Abstracts

The 27th Hiroshima International Symposium on Synchrotron Radiation

Materials Science using VUV-SX Synchrotron Radiation : Towards the future HiSOR-II project

March 9- 10, 2023

Faculty Club, Hiroshima University

Hiroshima Synchrotron Radiation Center, Hiroshima University

Supported by

The Japanese Society for Synchrotron Radiation Research

Particle Accelerator Society of Japan

The 27th Hiroshima International Symposium

on Synchrotron Radiation

Materials Science using VUV-SX Synchrotron Radiation : Towards the future HiSOR-II project

March 9 – 10, 2023
Hiroshima University Faculty Club

March 9 (Thursday)

08:45 – 09:30 Arrival and Registration

Opening

Chairperson: S. Ideta

09:30 – 09:35 Greeting

Shuhei HAYASHI (Deputy Director, Research Environment Division, Science and Technology Policy Bureau, Ministry of Education, Culture, Sports, Science and Technology (MEXT))

09:30 – 09:35 Greeting

Shinji KANEKO (Executive Vice President(Global Initiatives), Executive Vice President (Research and Academia-Government-Community Collaboration), Hiroshima University, Japan)

09:40 – 10:10 Overview of HiSOR Activities and Future Plan

Kenya Shimada

Director, Synchrotron Radiation Center, Hiroshima University, Japan

10:10 – 10:30 Symposium Photo

10:30 – 10:45 Coffee break

Oral Session 1

Chairperson: H. Sato

10:45 – 11:20 O 01 Teppei YOSHIDA

Kyoto University, Japan

"Electron-phonon coupling in correlated electron systems revealed by angle-resolved photoemission spectroscopy"

11:20 – 11:55 O 02 Yuita FUJISAWA

Okinawa Institute of Science and Technology Graduate University, Japan

"Laboratory-based in-situ photoemission spectroscopies of quantum material epitaxial films"

11:55 – 12:30 O 03 Meng WANG

RIKEN, Japan

"XAS study of spin-state related percolative dynamics in magnetic cobaltites"

12:30 – 13:40 Lunch

Poster Session

Chairperson: M. Sawada

13:40 – 14:40 Student Short Oral Session (1-2 min/each)

14:40 – 16:30

※Best Student Poster Award※

We will present the Best Student Poster Award. The winner will be announced during the welcome reception.

Oral Session 2

Chairperson: K. Matsuo and M. Ibrahim

16:30 – 17:05 O04 Martin ANDERSSON

Chalmers University of Technology, Sweden

"Engineering the Biology-Material Interface for Safer Medical Devices"

17:05 – 17:40 O 05 Marie-Christine AVERLANT-PETIT

LCPM, Lorraine University, France

"Self-Assembling of Peptide-Based Gels : A Multiscale Structural Analysis"

Chairperson: H. Namatame

18:00 – 20:00 Welcome Reception

LA Bohème(Faculty Club)

March 11 (Friday)

Oral Session 3 HiSOR-II Special Session
Chairperson: K. Miyamoto

09:30 – 09:45 O 06 Masahiro KATOH
Hiroshima University, Japan
"Design of HiSOR-II"

09:45 – 10:20 O 07 Akira MOCHIHASHI
The Karlsruhe Institute of Technology, Garmany
"KIT – Status of Test Facilities KARA and FLUTE"

10:20 – 10:55 O 08 Shan QIAO
Shanghai Institute of Microsystem and Information Technology, China
"The progress of spin-resolved photoelectron spectroscopy in Shanghai"

10:55 – 11:30 O 09 Dongang ZHANG
Shanghai Jiao Tong University, China
"THz-enhanced ultrafast electron diffraction"

11:30 – 13:00 Lunch

Oral Session 4 HiSOR-II Special Session
Chairperson: M. Katoh

13:00 – 13:35 O 10 Hirofumi YANAGISAWA
University of Tokyo, Japan
"Subnanometric optical control of electron emission sites"

13:35 – 14:10 O 11 Takayuki ICHIKAWA
Hiroshima University, Japan
"Material Science toward achieving Carbon Neutrality"

Closing
Chairperson: Ideta

14:10 – 14:25 Student Award Ceremony
14:25 – 14:30 Closing Remarks
15:00 – 15:30 HiSOR Tour (English)
15:30 – 16:00 HiSOR Tour (Japanese)

Oral Session

-Oral Session-

O01 Electron-phonon coupling in correlated electron systems revealed by angle-resolved photoemission spectroscopy

Teppei YOSHIDA
Graduate School of Human and Environmental Studies, Kyoto University, Japan

O02 Laboratory-based in-situ photoemission spectroscopies of quantum material epitaxial films

Yuita FUJISAWA, Anjana Krishnadas and Yoshinori Okada
Quantum Material Science Unit, Okinawa Institute of Science and Technology, Japan

