

ABSTRACTS

THE 46TH OKAZAKI CONFERENCE

**The 46th Okazaki Conference on
Application of Synchrotron Radiation to Molecular Science:
Present Status and Future Prospects**

**Institute for Molecular Science, December 16-18, 1992
(Room 101, Office Bldg.)**

December 16 (Wed.), 1992

Chairperson: Takehiko Ishii (ISSP, Univ. of Tokyo)

12:55 Welcome Address: Kyuya Yakushi, Director (UVSOR, IMS)

13:00 - 13:50 Samuel Krinsky (NSLS, BNL)
"Development of the VUV Storage Ring and Plans for a UVFEL"

13:50 - 14:15 Hisashi Kobayakawa (Photon Factory, KEK)
"Present Status of the Photon Factory Storage Ring"

14:15 - 14:40 Yukihide Kamiya (ISSP, Univ. of Tokyo)
"Present Status of SOR-Ring and Future Plans of a High-Brilliant VUV Ring"

14:40 - 15:05 Goro Isoyama (UVSOR, IMS)
"Present Status and Recent Developments of the UVSOR Storage Ring"

15:05 - 15:35 Coffee Break

Chairperson: Hideo Onuki (Electrotechnical Lab.)

15:35 - 16:25 Walter Braun (BESSY)
"Recent Instrumental Developments and Experimental Highlights at BESSY I, Future Prospects for BESSY II"

16:25 - 16:50 Masaki Yamamoto (Tohoku Univ.)
"Soft-X-Ray Multilayers for the Uses with Synchrotron Radiation"

16:50 - 17:15 Makoto Watanabe (UVSOR, IMS)
"Review of Recent Progress in Soft X-Ray Monochromators and Their Dispersive Elements"

Chairperson: Yoshihiko Hatano (Tokyo Inst. of Tech.)

17:15 - 17:40 Kiyohiko Tabayashi (IMS)
"VUV Photochemistry of Rare Gas-Dihalogen van der Waals Complexes Studied by Absorption and Fluorescence Spectroscopy"

17:40 - 18:40 Yuan T. Lee (Univ. of California, Berkeley)
"Application of VUV Undulator Beam Line to Chemical Dynamics at ALS"

19:00 - 20:45 Reception (Faculty Club, 2-nd Floor)

December 17 (Thur.), 1992

Chairperson : Inosuke Koyano (Himeji Inst. of Tech.)

9:00 - 9:30 Yukinori Sato (Tohoku Univ.)

"Resonance-Auger-Electron-Photoion Coincidence Studies on State-to-State Dissociation Dynamics of Inner-Shell-Excited Molecules"

9:30 - 10:00 Pascal Lablanquie (LURE, Univ. Paris Sud)

"Multiphotoionization Following Innershell Excitation"

10:00 - 10:40 Yoshihiko Hatano (Tokyo Inst. of Tech.)

"Spectroscopy and Dynamics of Superexcited Molecules"

10:40 - 11:10 Coffee Break (Room. 201) + Group Photo

Chairperson : Noriaki Itoh (Nagoya Univ.)

11:10 - 11:35 Koichiro Mitsuke (IMS)

"Negative-Ion Formation from Molecules, Clusters, and Condensed-Gas Surfaces"

11:35 - 12:25 Georg Zimmerer (DESY-HASYLAB, Univ. of Hamburg)

"Spectroscopy of Molecules in Gaseous and of Molecular Centers in Condensed Phase"

12:25 - 13:30 Lunch

Chairperson: Tadaoki Mitani (IMS)

13:30 - 13:55 Yoshinori Tokura (Univ. of Tokyo)

"Polarized Absorption Spectroscopy on σ -Conjugated Polymer: Polysilanes and Polygermanes"

13:55 - 14:20 Nobuo Ueno (Chiba Univ.)

"Molecular Orientation in Thin Films of Functional Molecules by Means of Angle-Resolved Photoemission"

14:20 - 14:45 Ken-ichi Kan'no (Kyoto Univ.)

"Time-Resolved Spectroscopic Study on the Self-Trapped Excitons in Alkali Halide Crystals"

14:45 - 15:10 Masao Kamada (UVSOR, IMS)

"Present and Future of Photoelectron and Photodesorption Spectroscopic Studies at UVSOR"

15:10 - 15:45 Coffee Break (Room 201)

Chairperson: Akito Kakizaki (ISSP, Univ. of Tokyo)

15:40 - 16:30 Ingolf Lindau (MAX-Lab, Univ. of Lund)
"High Resolution Photoelectron Spectroscopy on Solids: Past, Present and Future"

16:30 - 16:55 Akio Kotani (ISSP, Univ. of Tokyo)
"Can We Obtain X-Ray Absorption Spectra beyond the Core-Hole Lifetime Broadening?"

16:55 - 17:20 Tsuneharu Koide (Photon Factory, KEK)
"Magnetic Circular Dichroism in Core-Level Absorption of Magnetic Materials"

17:20 - 17:45 Takao Nanba (Kobe Univ.)
"Far Infrared Spectroscopy of Rare Earth Hexaborides"

17:45 - 19:00 Dinner

Chairperson: Masao Kamada (UVSOR, IMS)

19:00 - 21:00 Poster Session + (Laboratory Tour)

December 18 (Fri.), 1992

Chairperson: Shinri Sato (IMS)

9:00 - 9:25 Syozo Kono (Tohoku Univ.)
"A Future Direction of Synchrotron-Radiation Photoemission Study of Solid Surfaces"

9:25 - 9:50 Toshiaki Ohta (Univ. of Tokyo)
"XAFS Studies of Molecular Adsorbates on Metals"

9:50 - 10:40 Peter Weightman (Univ. of Liverpool)
"New Directions in the Study of Electronic Structure Using Synchrotron Radiation"

10:40 - 11:10 Coffee Break

Chairperson: Kosuke Shobatake (IMS)

11:10 - 11:35 Kenichiro Tanaka (Photon Factory, KEK)
"Photon Stimulated Desorption by Core Electron Excitation"

11:35 - 12:00 Tsuneo Urisu (IMS)
"Science and Engineering in Synchrotron Radiation-Excited Semiconductor Process"

12:00 - 12:10 Closing Remarks: Hiroo Inokuchi, Director-General (IMS)

Poster Session (December 17, 19:00 - 21:00)

Chairperson: Masao Kamada (UVSOR, IMS)

Place: Office Bldg. Room 201

- PS-I.** P. M. Raja Rao, B. N. Raja Sekhar, N. C. Das, S. Padmanabhan, P. S. Murty, G. D. Saksena, S. V. N. Bhaskara Rao, S. S. Bhattacharya, V. B. Kartha, A. K. Sinha, and S. Bhat (Bhabha Atomic Res. Cent., India)
"Design and Development of Spectroscopy Beam Lines at Indus I"
- PS-II.** P. -K. Tseng (Natl. Taiwan Univ. and SRRC, Taiwan)
"Present Status and Future Perspective of Synchrotron Radiation Center"
- PS-III.** C. Y. Xu (HESYRL, China and Riken)
"Present Status of HESYRL"
- PS-IV.** D. Xian, E. Tang, and Y. Hai (Beijing SR Facility, China)
"BSRF Status and Research Opportunities"
- PS-V.** S. Y. Rah, Y. Chung, and T.-N. Lee (Postech, Korea)
"Current Status of the PLS Project"
- PS-VI.** M. Watanabe (IMS)
"Synchrotron Radiation Sources in Japan"
- PS-1.** K. Yamashita (Nagoya Univ.)
"X-Ray Reflectivity of Au, Pt and Pt/C Multilayer"
- PS-2.** M. Sakurai (Kobe Univ.)
"VUV and Soft X-Ray Radiometry on the NIFS Beam Line BL5B"
- PS-3.** E. Ishiguro (Osaka City Univ.)
"Reflectance of Multilayer Gratings in Soft X-Ray Region"
- PS-4.** N. Watanabe (Univ. of Tsukuba)
"Soft X-ray Microscope with Zone Plates III"
- PS-5.** I. Ouchi (Tottori Univ.)
"Core Electron Absorption Spectra of Polyester Films"
- PS-6.** W.-F. Pong (Tamkang Univ., Taiwan)
"Soft X-Ray Absorption Studies of Diluted Magnetic Semiconductors $Zn_{1-x}Y_xS$ (Y=Mn, Fe, Co)"
- PS-7.** S. Nakai (Utsunomiya Univ.)
"Polarized Cu L Absorption Spectra of $Bi_2Sr_2Ca_{1-x}Y_xCu_2O_8$ (x=0.06)"
- PS-8.** S. Hasegawa, S. Tanaka, Y. Yamashita, H. Inokuchi (IMS), H. Fujimoto (Kumamoto Univ.), K. Kamiya, K. Sekiya (Nagoya Univ.) and N. Ueno (Chiba Univ.)
"Molecular Orientation in Thin Films of Bis(1,2,5-thiadiazolo)-p-quinobis(1,3-dithiole) on Graphite Studied by Angle-Resolved Photoelectron Spectroscopy"
- PS-9.** T. Masuoka (Osaka City Univ.)
"Dissociative Double Photoionization of Carbonyl Sulfide (OCS)"
- PS-10.** K. Furuya (Kyushu Univ.)
"Dissociation Dynamics of CH_4^+ in the A State Region"
- PS-11.** H. Yoshida, H. Hattori, and K. Mitsuke (IMS)
"Positive Ion-Negative Ion Coincidence Spectroscopy of Diatomic Molecules"
- PS-12.** H. Hattori, H. Yoshida, and K. Mitsuke (IMS)

- "Ion-Pair Formation from Hydrocarbons by Predissociation of the Rydberg States with C-2s Hole Characters"
- PS-13.** H. Yasumatsu, T. Kondow (Univ. of Tokyo), K. Tabayashi, K. Suzuki, and K. Shobatake (IMS)
"Dissociative Excitation of Alkali Cyanide Molecules"
- PS-14.** M. Kono, K. Tabayashi, and K. Shobatake (IMS)
"Photodissociative Excitation Process of CICN Studied by Fluorescence Polarization Measurements"
- PS-15.** H. Ogawa (Saga Univ.)
"Synchrotron Radiation Assisted Epitaxial Growth of ZnTe Using Metalorganic Sources"
- PS-16.** A. Yoshida, S. Umeda, and Y. Saito (IMS)
"Synchrotron Radiation-Induced Degradation of Metal-Insulator-Semiconductor Devices"
- PS-17.** S. Hirose and M. Kamada (IMS)
"Sputtering of Excited Alkali Atoms from Alkali-Halides Irradiated with Synchrotron Radiation"
- PS-18.** Y. Ukisu, H. Ogawa and S. Sato (IMS)
"Mechanism of the Photolysis of Iron Pentacarbonyl Adsorbed on Silver"
- PS-19.** S. Tanaka and M. Kamada (IMS)
"Co-Adsorption of K and Cl on the Si(100)(2x1) Surface"
- PS-20.** H. Nishikawa (Waseda Univ.)
"Photoluminescence and VUV Absorption Spectra in SiO₂ Glass"
- PS-21.** H. Kawazoe (Tokyo Inst. of Tech.)
"Crystal Structure and Electronic Structure-Design of Transparent Electrode Materials"
- PS-22.** M. Itoh (Shinshu Univ.) and H. Itoh (Kagawa Univ.)
"Light Amplification due to Population Inversion between the Valence and Outermost-Core Bands in BaF₂"
- PS-23.** H. Nakagawa (Fukui Univ.)
"Self-Trapped Excitons in CdBr₂ and CdCl₂"
- PS-24.** K. Nakagawa (Kobe Univ.)
"Origin of Photocurrent Structures of Anthracene Doped in Super Critical Xenon"
- PS-25.** S. Kubota (Rikkyo Univ.)
"Variation of Decay Curves for Auger-Free Luminescence in CsCl and BaF₂ against Exciting Photon Energies"
- PS-26.** M. Taniguchi (Nagoya Univ.)
"Time-Resolved Luminescence Spectroscopy of HMM Powders"
- PS-27.** T. Dodo (Ehime Univ.)
"Absorption and Reflection of FIR by Concentrated Electrolyte Solutions"
- PS-28.** M. Kobayashi (Osaka Univ.)
"Proton Order-Disorder Phase Transition in Ice Observed by Vibrational Spectra"
- PS-29.** H. Ohashi, K. Tabayashi, and K. Shobatake (IMS)
"Synchrotron Radiation-Excited Etching of Semiconductor Material Surface Studied by Velocity Distribution Measurements of Desorbed Species Using an Electron Bombardment Ionization Mass Spectrometer Detector"
- PS-30.** H. Hama, S. Takano, and G. Isoyama (IMS)
"Control of the Bunch Length on the UVSOR Storage Ring"

DEVELOPMENT OF THE VUV STORAGE RING AND PLANS FOR A UVFEL

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Abstract

The NSLS was initially funded in 1977 and VUV storage ring operations began in 1982. During the Phase II upgrade program in 1986, two insertion devices and an infrared beamline were installed. In 1989, a prototype real time global orbit feedback system was commissioned, stabilizing the orbit for all beamlines utilizing a single feedback system based upon harmonic analysis of the orbit fluctuations and correction dipole magnetic fields. The orbit feedback is facilitated by new RF receivers for processing the signals from the ring's pick-up electrodes. These receivers have a noise level below 10 microns. In 1992, RF receivers had been installed for all of the VUV ring's pick-up electrodes, allowing a real time orbit display. Also, the prototype global orbit feedback system was replaced by new horizontal and vertical orbit feedback systems with improved performance. Fast (5 Hz) and slow (once every two minutes) orbit histories are now logged on the computer to help follow up on user problems related to orbit stability.

The electron beam lifetime in the VUV ring, which operates at 750 MeV and is filled to 900 ma, is limited by Touschek (intrabunch) scattering. The lifetime was doubled in 1990 by installing a fourth harmonic RF cavity (211 MHz) and operating it passively in a manner to increase the electron bunch length. In Spring 1993, we plan to power the harmonic cavity and obtain an additional 50% increase in lifetime. We are also investigating the possibility that a further increase in lifetime can be achieved by increasing the ring's horizontal aperture.

Beamline development is continuing on the VUV ring. The success of the infrared beamline U4IR, has led to the building of a second infrared line on U2. The instrument of choice for high resolution soft x-ray spectroscopy is the spherical grating monochromator which was developed by AT&T Bell Labs on U4. This year the new SGM on the U13 undulator is supporting an active scientific program. Work has begun on the development of a beamline using the U13 undulator and standard normal incidence optics, for high resolution angle resolved photoemission in the 5 to 30 eV photon energy range. The normal bending magnet port on the VUV ring collects less than 50 milliradians of radiation. Consideration is being given to the development at ports U5 and U6 of special optics to collect and time focus close to 500 milliradians of radiation. This would provide an optimized source for projection x-ray lithography, and could also be used as a universal ionizer for state-of-the-art pump-probe experiments.

At the NSLS we are pursuing the development of a free electron laser operating in the wavelength range of 75-300 nm. Nanocoulomb electron pulses will be generated at a laser photocathode RF gun. The 6 ps pulses will be accelerated to 250 MeV in an s-band SLAC-type LINAC. We consider a subharmonically seeded single pass FEL amplifier utilizing two wiggler magnets separated by a dispersion section. To be specific, suppose the seed to be laser light at 300 nm. A first wiggler is

used to energy modulate the electron beam. This is followed by a dispersion section to produce spatial bunching, and a second wiggler resonant to 100 nm. Upon passing through the second wiggler the prebunched electron beam first radiates coherently, and then this radiation is exponentially amplified. Finally, a tapered section is used to extract additional power from the electron beam. In this manner we can achieve radiation pulses of 6 ps duration with 1 mJ energy per pulse in 10^4 bandwidth, with continuously tunable wavelength in the range 75-300 nm.

A proof-of-principle experiment in the infrared is presently in preparation to be carried out at the Accelerator Test Facility at BNL. In this experiment we will triple the frequency of a CO₂ seed laser by using two superconducting wigglers and a dispersion section. We plan to study the evolution of the various growth mechanisms as well as the coherence of the tripled and amplified radiation.

Present Status of the Photon Factory Storage Ring

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Abstract

The Photon Factory is a user-based facility for synchrotron-radiation research at the National Laboratory for High Energy Physics (KEK). Accelerators consist of a 2.5-GeV linear accelerator and a 2.5-GeV storage ring. Operating beam is positron. Initial stored current is 350-360 mA for user-runs and the beam lifetime is in excess of 60 hours at 300 mA. The average current is about 300 mA in 24-hour fill lengths. The injection rate of the positron beams is presently very high, 0.5-1.0 mA/sec. In 1991, 208 hours were provided for single-bunch users. The beam lifetime at 50 mA is 10-20 hours, which is limited by the Touschek effect. By using this vertical tune shifts, the beams in the neighboring buckets are cleaned to a factor of 10^{-5} - 10^{-6} .

Twenty-one beamports have been equipped with beamlines. Fifty-nine experimental stations are now operational; thirty-two of these are for X-ray studies, twenty-seven for VUV and soft X-rays and one for photon-beam position monitoring for diagnosis. Four beamlines were built by private companies. Six insertion-device beamlines have been operational.

Number of users is about 2300 including more than 500 users from industries. 69% of users is from universities, 7% is from national laboratories, and 24% is from industries. Number of proposals submitted every year is about 250; 48% of which is solid state physics and material science, 23% is chemistry and atomic or molecular sciences, 15% is biology or biochemistry, 6% is for technology or industrial uses.

The storage ring has been operational since 1982. Major upgrades made on the storage ring are (1) low emittance operation from 1987 in order to increase the brightness of synchrotron radiation, and (2) positron operation from 1988. A product of beam current and lifetime ($I\tau$) is a good standard of storage-ring performance. $I\tau$'s in present runs are very large more than 1000 Ampere-min.

An FEL-project using the Photon Factory storage ring is underway. This project involves FEL-research for developing the shorter-wavelength region. A gain measurement at 177-nm is our present goal.

We are planning to upgrade the storage ring with reducing the beam emittance by a factor of 5 and increase the brightness of synchrotron radiation by a factor of approximately 10. The present emittance is 130 nmrad, and new emittance will be 27 nmrad at 2.5 GeV. In this plan, we must add new quadrupole- and sextupole-magnets, which have smaller bore radius of 40 mm (present bore radius is 55 mm), and also their side-yokes are opened for the beamline ports. Since the bending magnets will not be changed, source points and lines of the synchrotron light do not change.

Present Status of SOR-Ring and Future Plans of a High-brilliant VUV Ring

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Abstract

Presented in this talk are two subjects; SOR-Ring status and future project of a high-brilliant light source. First I will give a talk about an overview of the SOR-Ring, operational status of the ring, and some accelerator studies and problems. Next I will report the future plans of a light source; an overview, accelerator parameters and ongoing accelerator R&D.

The SOR-Ring is located in the site of the Institute for Nuclear Study (INS) in the northwestern part of Tokyo Metropolitan, and operated by the Synchrotron Radiation Laboratory of ISSP. The construction of the SOR-Ring began in 1971, following productive activities of the INS-SOR, which utilized synchrotron light extracted from the ES, 1.3-GeV Electron Synchrotron. After the construction completed, the operational time of the ring was gradually increased and became up to about 2000 hours in the fiscal year of 1991. The ring is usually operated from morning to night and the weekly schedule is from Tuesday to Friday. There are five beamlines in the SOR-Ring, three of which are active ones: BL1 is for the experiments of photon reflection and absorption, BL2 for photoelectron spectroscopy, and BL5 is specifically dedicated to ultraviolet photobiology.

The injection energy and storage energy of the ring are 308 MeV and 380 MeV, respectively. The ring with an RF frequency of 120.83 MHz has 17.4-m circumference and consists of eight bending magnets and four quadrupole triplets. At 380 MeV the beam emittance is around 320 nm-rad and the critical photon energy 110 eV. In this summer shutdown, beam position monitors (BPM's) along with beam steerings have been installed to measure the closed orbits and to correct them. In this talk, I will present the BPM system, some results of orbit correction and also recent measurement of other machine parameters. Further I will talk about the accelerator problems in the SOR-Ring; ion-trapping phenomena, vacuum pressure growth around the RF-cavity and longitudinal instability presumably caused by a higher-order-mode in the RF-cavity. As every component of the SOR-Ring is aging rapidly, we eagerly hope to construct a new facility.

Our future project of a high-brilliant light source is one of the future plans for the whole ISSP, which is expected to move to a new campus in Kashiwa located northeast of Tokyo. The accelerator scheme of the new light source consists of a 50-MeV linac, a 1.5-GeV booster synchrotron and a 1.5-GeV storage ring that has a circumference of about 240 m, twelve long straight sections and an emittance of several nm-rad. Further presented in this talk are a plan view of the facility buildings, a layout of beamlines, principal parameters of the accelerators, photon brilliance and so forth. Because of the very small emittance and relatively low energy of the beam, the beam lifetime will be mainly determined by the Touschek effect even for multi-bunch operation. The lifetime is then estimated to be around 10 hours.

Two accelerator R&D's are now under way. One is a BPM system with PIN diodes used as signal switching, being intended to be more high-speed and reliable than ever. This BPM system is already working in SOR-Ring. Relative accuracy of the system obtained so far is the order of a few microns, but large unevenness of BPM data that would unexpectedly occur for mechanical switches has never been observed. The other R&D is that for RF-cavities, the purposes of which are to find out a suitable cavity structure not so as to cause coupled-bunch instabilities, and to adopt a simple structure in order to get a reliable operation at high RF power. The specific feature of the present design is that resistive material, SiC, is attached on the beam pipes near a cavity to damp some higher-order-modes that are propagated out of the cavity. A cold model of cavity has already been delivered from a company and its test is about to begin this December. I will report some details of these R&D's and beam instabilities related to this designed cavity.

Present Status and Recent Developments of the UVSOR Storage Ring

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The accelerator system of the UVSOR facility is introduced, and recent developments of the control system and a superconducting wiggler are described. The present status, experiments of control of the bunch length and a free electron laser on the storage ring are given in other parts of this report.

Construction of the accelerator system started in 1981, and the first electron beam was stored on November 10, 1983. Since then, the light source has been running for 9 years. The accelerator system consists of a 750 MeV electron storage ring and a 600 MeV injector synchrotron with a 15 MeV linac. The magnetic lattice of the storage ring is the double bend achromat. There are four long straight sections of 3.5 m long, where a superconducting wiggler and two undulators are installed.

Recently, a new control system was installed for the accelerator system. It is a distributed control system based on two mini-computers as process computers. One of the computers controls the storage ring and the other takes care of the beam transport line from the synchrotron. The system was designed with the emphasis on its reliability and flexibility. To ensure reliability, the dual disk system was employed. It is possible to operate the accelerator system with one computer though performance of the control system becomes slightly worse. To ensure flexibility, we employed a file-operating system. In a conduct file, names of data files are written, while names and setting values of devices are written in data files.

A 4 T superconducting wiggler of the wavelength shifter type was recently installed on the storage ring. Two thermal shielding plates for the helium vessel are cooled with one of the refrigerators equipped on the top, and evaporated helium gas is liquefied again with the other refrigerator. Therefore, this wiggler can be operated without adding liquid helium.

Recent Instrumental Developments and Experimental Highlights at BESSY I, Future Prospects for BESSY II

W. Braun

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The BESSY company was founded in 1979 after the federal government had decided to build a dedicated 800 MeV XUV source in Berlin. The purpose of the company is the operation and development of synchrotron radiation sources for basic and applied research as well as technology: in particular microlithography for microelectronics and micromechanics and radio-metry for the federal governments standards institute. The first beam was stored in December 1981 and user operation started already in February 1982. From mid 1985 onwards the storage ring was operated in the small emittance mode. About 130 user groups perform their experiments at BESSY per year. These groups originate from national and international (mainly European) universities, research institutes, industry and the national institutes of standards. Presently BESSY operates 33 experimental stations with 25 monochromators and 2 X-ray microscopes in the basic research area, 5 experimental stations with 5 monochromators are operated by the Physikalisch-Technische Bundesanstalt (German standards institute) and 4 white light beam lines are dedicated for X-ray lithography purposes.

In the following some recent developments and highlights will be discussed. After commissioning in 1986, the first undulator (a 35 period device) was equipped with two toroidal grating monochromators. These instruments are now used for photoemission spectroscopy in surface and solid state physics as well as for atomic and molecular physics. In particular two photon experiments to determine the angular distributions of photoelectrons of laser excited aligned atoms are performed with high count rates and high resolution (1000 cts/sec and 17.5 meV at 31 eV in the gas phase). In 1992 very high resolution (4 meV at 65 eV) was obtained in first order with a plane grating monochromator (SX-700 II) at a dipole source using a 2400 ℓ /mm grating. Theoretically predicted but hitherto unseen Rydberg states of doubly ionized He were observed [1]. Magnetic X-ray dichroism of deep core levels was observed for the first time in photoelectron spectroscopy [2]. In 1991 the first crossed undulator (6.5 and 7.5 periods) of the Nikitin-Kim type [3] went into operation and its polarization characteristics were determined. As expected, the quality of the circular polarization of this device is determined by the emittance of the storage ring and also decreases as the wavelength decreases, as theoretically predicted. The spherical grating monochromator beam line optimized for operation on this undulator showed its excellent performance. A resolving power in excess of 17000 was obtained at 65 eV. The combination of these devices makes new experiments like magnetic circular dichroism possible, not only in the solid state but also in the gas phase.

Even spin resolved measurements will be possible for photon energies between 30 eV and 200 eV.

A special plane mirror device was developed by H. Petersen and M. Willmann of BESSY to select right and left handed circular polarization from a dipole magnet source. This device was combined with a standard SX-700 monochromator to produce circularly polarized light up to 1000 eV. The degree of circular polarization as a function of off plane angle was determined at 265 eV using a multilayer polarimeter [4]. The measured Stokes parameter S_3 clearly follows the theoretically expected curve. A commercial photoelectron microscope was adapted to this beam line. With this instrument H^+ -ion bombarded organic films as well as magnetic domains of ion single crystals have been imaged. In the latter, topography effects can be eliminated by measuring the domains with different helicities. Thus, photoelectron microscopy will help to study magnetic domain properties. Recently, the X-ray microscopes of Prof. Schmahl's group from Göttingen have been further developed. Now specimens can be put in a special preparation chamber and brought into the light path in air. The implementation of a CCD camera helped to reduce the measuring time per picture to below 200 msec. New developments at BESSY also include the test of new designs of monochromators such as Rowland circle and variable line spacing monochromators. Test stations will be set up in the near future.

In July 1992 the construction of the 1.7 GeV third generation synchrotron radiation source, BESSY II, was approved. The project started already in September 1992 in Berlin-Adlershof in the former GDR. New science will be possible in atomic and molecular physics, depth lithography, high resolution X-ray microscopy and photoelectron microscopy for applications in particular in material sciences, catalysis and biology. It will be a storage ring of double achromate symmetry with two different length straight sections. The emittance of that new storage ring will be about 6×10^{-9} m-rad, an order of magnitude smaller than that for the present ring BESSY I. The first beam is scheduled for end of 1997.

- [1] M. Domke, G. Remmers and G. Kaindl, Phys. Rev. Lett. 69, 1171 (1992)
- [2] L. Baumgarten, C.M. Schneider, H. Petersen, F. Schäfers and J. Kirschner, Phys. Rev. Lett. 65, 492 (1990)
- [3] K.-J. Kim, Nucl. Instrum. Meth. 222, 11 (1984)
M.B. Moisey, M.M. Nikitin and N.I. Fedosov, Sov. Phys. Journal 21, 332 (1984)
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Soft-X-Ray Multilayers for the Uses with Synchrotron Radiation

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Soft-x-ray multilayers have been used as novel optical elements such as a reflection filter, a power filter, a polarizer, and a phase shifter. With development of fabrication technique, the multilayer structure is made possible to realize constructive interference of soft-x-ray[1].

The multilayer differs from that in visible region in two respects. Absorption of layer elements limits the attainable reflectance level and interface roughness scatters light, which necessitates a use of super-polished substrate. At present, we can fabricate a multilayer mirror having a high enough reflectance over 50% for various applications at a photon energy up to 100eV.

Figure 1 shows reflectance spectra of Mo-Si multilayer measured at various angles of incidence with s-polarization. Such a multilayer can be used as a reflection filter with a 10eV FWHM pass band whose center is tunable by adjusting the angle of incidence. This has been utilized at beamline 11A, PF-KEK, where a multilayer reflection filter delivers high flux photon to a station of photo CVD experiments[2]. In these application with SR, multilayers have been proved to be durable for irradiation of SR of a bending section at a power level of 20W/cm². For a power filter application to reduce heat load to beamline optics, irradiation test was carried at BL-28 multipole wiggler, PF-KEK. A Mo/BN multilayer was found survived after 10min exposure of 2.3W/mm² irradiation[3].

Another use of the multilayer is in polarization measurements. At near 45° angle of incidence, a multilayer acts as a polarizer since p-reflectance is much smaller than s-reflectance. At a photon energy of 97eV, polarizance of over 97% is easily obtained[4]. With the polarizer, we evaluated the state of polarization of SR coming out of a grasshopper monochromator at BL11A, PF-KEK. It was found that the alignment of beamline optics to the maximum intensity gave elliptical polarization whose axis was not horizontal[5]. This demonstrated that for the best alignment to linear polarization at the center of SR, polarization should be observed.

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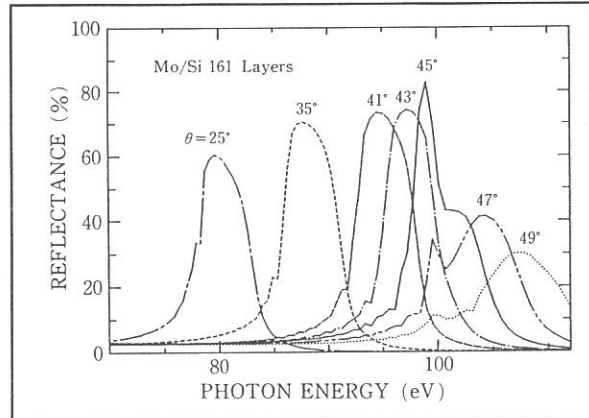


Figure 1 S-reflectance spectra of a Mo-Si multilayer at various angles of incidence

Review of Recent Progress in Soft X-Ray Monochromators and Their Dispersive Elements

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The soft X-ray region from 40 Å to 6 Å had been somewhat dark. The soft X-ray optics is now being developed from two sides, one of which is long wavelength side using grating monochromators and, the other, short wavelength side using crystal monochromators. It had been suggested that grating monochromators can supply monochromatic light down to 6 Å.¹⁾ Recently, high resolution spectrum of K-absorption on condensed N₂ was obtained with E/ΔE of 10⁴ by the use of Dragon monochromator.²⁾ The high resolution has been achieved by the use of a grating with a large radius. Further high resolution will be realized by the use of gratings with high groove density or varied space.³⁾

In Japan, two types of SiC gratings have been developed. One is the mechanically ruled grating on Au film evaporated on SiC substrate.⁴⁾ The other is the holographic grating with the grooves directly ruled on the SiC substrate by ion-beam etching and coated with Au.⁵⁾ In both cases, the SiC substrate is durable against the heat load of undulator radiation, but the Au coating is not. Effective cooling system should be developed.

Usually, double crystal monochromators equipped with beryl crystals have supplied monochromatic light with E/ΔE of 10³ below 15 Å. Since the beryl is not strong against highly bright radiation, new crystals of β-alumina⁶⁾ and YB₆₆⁷⁾ have been developed. However, it is a future subject to grow large crystals with good crystallinity.

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VUV Photochemistry of Rare Gas-Dihalogen van der Waals Complexes Studied by Absorption and Fluorescence Spectroscopy

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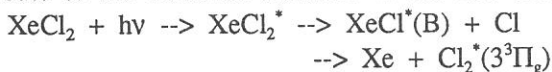
One of the merits for the application of SOR light to photochemistry of van der Waals (vdW) complexes lies in that spectral measurements for both direct absorption and fluorescence can be easily carried out in the wide vacuum UV energy regions. In the VUV regions, however, not much work has been done for all a variety of the excited states and opening of new reactive channels for the excited vdW complexes.

Present paper summarizes current VUV photochemical studies[1,2] of rare gas-dihalogen Rg-Cl₂(Rg=Xe,Kr) complexes made in UVSOR(BL2A) using both absorption and fluorescence excitation spectroscopy. As the topics, two types of new vdW bands for Rg-Cl₂ are presented and principal decay processes from the relevant excited states are proposed on the basis of the fluorescence quantum yields determined.

Both bands observed are originated from (1:1)Rg-Cl₂ complex and are attributed to the excitation in Cl₂ moiety. Broad absorption band in the 125-150nm region is assigned to a transition to the excited state of ion-pair RgCl⁺Cl⁻ type. Low fluorescence quantum yield ≤ 0.05 for the band indicates predominant dissociation of the photoexcited vdW complex to the non-fluorescent products,



Another complex band in the fluorescence excitation spectrum in the 138-145nm region has a vibrational structure ($\Delta v \sim 640 \text{ cm}^{-1}$) and can be assigned to the excitation to the Cl₂^{*} state of Rydberg character. We propose two kinds of excimer formation channels contribute to the observed emission in the 230-400 nm region,



It should be complemented that BL2A was designed to conduct both absorption and fluorescence measurements for gaseous samples such as molecules in a gas cell and molecular complexes in free jets. Although a LiF window has been placed to eliminate higher order of excitation light and isolate sample region from the vacuum systems, fundamental but important spectroscopic data have been accumulated[2] in the energy region below the LiF cut-off. Since detection efficiency of absorption measurements is generally not so high, special precautions have been taken to cover the present experiments, by increasing and controlling the concentration of the complexes and clusters. In order to check directly on the complex size distribution, beam characterization such as TOF photoion-mass analysis should be next programmed in the separate measurements. Ionization of the complexes and clusters without LiF window might be required for the characterization of such kind. Users outside our Institute also have a request to extend the energy range upward, then modification of the setup and measurements without window are our next future projects for BL2A.

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APPLICATION OF VUV UNDULATOR BEAM LINE TO CHEMICAL DYNAMICS AT ALS

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Purpose

A new program will be initiated at the Lawrence Berkeley Laboratory (LBL) to explore applications of synchrotron radiation at LBL's Advanced Light Source (ALS) in chemical dynamics, which encompasses all phenomena in which molecules undergo energetic or chemical transformations and to provide the experimental facilities needed for the exploration. The ALS will be used as a photo-analysis source to produce high yields of vacuum ultraviolet photoionized products. If operated in conjunction with powerful lasers, the Light Source will additionally be a powerful tool for the study of chemical processes induced by multiphoton absorption. Its time structure permit the study of ultrafast processes. These studies will culminate in research to determine the microscopic details of the mechanisms and dynamics of primary dissociation processes and elementary chemical reactions, to explore the chemistry of molecules excited to a Rydberg state or to other superexcited states, to study the structure, energetics and chemical reactivity of highly reactive polyatomic radicals and unusual transient species, to probe the nature of inter- and intra-molecular energy relaxation, and to search for bond-selective means to modify and manipulate chemical reactivity.

Approach

The experimental approach involves combining a synchrotron radiation source, lasers, molecular beams, and molecular and spectroscopic detection techniques to carry out the proposed research. The ALS U8.0 undulator beamline will be modified and a new branchline constructed to deliver a high intensity (10^{15} photons/sec), low resolution (2.5%) VUV beam for selective photoionization and product detection in primary photodissociation and photofragmentation studies. This branchline will feature a differentially pumped gas filter to suppress unwanted orders of the undulator radiation, and torroidal mirrors that focuses the synchrotron light to a spot of $\sim 100 \mu\text{m}$. The ability to focus a small spot size is a special characteristic of undulator radiation. It will lead to highly improved mass and energy resolution in ion and electron detection in the proposed experiments.

Standard lasers in the IR, Visible, and UV, and specially fabricated high-power, high-resolution lasers in the mid-IR and VUV will be used in conjunction with the undulator beamline to carry out pump-probe and state-to-state selective dynamics experiments throughout the optical region of the electromagnetic spectrum.

Projects of 1993

1. Design and fabrication of branchline at the ALS U8.0 undulator beamline. It is necessary to modify the existing U8.0 beamline so that VUV photons can be deflected, filtered, and refocused into the molecular beam chamber. A new torroidal mirror and associated

vacuum chamber will be inserted as the deflector that also serves to squeeze the photon beam through a differentially-pumped high-order suppressor. This high-order suppressor is used to absorb unwanted high energy photons that are found in abundance in the undulator beam. A second torroidal mirror then recollimates the beam to a cross-section of the order of $100\ \mu\text{m} \times 0.5\ \text{mm}$ located at the detector ionization region or at the point where two molecular beams cross in the sample chamber. The VUV beam is then sent through a normal incidence monochromator to provide light for experiments that require higher resolution than the undulator can produce.

2. Design and fabrication of molecular beam experimental station. Two stations are planned. One will be designed for experiments requiring the highest available VUV fluxes and one will be for experiments that need to utilize higher resolution than the 2.5% bandwidth that the U8.0 undulator normally provides. It is anticipated that the majority of experiments will fall in the former category.

The first station will be a universal rotating-source crossed-molecular-beam apparatus designed to use the ALS as a photoanalysis source. The tunable output from the U8.0 undulator will be used directly, without additional frequency filtering. The apparatus will be designed for studying primary photochemical processes and the dynamics and reactivity of polyatomic molecules, ions and clusters, using photofragmentation translational spectroscopy. The ALS beam will be shaped and transmitted through the ionizer region of the conventional TOF mass analyzer and serves to ionize photodissociation products. This unique approach is advantageous for product detection because it provides both improved species selectivity and reduced background detection. Alternatively, for certain experiments, the ALS beam will be directed to the molecular-beams interaction region to be used as an excitation source. In this case, an electron impact ionizer will be used in the same TOF apparatus. Differential pumping will be employed extensively to protect against systematic and accidental contamination of the synchrotron beamline and storage ring apparatus.

Experiments that require a higher resolution than the 2.5% bandwidth that the U8.0 undulator can provide will be performed in a second station. The ALS beam exiting from the first station will be passed through a 1-m normal incidence monochromator to obtain a 100-fold improvement in wavelength resolution. This monochromatized beam will be collimated and delivered to a molecular beam apparatus. The apparatus will be "conventional" in design, equipped with a TOF mass spectrometer and a zero-electron-kinetic-energy (ZEKE) spectrometer. Since this station will be located further downstream from the storage ring, the vacuum protection requirements will be less stringent. This station will be particularly useful for studying VUV and IR spectroscopy of superexcited molecules, free radicals, and other transient species.

Molecular source chambers for generating radicals, ions and clusters, both CW and pulsed, will be constructed to be used at both stations. Oil-free vacuum equipment will be employed for all chambers. Tunable lasers for pump-probe experiments will be included.

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RESONANCE-AUGER-ELECTRON-PHOTOION COINCIDENCE STUDIES ON STATE-TO-STATE DISSOCIATION DYNAMICS OF INNER-SHELL-EXCITED MOLECULES

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Decay of a core-excited molecule is a complex of a variety of processes including the electronic processes as well as the relaxation in nuclear degrees of freedom. In most cases, the primary decay of a core-excited molecule occurs electronically with the ejection of Auger electrons, and the resultant cation may then be subject to dissociation processes. We have started a series of coincidence experiments between the Auger electrons and the photofragment ions of core-excited molecules, using the SR of the 2.5 GeV storage ring at the Photon Factory of KEK in Tsukuba [1-3]. I present here the study on the decay of the core-excited resonance of BF_3 produced by the photoexcitation of the B- K electron into the lowest unoccupied $2a_2''(2p_{z,B})$ orbital [3].

The time-of-flight mass-analysis of the fragment ions is performed in coincidence with the energy analysis of the B: KVV normal- and resonance-Auger electrons as well as the valence photoelectrons. The results are summarized as follows:

(a) Direct photoionization of the valence electrons or the participant-resonance-Auger decay of the core-excited resonance results in the BF_3^+ states with one hole in an outer-valence orbital. The resultant BF_3^+ states dissociate to yield the BF_2^+ ion.

(b) The spectator-resonance-Auger decay of the core-excited resonance results in the excited BF_3^+ states having one excited (a_2'') electron and two outer-valence holes. The resultant BF_3^+ states dissociate to yield the B^+ ion as the predominant ionic fragment.

The results (a) and (b) demonstrate a dramatic change of dissociation induced by one electron excitation from an outer-valence orbital to the a_2'' orbital in the BF_3^+ states.

(c) The excited BF_3^+ states having one excited (a_2'') electron, one outer-valence hole, and one inner-valence hole are energetically allowed to autoionize into the dicationic BF_3^{2+} states but are subject to a primary fast dissociation before the autoionization.

(d) The spectator-resonance-Auger-final BF_3^+ states have been assigned to have two types of two-hole locations; one is localized at a single F atomic site and the other at different F atomic sites. However, no significant difference is observed in dissociation between the two types of two-hole locations.

In conclusion, the coincidence measurements between the resonance-Auger electrons and the fragment ions provide us with a new method to investigate the state-to-state dissociation dynamics of various excited monocationic states.

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MULTIPHOTOIONISATION FOLLOWING INNERSHELL EXCITATION

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Multiphotoionisation processes have recently become the subject of many detailed investigations. Here we will just stress a part of this wide field, and give a few examples to illustrate the special case where they are produced through innershell excitation. As opposed to the "direct" multiphotoionisation case in the valence region (where the dominant process is single photoionisation), it is a very intense and effective way to create multicharged ions.

As suggested in the title, a useful guide to describe the processes is to use the time evolution of the system, which can be considered to occur in the following successive steps: 1) photon absorption giving rise to the excitation of an innershell electron 2) electronic relaxation -or "creation" of a multicharged species- 3) nuclear motion -that is vibration, rotation and possibly dissociation of the excited ion. Here are given some examples extracted from the work performed in our laboratory, to illustrate this description and its limits:

-1) the different kinds of innershell excitation processes can be visualised through absorption measurement; due to the high energy range (typically 100 to 1000eV) such high resolution experiment have only recently been possible¹. In LURE, a high resolution plane grating monochromator in the 20-200 eV photon energy range was constructed recently. Its high resolving power (routinely 5000) enables to study the broadening of these innershell resonances, and consequently gives us the lifetime of the transient excited state; for H₂S, the excited state vibrational structures could also be resolved for the first time².

-2) The well known Auger effects (resonant or not) then give lead to the formation of multicharged ions. Though studied since a long time, we just begin to have a clear view of the branching ratios between the different production mechanisms and ionisation degrees of the final state. An example is the relaxation of the $3d_{5/2} \rightarrow 5p$ transition in Krypton; we showed³ that its relaxation gives dominantly doubly charged ions, produced in a 2 step electron emission.

Electronic relaxation in molecules is furthermore complicated by the nuclear motion of the squeueleton. However, in a good first approximation, it can generally be considered that electronic relaxation occurs with nuclei fixed, the subsequent motion of these occurring later, in the

multicharged environment. Caution is however essential: P.Morin et al⁴ showed that in HBr, rapid loss of an H atom can sometimes efficiently compete with the electronic relaxation. Since then, other examples have been found, usually involving a rapid H release prior to electronic relaxation.

-3) The multicharged molecule we then obtain is usually, (but not always) unstable. It is precisely the mechanisms of these dissociations we want to analyze. In order to visualize all ionization degrees and dissociation paths, we developed a multidimension mass spectroscopy experiment "EPICE" described in ref ⁵ whose advantage is to be able to detect, in coincidence, all the ionic fragments from the same ionisation event, and their time correlation. Analysis of these correlations is a very powerful tool to observe the dissociation mechanisms, it was first developed by John Eland, and deeper understanding is constantly gained⁶.

As an example we will mention here the case of the Fe(CO)₂(NO)₂ molecule. We were interested to see whether excitation of an innershell electron from the metal Fe or from one of the ligands NO or CO gave rise to a specific dissociation process, or in other terms whether some selective fragmentation could be initiated. Our results⁷ showed that extensive fragmentation is experienced, that occurs through successive evaporation of the ligands (charged or not); moreover whatever the innershell electron we excite, the same final state is observed; it shows that the memory of the excitation route is lost at the end; explanation is that, after electronic relaxation, the multicharged ion has time to vibrate and redistribute its internal energy in vibrational modes, prior to a statistical dissociation.

As a conclusion, we showed that the innershell photoexcitation mechanism is a powerful means to produce multicharged species in order to investigate their dissociation mechanisms. Coincidence technique is essential and will certainly be greatly developed in the future. One such extension is the Auger electron / ion(s) coincidence experiment developed in Tsukuba, USA and also in LURE.

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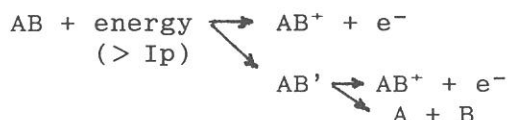
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Spectroscopy and Dynamics of Superexcited Molecules

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A survey is given of the entitled subject based mainly on the author's recent review articles and talks[1-4].

After introducing briefly a historical background of the entitled subject such as the Platzman's theoretical idea of a scheme of the formation and decay of superexcited states AB' ,



and the electron impact studies of this scheme[5], recent advances in synchrotron radiation studies of the spectroscopy and dynamics of superexcited molecules are surveyed by choosing some typical examples of molecules from the recent investigations by the author's group summarized as follows.

- (1) Dissociation dynamics of doubly excited molecular hydrogen[6,7],
- (2) Angular momentum population of excited hydrogen atoms produced by the dissociation of H_2 [8],
- (3) Dissociation dynamics of N_2 [9], O_2 [10], CO_2 [11], SiH_4 [12], Si_2H_6 [13], and C_2H_2 [14] in the superexcited states, and
- (4) Absolute measurements of photoabsorption cross sections, photoionization cross sections, photodissociation cross sections, and photoionization quantum yields of hydrocarbons[14-17], Si-containing molecules[12,13], ethers[17-19], and alcohols[17-19].

It is concluded from these investigations that the electronic structure of superexcited molecules is characterized with their decaying processes of the dissociation into neutral fragments in competing with autoionization and is classified into the following four types.

- 1) Vibrationally excited,
- 2) Doubly excited, or
- 3) Inner-core excited high Rydberg states converging to each ion state, or
- 4) Inner-core excited non-Rydberg states.

Finally, comments on future prospects and problems as divided into those of experimental techniques and research objectives are presented from the viewpoint of the application of synchrotron radiation to molecular science.

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Negative-Ion Formation from Molecules, Clusters, and Condensed-Gas Surfaces.

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Ion-pair formation is a very common process of highly-excited molecules in the photon energy range of 10 - 50 eV. Negative-ion mass spectrometry (NIMS) enables us to study ion-pair processes in various molecules:¹⁾ diatomic [O_2 , H_2 , CO , NO], triatomic [N_2O , OCS , CO_2 , SO_2], saturated and unsaturated hydrocarbons [C_nH_{2n+2} ($1 \leq n \leq 5$), C_2H_4 , C_2H_2], and halogenides [SF_6 , CF_4 , CH_3F , CH_3Cl , CH_3Br]. We have measured the efficiency curves of negative ions using monochromatized synchrotron radiation. A series of works demonstrates that NIMS provides a sensitive probe to investigate the properties of Rydberg states lying in the vacuum ultraviolet — not only their spectroscopy but also their dynamical behavior in predissociation — if the ion-pair continuum interacts strongly with these discrete states. A great interest has also been taken in the dynamics of the ion-pair formation as half-collisional version of the electron-transfer reaction. In the case of clusters or condensed gas-surfaces, it is probable that the ion-pair formation plays an important role in the vacuum UV photoscience, since the electronic couplings with the neighboring molecules or substrate change the high-energy relaxation dynamics in superexcited states. For example, the $O^+ + O^-$ production from quasi-bound positive-energy excitons has been observed in the condensed oxygen.²⁾

Last year, We developed a new coincidence technique, PINICO, which utilizes the flight-time correlation of a pair of positive and negative ions produced by single photon excitation.³⁾ This method is likely to prove eminently useful to study the ion-pair formation process. In this conference, we presented our molecular-beam photoexcitation apparatus, recent results on NIMS and PINICO, discussion on the spectroscopy and dynamics of molecular superexcited states, and future prospects of applying these experimental methods to clusters and condensed-gas surfaces.

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SPECTROSCOPY OF MOLECULES IN GASEOUS AND OF MOLECULAR CENTERS IN CONDENSED PHASE

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Very early luminescence experiments on rare gas solids (RGS) and rare gas liquids yielded close similarities between the dense gaseous phase and the condensed phases [1]. The similarities arise from the fact that an emitting center in the condensed phases exists which corresponds to a rare gas dimer, R_2^* , embedded into a matrix of the same kind of atoms. This was the starting point for spectroscopic investigations of the emitting species with SR of the storage ring DORIS at DESY, Hamburg. It turned out that time- and spectrally resolved luminescence spectroscopy under selective photon excitation is a powerful method to investigate the properties of the R_2^* molecules in the gas phase and of the R_2^* -type centers in the solid phase. After an initial period of experiments at the HIGITI station of HASYLAB, the experimental station SUPERLUMI was constructed for this purpose [2].

Another starting point was the unique contribution of Toyozawa at the VUV-4 conference in 1974 [3]. In Toyozawa's theory, the formation of the R_2^* centers was attributed to the peculiarities of exciton lattice interaction. Moreover, the co-existence of free excitons (FE) in the unrelaxed lattice, and of so-called selftrapped excitons (STE) like the R_2^* centers in a locally distorted lattice was predicted. This co-existence should show up in the luminescence spectra, and, indeed, was found later on. The early work has been described elsewhere [4]. Several examples of our gas-phase work have been published in [5].

In this contribution, a few very recent solid-state results are presented which are of great relevance for the fundamental properties of RGS-excitons.

(i) FE-spectroscopy: in the early work [4], an order-of-magnitude discrepancy between the intensity ratio of FE versus STE luminescence on one side, and the measured FE-lifetime was reported. Very recently, it was possible to prepare Xe samples in which the FE line is so intense that this discrepancy can be removed [6]. Fig. 1 shows that the peak-to-peak ratio is $\cong 50$, and the ratio of the wavelength-integrated spectra is $\cong 1$. A typical decay curve of the FE line is shown in the inset, together with a time-resolved spectrum of the STE band. Superimposed to a background originating from the triplet state, a signal with fast rise and decay is observed (singlet state of STE). The temporal behaviour of the singlet emission can be quantitatively fitted convoluting the temporal FE-spectrum with the exponential singlet decay. In other words, in a high-quality Xe crystal, the STE precursor is indeed the FE. Only then it is possible to deduce the self-trapping rates from the intensity ratio and the FE decay rate [6].

(ii) Exciton-induced desorption: The microscopic mechanism of desorption of neutral atoms from the surface of a pure or a rare gas doped RGS is closely related to exciton-lattice interaction [7]. Luminescence spectroscopy is especially well suited to detect desorbed excited atoms which emit resonance fluorescence after desorption. The SUPERLUMI station is so sensitive that even desorption from doped systems can be investigated. Metastable and neutral ground-state atoms have been detected as well [7]. It was even possible to measure the partial yield spectra of each desorption channel. First theoretical calculations of the interaction potentials of an excited Kr sur-

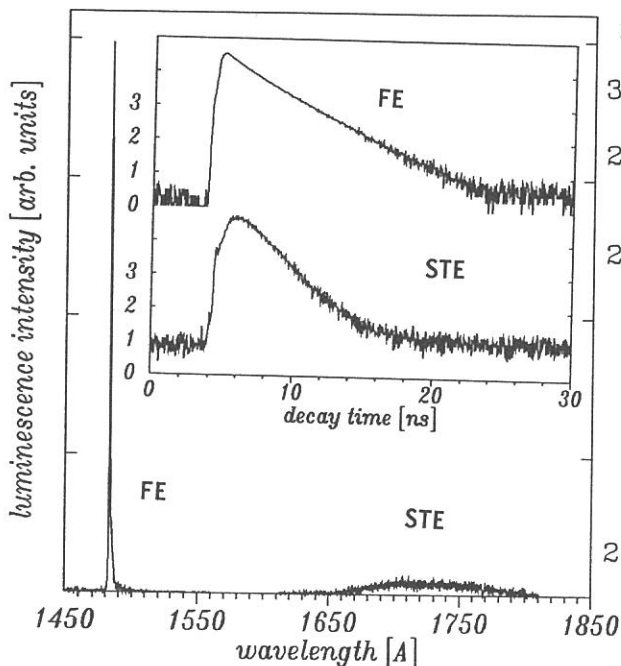


Fig. 1 Luminescence of solid Xe at $T=4.7\text{K}$, excited with 1400\AA -light. Note the logarithmic intensity scale of the inset.

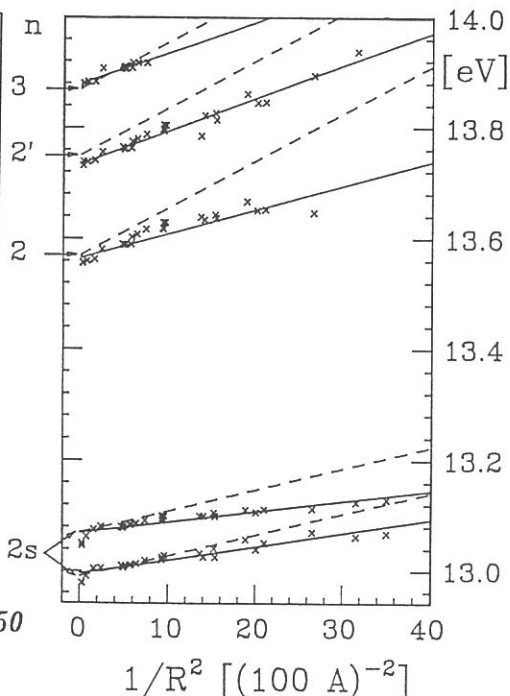


Fig. 2 Energetic positions of excitons in Ar clusters. R = cluster radius

face atom with an Ar host have been carried out leading to a microscopic understanding of the sputtering process [8].

(iii) Confined excitons in rare-gas clusters: it is a fundamental question, how the Wannier-type excitons of RGS develop as a function of particle size starting from the atoms or molecules. A powerful cluster-beam apparatus has been constructed in which the skimmed beam is crossed with monochromatized SR. The emitted clusterluminescence is detected either wavelength-integrated or spectrally and even time resolved [9]. Fig. 2 shows the energetic positions of surface ($n=2(s)$) and of bulk Wannier-type excitons ($n=2, 2', 3$) of Ar clusters as a function of $1/R^2$ (R : cluster radius) [10]. The straight lines observed can be explained with confinement models. The luminescence methods can be used as well to investigate fragmentation and relaxation processes.

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Polarized Absorption Spectroscopy on σ -Conjugated Polymers: Polysilanes and Polygermanes

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Polysilanes (and polygermanes) are extended Si(Ge) polymers with organic substituent in which σ electrons are considered to be delocalized on the Si (Ge) backbones. Ideal polymer structures with regular sequences may be viewed as ultimate quantum wires made of Si (Ge). To elucidate their overall electronic structures, polarized absorption spectra on highly oriented films of polysilanes and polygermanes have been investigated over a wide photon-energy region by utilizing synchrotron radiation from the UV-SOR ring at IMS.

Polarized absorption spectra (77K) with polarization parallel ($E//$) and perpendicular ($E\perp$) are shown in Fig.1 for the *trans* planar forms of polydihexylsilane (PDHS) and polydihexylgermane (PDHG). The both spectra show very common features for spectral shapes, polarization dependence and energy positions, indicating nearly identical electronic structures. The polarized absorption spectra can be well compared with the theoretical band calculation, as demonstrated in Fig.2. The results indicated that the one-dimensional (1D) band model works well in polysilanes and polygermanes. Detailed results and discussion have been reported in the references listed below.

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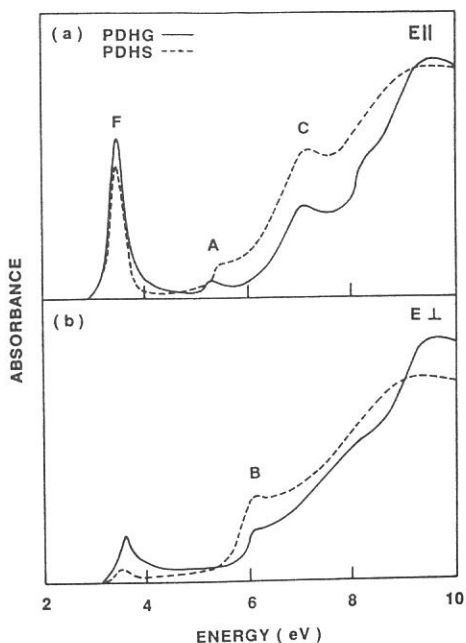


FIG. 1. