity model. This study provides important information on the Cu partial density of empty states in this correlated material and its dependence on doping.

Phonon dispersion and lifetimes in MgB_2

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We measure [1] phonon dispersion and linewidth in a single crystal of MgB_2 along the $\Gamma \rightarrow A$, $\Gamma \rightarrow M$ and $A \rightarrow L$ directions using inelastic x-ray scattering. We use density functional theory to compute the effect of both electron-phonon coupling and anharmonicity on the linewidth, obtaining excellent agreement with experiment. Anomalous broadening of the E_{2g} phonon mode is found all along $\Gamma \rightarrow A$. The dominant contribution to the linewidth is always electron-phonon coupling.

[1] Phys. Rev. Lett. **90**, 095506, (2003)

Compton scattering of gas hydrates

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Gas hydrates are inclusion compounds in which small hydrophobic guests are trapped in cages formed by water molecules. These compounds have attracted considerable interest because large deposits of natural methane hydrates have been found on the ocean sea floor and in permafrost regions. The hydrate cages are stabilized by the repulsive interaction between the guests, e.g., methane or noble gases, and the host lattice, i.e., hydrate structures without guests do not exist.

We performed Compton profile measurements of several gas hydrates, as well as of hexagonal ice, to find indications for the guest-host interaction in these compounds. The Compton profiles have been measured at beamline ID15b of ESRF with a momentum space resolution of 0.38 a.u. at 56.4 keV incident energy at a 173° scattering angle. The sample temperature was about 80K during the measurements, and the stability of the samples has been checked by taking diffraction patterns before and right after the measurements. The resulting Compton profiles have been analyzed using Hartree-Fock Compton profiles and LCAO calculations for the noble gases and the methane guests, respectively, showing good overall agreement between experiment and theory. However, small differences between experimental and theoretical Compton profiles remain, which will be discussed in terms of deviations of empty hydrate from hexagonal ice LDA Compton profiles.

3*d* Spectator hole satellites of the Cu $K\beta_{1,3}$ and $K\beta_{2,5}$ emission spectrum

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Multielectron excitations during inner shell vacancy creation have been extensively studied within the isothermal regime far above the excitation threshold. With the advent of 3rd-generation synchrotron sources, x-ray fluorescence spectroscopy became a prominent tool to investigate these excitations in a wide range of excitation energies from the excitation threshold (adiabatic regime) up to the saturation limit (isothermal regime). One of the best studied materials with respect to multielectron excitations using x-ray fluorescence is Cu.

We present measurements of the intensity evolution of the Cu $K\beta_{1,3}$ and $K\beta_{2,5}$ emission spectrum as a function of excitation energy using resonant inelastic x-ray scattering. The contribution from 1*s*3*d* shake satellites to both emission spectra is extracted. The saturation behaviour of the satellites is shown to be independent on the re-emission shell of the shake process. The saturation limit as a function of excitation energy is reached rapidly in contrast to the Cu 1*s*1*s* and 1*s*2*p* shake satellites. An upper limit of the shake-up contribution to the total shake intensity is found to be 20%. Furthermore, significant contributions from the KMN and KNN radiative Auger satellite to the Cu $K\beta_{1,3}$ and $K\beta_{2,5}$ fluorescence spectrum are found, respectively. The KNN radiative Auger satellite is shown to play an important role within the interpretation of valence emission spectra.

Use of quartz crystals as backscattering monochromators

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Quartz crystals offer a possible alternative to the silicon backscattering monochromators presently used in IXS experiments, particularly in the photon energy range of 5-10 keV. Because the quartz crystal lattice is trigonal (space group $P3_121$ or $P3_221$) as opposed to the silicon crystal's cubic diamond structure, quartz has fewer forbidden reflections and thus more backscattering reflections per unit photon energy range. Different backscattering reflections in quartz can also differ greatly in bandpass, even if their photon energies are nearly equal. This is very different from silicon, in which the bandpasses of the even reflections and of the odd reflections form two simple curves that decrease monotonically with increasing photon energy. As a result, quartz allows the photon energy and the energy resolution to be more readily tailored to experimental needs. The main issue at this point is whether sufficiently pure and undistorted quartz crystals can be obtained for the proposed purpose. Topographs of commercially made synthetic quartz crystals published by other authors have shown such crystals to be divided into several zones of different impurity levels and degrees of lattice distortion. Tests of synthetic quartz crystals with synchrotron radiation are planned at SPring-8 this year.

Theory of resonant inelastic x-ray scattering in cuprates

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Resonant inelastic x-ray scattering (RIXS) has received much attention as a powerful technique to investigate elementary excitations in strongly correlated electron systems. In particular, the momentum-dependent spectra of Cu *K*-edge RIXS in high-T_c cuprates have been obtained by several experimental groups. The knowledge of these excitations across the gap, as well as single-particle excitations, is of importance for understanding the electronic properties in cuprates.

We demonstrate theoretically momentum dependences of the RIXS in insulating and doped cuprates. The RIXS spectra are calculated by using the exact diagonalization techniques on small clusters in two-dimensional Hubbard models with 1*s*-core bands. In the insulating case, we find the anisotropic momentum dependence in the RIXS spectrum. The dependence is explained by the particle-hole excitations in which the antiferromagnetic correlation of the ground state plays a crucial role. Upon hole-doping, the spectrum from the lower Hubbard band to the upper Hubbard band becomes broad and less momentum dependent. This is in contrast to the case of electron-doping, where the momentum dependence of the spectrum in the undoped system remains, except that along the <1,0> direction. The difference in the spectra between hole- and electron-doped systems follows the carrier dependence of short-range AF spin correlations.

Development of X-eX spectrometer at KEK-PF-AR

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To obtain the two-dimensional and three-dimensional momentum density directly from an experiment, an X-eX spectrometer has been developed at KEK-PF-AR. The spectrometer is equipped with a time-of-flight energy analyzer to record the flight direction and the kinetic energies of recoiled electrons, and a position-sensitive photon detector to record directions of Compton scattered photons. The signals from the electron branch and those from the photon branch are processed in coincidence mode. The measured two-dimensional momentum density on the [100] plane in Si and the three-dimensional momentum density on some major symmetry axes will be presented and compared with FLAPW theoretical results obtained by Kubo (private communication).

Observation of quadrupole transitions of lanthanide compounds by high-resolution lifetime-broadening-suppressed XANES spectroscopy

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Determination of energies and relative strength of the dipolar and quadrupolar transitions in L_3 XANES are essential for understanding of the properties of lanthanide compounds. Weak pre-edge features arising from the 2*p*-4*f* quadrupole transitions are, however, often smeared out within the lifetime broadening (~4 eV) of the 2*p*-5*d* dipolar transitions. We have recently shown that through analyses of resonant inelastic x-ray scattering (RIXS) in terms of a formula derived from the Kramers-Heisenberg equation, lifetime broadening can be circumvented [1]. However, limited resolution of the spectrometer employed prevented us from obtaining very sharp bands.

RIXS measurements with higher resolution make it possible to observe fine structures in absorption spectra more distinctly. In this study, we apply lifetime-broadening-suppressed spectroscopy to L_3 XANES of lanthanide compounds, $Dy(NO_3)_3$ and Ho_2O_3. It is demonstrated that analyses of highly resolved RIXS spectra provide several very sharp (~0.1 eV) 2*p*-4*f* peaks, separated from the 2*p*-5*d* main band by a few eV, offering a unique and powerful method for studies of electronic states of lanthanide compounds.

[1] H. Hayashi et al., Phys. Rev. B **68**, 45122 (2003)

Spin transitions studied with x-ray emission spectroscopy

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Transition metal ions in octahedral surroundings with electron configuration *d*4 ... *d*7 can be in low spin (LS) or in high spin (HS) states, depending on the energy separation of the t_{2g} and e_g levels caused by the crystal field. An interesting class of molecular compounds of these ions shows spin transition upon external perturbations. In these systems, the spin state can be switched back and forth between the LS and the HS states by triggering a redistribution of the 3*d* electrons on the t_{2g} and e_g levels. We have studied such spin transition compounds of Fe^{3+}, Fe^{2+} and Co^{2+}, which cover almost the entire *d*4...*d*7 range, have unambiguous spin states and show diverse spin transitions, to demonstrate that techniques based on x-rays emitted after 1*s* core ionization of the metal ion are true spectroscopic probes of the local magnetic moment, as well as the electronic state. Our x-ray emission spectra, which reflects the variation of the spin states of different transition-metal ions of well-defined 3*d* configurations with preserved chemical environment and valence state, can be regarded as benchmark measurements in studying magnetism with XES. Applications to other spin transition systems will also be discussed.

Compton scattering on alkali-metal-doped silicon clathrates

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Silicon clathrates are guest-host materials in which a dopant is trapped in cage-like structures built up from covalently bonded Si atoms. Using the Compton-scattering technique, we studied the guest-host interactions of the silicon clathrates, which are of special importance to reach a deeper understanding of the electronic properties of these candidates for thermoelectric applications. Compton scattering gives a valuable tool at hand to investigate how the electronic ground state along with the electronic wave functions of the host lattice is changed by the different alkali-metal guests.

Compton profiles of the empty-caged Si_{136} structure II clathrate and of the alkali-metal-doped M_8Si_{46} (M = Na, K, Rb) structure I calthrates, as well as polycrystalline Si, have been measured at the Compton-scattering beamline ID15B of the ESRF using an incident photon energy of 56.4 keV with a momentum space resolution of 0.25 a.u. The Compton-profile differences between the alkali-metal-doped Si clathrates and the empty-caged structure are compared with LDA calculations of these systems, and the valence electron Compton profile is discussed in terms of charge transfer between the guest and the host lattice.

Nuclear resonant vibrational spectroscopy of *Pyrococcus furiosus* rubredoxin

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Rubredoxins are small (~50 amino acid) electron-transfer proteins that contain a single Fe(S-*cys*)$_4$ redox center that occur in several anaerobic bacteria. Apart from their role in specific biological catalytic reactions, rubredoxins serve as model systems for understanding the factors that determine reduction potentials in metalloproteins.

Nuclear resonant vibrational spectroscopy (NRVS) is an important new technique for understanding iron metalloproteins through their vibrational spectra based on the high brilliance third-generation synchrotron sources and development of tunable monochromators with sub-meV resolution, sensitive only to those vibration modes involving the iron atoms that provides useful site selectivity.
The vibrational spectra of oxidized rubredoxin and reduced Rubredoxin were measured by NRVS, resonance Raman spectra for the oxidized protein are also presented. Normal mode calculations are used to reproduce and interpret the experimental spectra because the NRVS intensity is directly related to the mean-square displacement (msd) of Fe motion. Both the frequency and the intensity of the NRVS bands were used as constraints. In both proteins, the T2 modes of tetrahedral symmetry have been degenerated to three components because of the lowing of symmetry. The Fe-S stretch force constant is decreased from 1.4 mdyn/Å for oxidized rubredoxin to 1.04 mdyn/Å for reduced rubredoxin due to the diminishment of this interaction in reduced protein compared to the oxidized one.

Phonon dispersion curves by thermal diffuse x-ray scattering: A case study of an fcc Pu-Ga alloy

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Thermal diffuse x-ray scattering has been used to study the phonon dispersion curves (PDCs) of an fcc Pu-0.6 wt% Ga alloy. By focusing an 18 keV undulator x-ray beam at the APS to a diameter of ~30 μm, it was possible to selectively probe single grains of a large-grained polycrystalline foil. Three TDS intensity patterns from grains oriented in approximately the <100>, <110>, and <111> directions were simultaneously fit to a Born-von Karman force constant model using a least-squares fitting routine. The resulting PDCs are in good agreement with those obtained from IXS measurements performed at the ESRF [1]. In particular, a pronounced softening of the transverse acoustic branch along the <111> direction is clearly seen. The rapid data collection rates of TDS as compared to IXS make it well suited for studying the evolution of the PDCs as a function of external parameters, such as temperature or pressure. Initial results on the temperature and composition dependence of the PDCs will be presented, and the future directions for this research will be discussed.

[1] J. Wong et al., Science **301**, 1078 (2003).

Collective dynamics of supercritical water

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Water has recently been revealed to be a unique medium for chemical processes in the supercritical condition. The usefulness of supercritical water is related to the drastic change in its properties as a solvent from the ambient condition.

We have measured IXS on sub- and supercritical water (or expanded water) with the density of 1-0.26 gcm^{-3} in the Q range 1.3-10.7 nm^{-1} using a high-resolution spectrometer installed at BL35XU/SPring-8 and using a high-pressure vessel made of Inconel625 alloy with thin diamond windows. From this experiment, we have investigated high-frequency phonon excitations in water with decreasing density, where a suppression of the hydrogen bonding nature has been reported.

At room temperature, the features of the present spectra are in good agreement with previous IXS data, i.e., phonon excitations can be seen as shoulders at both sides of the central peak, and the excitation energies are much faster than the hydrodynamic values. With decreasing density, the magnitude of the positive deviation of the high-frequency phonon excitations from the hydrodynamic value rapidly decreases from about 100% (about 1 gcm^{-3}) to about 10% (about 0.8 gcm^{-3}). With a further decrease of density, it becomes large again.

Sapphire analyzers for RIXS?

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Backscattering analyzers for inelastic x-ray scattering experiments have been under development for over two decades. Large angular acceptance and good reflectivity make this geometry attractive. So far Si and Ge have been successfully used, due to the availability of good crystals. However, there is a need to find other crystals, as IXS experiments at specific energies near the atomic absorption edge may provide element-specific electronic state information. Hence crystals of lower symmetry containing more than one element are of great interest. In this study, we have developed new manufacturing techniques to build spherically bent, diced sapphire analyzers. Procedures regarding dicing, etching and bonding will be discussed, and initial test results for Al_2O_3 (0 4 14) at 8.9 keV will be presented.

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