O03 XAS study of spin-state related percolative dynamics in magnetic cobaltites

Meng WANG
RIKEN Center for Emergent Matter Science (CEMS), Japan

O04 Engineering the Biology-Material Interface for Safer Medical Devices

Martin ANDERSSON
Dept. Chemistry and Chemical Engineering, Applied Chemistry, Chalmers University of Technology, Sweden

O05 Self-Assembling of Peptide-Based Gels : A Multiscale Structural Analysis

Loïc Stefan[a], Guillaume Pickaert[a], Mohamed Ibrahim[b] and Marie-Christine Averlant-Petit[a]
[a]Laboratoire de Chimie Physique Macromoléculaire (LCPM), Université de Lorraine, France.
[b]Hiroshima Synchrotron Radiation Center (HiSOR), Hiroshima University, Japan.

O06 Design of HiSOR-II

Masahiro Katoh[a,b]
[a]Hiroshima University, Japan
[b]Institute for Molecular Science, National Institutes of Natural Sciences, Japan

O07 KIT – Status of Test Facilities KARA and FLUTE

Akira MOCHIHASHI
Karlsruhe Institute of Technology (KIT), Institute for Beam Physics and Technology (IBPT), Germany

O08 The progress of spin-resolved photoelectron spectroscopy in Shanghai

Shan QIAO
Shanghai Institute of Microsystem and Information Technology, China

O09 THz-enhanced ultrafast electron diffraction

Dongang ZHANG
School of Physics and Astronomy, Shanghai Jiao Tong University, China

O10 Subnanometric optical control of electron emission sites

Hirofumi YANAGISAWA[a-d]

[a]*Japan Science and Technology Agency, Japan*
[b]*The University of Tokyo, Japan*
[c]*Ludwig-Maximilians-Universität Munich, Germany*
[d]*Max Planck Institute of Quantum Optics, Germany*

O11 Material Science toward achieving Carbon Neutrality

Takayuki ICHIKAWA

Graduate School of Advanced Science and Engineering, Hiroshima University, Japan

Electron-phonon coupling in the correlated electron systems revealed by angle-resolved photoemission spectroscopy

Teppei Yoshida

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Electron-phonon coupling is one of the fundamental many-body interactions and has been discussed as the key to the enhancement of the superconducting temperature T_c in a wide variety of materials such as A-15 compounds, high-T_c cuprates, iron pnictides/chalcogenides, and hydrogen sulfide. The signature of electron-phonon interactions appears in the kink and spectral linewidth of the quasiparticle dispersion and can be investigated by angle-resolved photoemission spectroscopy.

Here we present the signature of electron-phonon coupling observed in the electronic states of $Ca_{2-x}Sr_xRuO_4$ (CSRO) [1] and $BaIr_2Ge_7$ [2]. CSRO shows a metal-insulator transition with a structural phase transition. In the region of small x, the bulk of CSRO is in the insulating phase at low temperatures. We have performed angle-resolved photoemission spectroscopy (ARPES) of CSRO (x = 0.06) and revealed that the surface is in a metallic state while the bulk is in an insulating state. The observed band dispersion of the surface metallic state exhibits kink structures with the energy scales of 35 and 60 meV. The distinct kink structures suggest a strong electron–phonon coupling compared with Sr_2RuO_4.

We also performed ARPES on $BaIr_2Ge_7$ with cage structures and observed the temperature dependence of the ARPES spectra near the Fermi level. We found that the width of the spectral peak shows a concave-downward behavior with temperature similar to the electrical resistivity. Considering the effect of anharmonic phonon modes, this behavior was well reproduced in our simulations. Our results suggest the existence of the weak anharmonic phonon modes in $BaIr_2Ge_7$.

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Laboratory-based *in-situ* photoemission spectroscopy of quantum material epitaxial films

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Epitaxial film technology allows us to design and control the physical properties of quantum materials beyond the bulk properties. It also makes it possible to investigate materials that have been difficult to synthesize their bulk single crystals by such as angle-resolved photoemission spectroscopy (ARPES). To reveal the electronic states of exotic quantum material epitaxial films, we have constructed a so-called vacuum cluster system where a pulsed laser deposition (PLD) system and an APRES system are connected under ultra-high-vacuum (see **Figure 1a**)[1,2]. In this talk, I'd like to introduce one of the recent studies on an oxide superconductor, $LiTi_2O_4$ (LTO).

LTO is a unique spinel oxide with a high superconducting transition temperature of 13 K (see **Figure 1b**). While it is expected to have intimate relation between superconductivity and orbital degree of freedom, less is understood about this material because large size single crystal has not been available. Recently, epitaxial film growth using PLD has been reported [3]. However, direct observation of the electronic structure by APRES has not been accomplished.

This work presents the first observation of the band structure of LTO (111) thin films grown by PLD. The hexagonal Fermi surface with corners on the Brillouin zone corner implies that a saddle point exists near the Fermi energy (E_F). The band dispersion shows a distinct kink structure at 50 meV below E_F, suggesting the enhanced many-body effects. Its temperature dependence reveals a phase transition around 150 K accompanied by the disappearance of the kink. We will discuss the origin in detail.

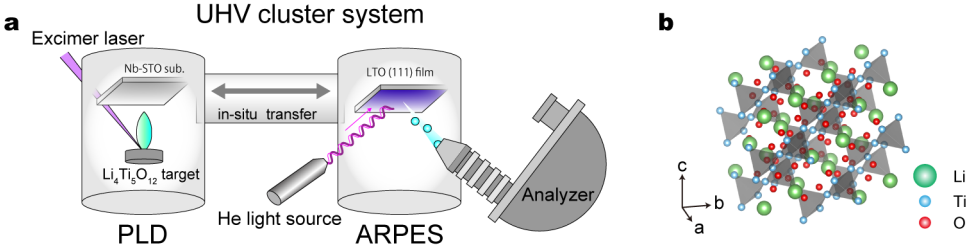

FIGURE 1. (a) Schematics of our UHV cluster system connecting the PLD and the ARPES systems under ultra-high vacuum. (b) Crystal structure of the spinel oxide superconductor $LiTi_2O_4$.

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XAS study of spin-state related percolative dynamics in magnetic cobaltites

Meng Wang [a]

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Mixed-valent cobaltite is a double-exchange ferromagnetic system, as analogous to the double-exchange manganite. However, the colossal magnetoresistance (CMR) associated with a magnetic-field-driven insulator-metal transition (IMT) at the phase boundary has not yet been reported in cobaltite. Combining magnetic transport, magnetization, magnetic-force-microscopy (MFM), and X-ray absorption spectroscopy (XAS) measurements, we conducted a systematic research on the $La_{0.7}AE_{0.3}CoO_3$ (AE = Ca, Sr, and Ba) films and unveiled the hidden mechanisms that dominate the phase transition dynamics in cobaltite. First, in contrast to utilizing the bulk crystal, we fabricated films on a $SrTiO_3$ substrate with tensile strain to drive it to the insulator-metal phase boundary. All films exhibit a ferromagnetic and non-ferromagnetic phase separation, which is robust against an isothermal magnetic field sweeping, while a percolation induced insulator-to-metal transition can be achieved by a field-cooling process. Such a thermodynamic-history-dependent properties signify a nonergodic feature associated with the dynamics of magnetic domains. By further comparing the nonergodic properties and the spin-sates among $La_{0.7}AE_{0.3}CoO_3$ films by the transport and XAS measurements, respectively, we reveal that the mixed low-spin Co^{3+} forms a key factor to enhance the energy barrier for domain-wall motions during domain percolation. Such a spin-state degree of freedom is absent in manganites, probably resulting in the large difference of the phase evolution kinetics in the magnetic-field-induced IMT between cobaltite and manganite. [1]

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Engineering the Biology-Material Interface for Safer Medical Devices

Martin Andersson

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SE-412 96 Gothenburg, Sweden

In this presentation, two different concepts of engineering the interface between artificial materials and biology will be demonstrated. The first example is an attempt to form synthetic bone materials, intended for use in medical devices as well as a model system to study bone mineralization, to shed light on *in vivo* bone formation mechanisms. In the second example, controlled surface topography and its impact on protein interaction with surfaces is in focus. Specifically, topographical alterations on similar length scale as proteins has shown to largely affect the interactions, giving us a tool to regulate how foreign materials are integrated with living tissue. This is for example of great interest in the development of medical devices, such as implants, and how they are accepted in the human body.

A novel synthetic approach, highly inspired by the architecture of natural bone, to design mechanically stable nanocomposites incorporating aligned apatite nanocrystals will be demonstrated.[1] To mimic the nanostructure of natural bone, we first combine molecular self-assembly and intermolecular crosslinking to create resilient polymeric matrices with long-range periodicity; then we employ compartmentalized mineral growth via a transient amorphous phase for the biomimetic formation of bone-like apatite. The nano-domains and their alignment has been investigated using 3D small angle X-ray scattering (3D-SAXS)[2] and the crystallization process has been studied using transmission electron microscopy (TEM).[3]

By using silica nanoparticles of various sizes immobilized onto surfaces, the nanotopographical effect on the classical immune complement activation through adsorption of IgG and the following binding of C1q, was examined.[4] In another example, using silica nanoparticles deposited as a gradient in nanostructure density on a surface, the initial attachment of bacteria with or without the presence of human fibrinogen was examined.[5] By using a parallel plate laminar flow chamber, we found a near-linear positive correlation between the adhesion of S. epidermidis with increasing nanoparticle density. However, if the nanostructured gradient was precoated with human fibrinogen the opposite relationship was observed, although the adsorbed amount of fibrinogen was found to be higher on nanostructured than on smooth surfaces. This latter observation correlated well with protein conformation studies using circular dichroism (CD), where the nanostructured surfaces preserved the protein secondary structure, similar to in solution, as compared to the smooth surfaces.

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Self-Assembling of Peptide-Based Gels: A Multiscale Structural Analysis

Loïc Stefan[a], Guillaume Pickaert[a], Mohamed Ibrahim[b] and Marie-Christine Averlant-Petit[a]

[a]*Laboratoire de Chimie Physique Macromoléculaire (LCPM), Université de Lorraine, France.*
[b]*Hiroshima Synchrotron Radiation Center (HiSOR), Hiroshima University, Japan.*

Supramolecular hydrogels have drawn much attention in the past years especially because of their broad range of applications from material science to medical science domains. Peptide-based gels have been developed lately [1, 2], mainly thanks to their higher modularity and possibilities of functionalization compared to polymer gels [3, 4]. Mechanisms of forming peptides hydrogels are starting to be examined: first is the gelation of nanofibrous peptides assemblies and is observed predominantly with oligopeptide precursors. Gel formation in such systems involves supramolecular assembly of precursors into nanofibers, -tapes, -tubes, or -ribbons that entangle and form nonspecific.

The capability of peptides and proteins to form gels is long time known, as gelatine used in cooking. But the development of gel materials was mostly built on serendipity. Moreover, only a few publications are found on relationships between the mechanical properties of the gel materials and their self-assembling [5-7], although the mechanical properties are very important for the applications. As a mesh has a different appearance depending on whether the knitting is tight or loose, there is a correlation between morphology and number of fibrils and mechanical properties of the obtained material. But so far, no rules were found that can predict which peptide sequence, or peptide modification leads to self-assembling in a gel and what kind of soft material it will give. This observation is the starting point of our project.

The assumption is the following: the self-assembling process and the interactions involved in the first stages has an impact on the size, morphology, number of fibrils and, subsequently, on the material properties. study the interactions from the inter-molecular level to supra-molecular, meso-level, and macroscopic properties, to investigate the relationships between self-assembling of the peptide-based molecules and the resulting mechanical properties of gels. In the Laboratoire de Chimie Physique Macromoléculaire, we associate synthesis of gelling molecules, physical chemistry analysis, structural and 3D conformational modelling studies, imaging, and rheology experiments to evaluate correlation between the structural and self-assembling to mechanical properties of the resulting soft material.

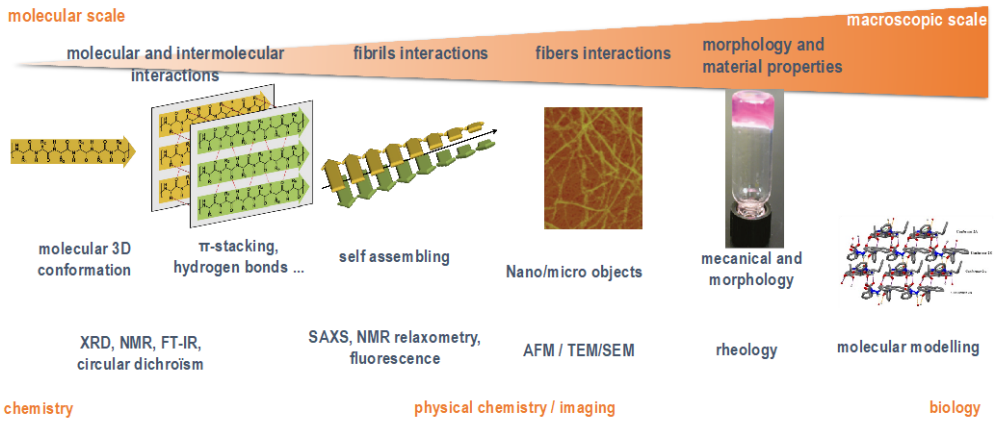

FIGURE 1. Multiscale structural analysis of self-assembling peptide-based gels.

To that end, a multiscale approach has been undertaken from molecular scale to macroscopic scale the interactions involved in the materials (Figure 1) to decipher their influence on the soft material formation and guide chemists to the next generation of gelling molecules.

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Design of HiSOR-2

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Keywords: Synchrotron light source, electron storage ring.

HiSOR, a low energy and compact synchrotron light source in Hiroshima University, has been operational since the middle of 1990's. It equipped with two undulators which produce high-brightness light in the vacuum ultraviolet range. It has two normal conducting bending magnets with high field strength of 2.7 T, which produce synchrotron radiation in a wide range including tender X-rays even with the low electron energy, 700MeV. On the other hand, the emittance is 400 nm, which is larger by two orders of magnitudes than the 3rd generation sources and results in the low brightness. This large emittance is caused by the simple lattice structure which consists of two 180 degree bending magnets. To make the beam injection system simple and compact, the injection is made at the energy of 150 MeV. Consequently, the ring cannot be operated in the top-up mode, which has become a standard operation mode in modern light sources. Since the HiSOR electron storage ring has a rational design without redundancy, it is difficult to make a major modification to improve the performance or introduce new technologies. This is in contrast with other light sources in Japan, such as Photon Factory [1], UVSOR [2] and SPring-8 [3], which already made or is planning major upgrades.

For the future plan of HiSOR, we designed a completely new ring, HiSOR-2 [4]. The circumference is about 50 m, the electron energy 500 MeV and the emittance around 10nm. It has six straight sections and four of them can be used for undulators. The small emittance gives much higher brightness of undulator radiation by two orders of magnitudes than the present one. It would have a new full energy injector to realize the top-up operation, which consists of a linear accelerator and a booster synchrotron. Such a completely new facility is ideal for further developing the researches based on the high brightness undulator radiation in the vacuum ultraviolet range. However, we have to prepare responding flexibly to changes in the environment surrounding synchrotron radiation science in Japan. As leaving this plan as one candidate, we have started designing alternative plan, which is more compact and hopefully can be realized with less budget [5].

An example of the design is shown in Fig. 1. The circumference is about 30 m and the electron energy is 500 MeV. The emittance is 17 nm. The ring has six 2.2 m straight sections, four of which can be used for undulators. To realize such a simple lattice, we have to develop combined function multipole magnets. Another example has similar lattice structure as in Ref. [4] but is more compact with the circumference of about 40m and the emittance of about 10 nm. An example of the accelerator layout with this second design is shown in Fig. 2, which requires construction of a new building for the storage ring and experimental hall but the full-energy booster synchrotron would be constructed in the present injector room.

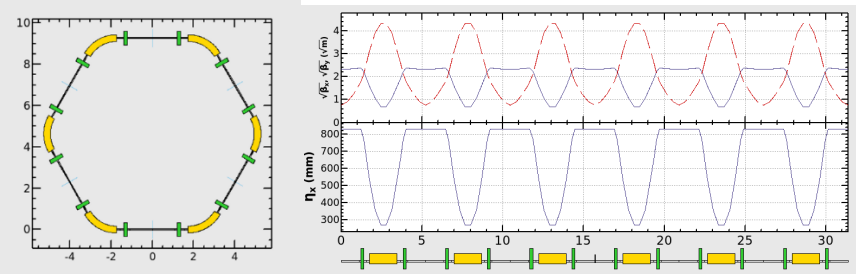

FIGURE 1. Magnetic lattice (left) and optical functions (right) of the new lattice design for HiSOR-2.

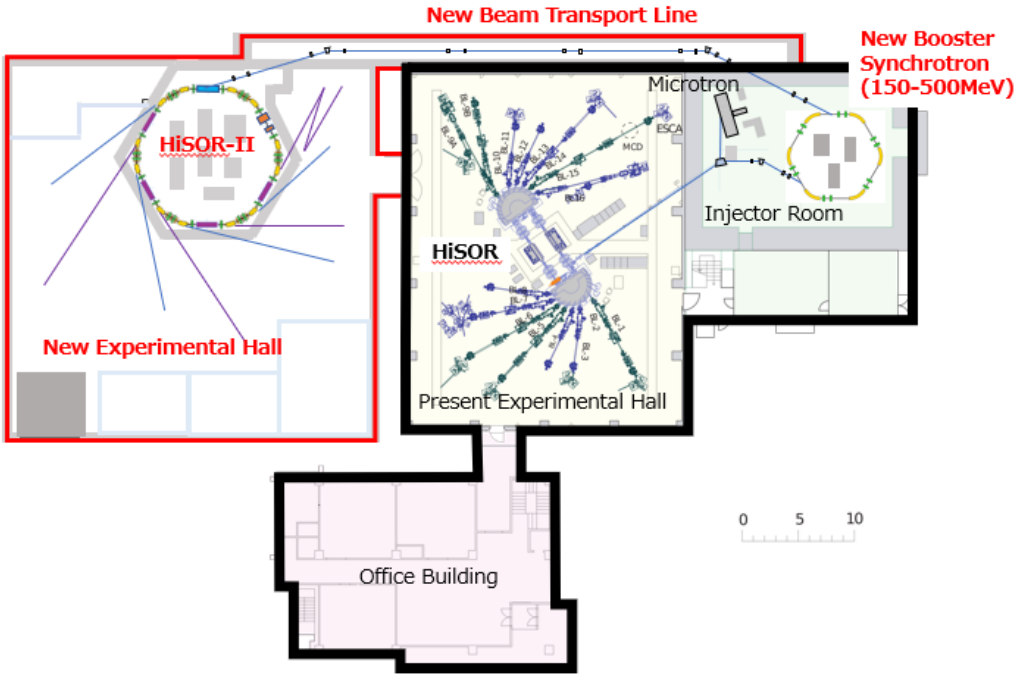

FIGURE 2. An example of the layout of the facility with a design of HiSOR-2 storage ring with 40 m circumference.

It should be noted that, in HiSOR-2, the bending magnets will be normal conducting and have ordinary field strengths such as around 1 T. In addition, the electron energy is lower than the present HiSOR. The bending radiation will not cover the X-ray range. This may strongly limit the application fields of new facility. The accelerator layout shown in Fig. 2 enables us to operate the present HiSOR even after the construction of HiSOR-2.

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5. Y. Lu *et al*., in these proceedings

KIT – Status of Test Facilities KARA and FLUTE

Akira Mochihashi[a], on behalf of the accelerator team at KIT IBPT

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In the Institute for Beam Physics and Technology (IBPT) [1] at the Karlsruhe Institute of Technology (KIT) in Germany, the accelerator complexes KARA and FLUTE are in operation as test facilities where various scientific activities for accelerator physics and technology take place now. The Karlsruhe Research Accelerator (KARA) is a high-energy electron storage ring, which provides electron beams with an energy range between 500 MeV to 2.5 GeV and a synchrotron radiation source, the KIT Light Source. The FLUTE (Ferninfrarot Linac- und Test- Experiment) facility serves as an accelerator test facility for various accelerator physics studies, whose core consists of a femtosecond chirped laser-driven RF photo injector, a linear accelerator, and an electron bunch compressor to provide ultra-short electron bunches for THz generation studies and non-linear physics investigations.

As test facilities, KARA and FLUTE and other research infrastructures within the Accelerator Technology Platform (ATP) [2] at KIT support the R&D of technologies for tomorrow's accelerators and detectors. Access to KIT-based accelerators via IBPT is augmented by European Transnational Access via several international projects such as EURO-LABS [3]. ATP provides a single point of contact (SPOC) and central access point for large-scale accelerator projects to the accelerators (KARA and FLUTE) and know-how located at KIT institutes.

IBPT provides an educational and hands-on environment for students and the next generation of accelerator scientists at KIT. Doctor and master candidates and bachelor students are currently engaged in research and development for the projects at KARA and FLUTE and other projects, where the latest frontiers of accelerator physics are promoted enthusiastically.

Following an introduction to KIT and IBPT, the presentation introduces the status of our accelerator complexes, KARA and FLUTE and current research topics and ongoing projects. The international projects associated with the activities are introduced in the context of the research topics at KARA and FLUTE. The educational environment and related outcoming products, such as theses and presentations at international conferences, are shown in the presentation.

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The Progress of Spin-Resolved Photoelectron Spectroscopy in Shanghai

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Chinese Academy of Sciences
863 Changning Road, Shanghai, China

Keywords: spin polarimeter, laser

The performances of two new image type VLEED spin polarimeters and 21 eV laser will be reported. The energy resolution of second version with permanent magnets and quadrupole lenses achieves 12 meV. The possibility to use 45 degree reflection for VLEED spin measurements was also checked and a higher efficiency was obtained at 3.5 eV. This type polarimeter with simple structure can achieve small aberration and have the ability to measure the three dimensional spin polarization. The construction of a time of flight spin polarimeter will also be reported.

Generating a laser with a short wavelength is a bottleneck problem in laser technology. The current applicable extreme ultraviolet (EUV) lasers generated by the multi-photon process, with low efficiency and the record short wavelength of 113.8 nm, do not meet some actual needs. we will report the development of a practical 58.4 nm laser by a single-photon-excitation related anti-Stokes Raman scattering (ASRS). The conversion efficiency is much higher than that of high harmonic generation (HHG). The almost same divergence of 1.9 mrad as that of excitation laser indicates its coherent and stimulating characters. Our results show an applicable path towards up-conversion by a single-photon process to generate intense EUV lasers.

The spin-resolved photoelectron measurements on some systems showing the ability of image type spin polarimeter will also be reported.

THz-enhanced ultrafast electron diffraction

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Ultrafast electron diffraction (UED) has gained tremendous interest in the ultrafast community in the last decades because of the ability to provide atomic-level material structure information on the femtosecond time scale. Terahertz laser-based accelerators are prominent candidates for driving next-generation compact light sources, promising high-brightness, ultrashort x-ray and electron pulses. Here, I will present on the development of key components in the development of THz based electron sources. Different THz based devices that are capable of performing multiple high-field operations on the 6D-phase-space of ultrashort electron bunches will be introduced, that includes electron acceleration, compression, focusing and streaking [1,2].

The first application with THz-powered electron source in ultrafast electron diffraction will be discussed [3]. In proof-of-principle experiments, we leverage high-field THz pulses to compress the electron bunches by 10x to ~180 fs. The high-quality diffraction patterns and enhanced temporal resolution are benchmarked using ultrafast structural dynamics measurements of silicon. We show that optimization of this technology may enable temporal resolution in the few-fs regime.

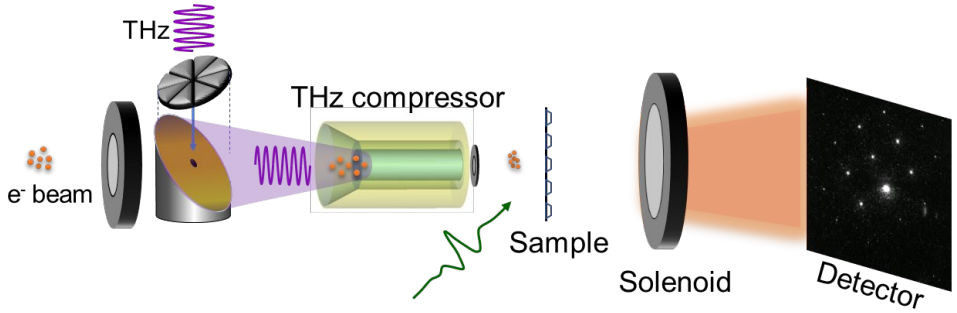

FIGURE 1. THz-enhanced UED setup. A small fraction of the 1030 nm infrared optical beam is converted to 257 nm based on two-stage second harmonic generation. The 257 nm UV pulse is directed onto a gold photocathode generating electron pulses, which are accelerated to 53 keV by the DC electric field. The same infrared laser also drives a multicycle THz generation stage, two single-cycle THz stages, and pump laser for the electron manipulator, the streaker, and sample excitation, respectively. The streaker and the sample are on the same manipulator which can be exchanged for checking the pulse duration at the sample position or performing the ultrafast electron diffraction experiment.

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Subnanometric optical control of electron emission sites

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In this presentation, we will provide an overview of our recent development of the optical control of electron emission sites.

By irradiating a sharp metallic needle with femtosecond light pulses, optical fields can be concentrated on the needle's apex, and these localized optical fields then generate electron emissions from the apex [1], as shown schematically in Figure 1(a). Such electron emissions can be used as optically-controlled ultrafast switches that are three to six orders of magnitude faster than current switching devices in modern computers. Concurrent plasmonic effects can spatially control the electron emission at its source on a scale of a few tens of nanometers [2]. For example, one can select emission sites A or B, as shown in Figure 1(b). The optical control of emission sites yields a device equivalent to multiple switches integrated into a nano-object, whose corresponding electronic circuit is shown in the right panel of Figure 1(b). Further acceleration of such a switch would be possible with advances in laser technology. However, further miniaturization of such a spatially controllable electron source is fundamentally difficult via plasmonics, and a paradigm shift is required.

Here, we realized that paradigm shift by employing a recently identified single-molecule electron source that generates electron emissions from individual fullerene molecules deposited on a metallic needle [3], as shown schematically in Figure 2. By illuminating the molecules with light, we discovered that largely modulated emission patterns appeared from a single molecule, approximately one nanometer in size [4]. These are quantum-mechanical phenomena that use variations of molecular orbitals. This scenario is well supported by simulations using density functional theory, which also explains the physics of electron emission patterns from single molecules via DC electric fields—an intractable question for

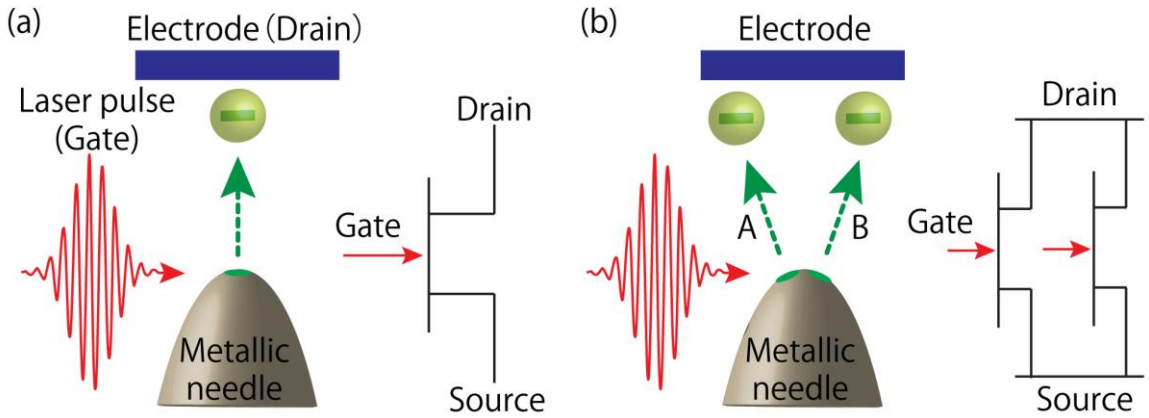

FIGURE 1. Conceptual diagram of how to induce ultrafast electron emission from a nano-object by irradiating a light pulse (a) and optical control of emission sites (b). Electronic circuits equivalent to these electron sources are drawn alongside the figures.

more than seven decades. In addition, we will further discuss optical controllability over emission sites at a single molecule. Our work will open the door to multiple ultrafast switches integrated into a single molecule.

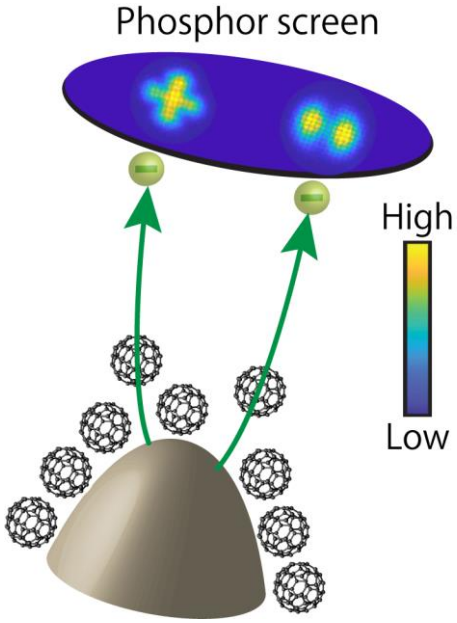

FIGURE 2. Schematic diagram of electron emissions from single fullerene molecules.

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Material Science toward achieving Carbon Neutrality

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Growing global energy demand and exhaustion of fossil fuels are gradually becoming a big concern for all the people on the Earth. Meanwhile, the deteriorating environmental pollution and global warming with the emergence of recent extreme weather make us re-recognize the importance of the usage of renewable resources with carbon-free emission and energy storage with high efficiency. A secondary battery to store the fluctuating renewable energy attracts a lot of attention and seems to fulfill the requirements of human beings. Since these battery technologies are only suitable for short-term energy storage daily or weekly due to their high cost, and cannot be used for leveling seasonal fluctuations. Due to economic requirement, it is important to establish hydrogen utilization technology as a countermeasure against long-term fluctuations in renewable energy. Therefore, in order to achieve carbon neutrality, it is impossible to avoid the development of high-performance secondary batteries and the establishment of a hydrogen-utilizing society.

Our group has so far focused on various kind of metal hydrides and focused on exploring their functions to solve the above problems. As an example, metal hydrides are considered to be a potential anode material for all-solid-state Li-ion batteries, because of its high theoretical Li storage capacity, relatively low volume expansion, and suitable working potential with very small polarization by the “hydride conversion reaction”. On the other hand, as characteristic properties related to hydrogen gas, not only for high capacity hydrogen storage but also for obtaining high pressure H_2, producing heat by control of H_2 pressure, and absorbing NH_3 with relatively low pressure, we focused on various kinds of hydrides related materials, such as MgH_2, TiFe intermetallic compound, TiH_2, and $LiBH_4$. And then, for high performance properties, “nano-composite techniques” played an important role. Of course, material modification to achieve required performance can only be accelerated by precise and accurate characterizations based on materials science.

The synthesis of hydrogen gas from renewable energies is also quite important technology to be developed with a reasonable cost (in Japan, target cost for hydrogen production is about 2 USD/kg). To achieve this economic requirement, thermochemical method to produce hydrogen is attracting a significant attention. The reaction cycles for water-splitting based on redox reactions of metallic phase of Na are focused in our group, which is composed of three reactions, that is hydrogen generation by solid-liquid reaction, metal separation by thermolysis, and oxygen generation by hydrolysis, where we are able to expect to have the effect of mass production. As is well known that sodium oxides, Na_2O and Na_2O_2 show highly reactive properties to any kind of metals and ceramics at high temperature conditions around 500 °C, it is quite difficult to control the target reaction, which lead to serious corrosion of the vessel materials. In this work, thermodynamic analyses are performed by using the parameters such as operating temperature and partial pressures of the products obtained by the experiments to determine that the Na metal redox cycle is potential hydrogen production technique as thermochemical energy storage. And some suitable way to control this promising reaction by minimizing the corrosion effect would be demonstrated.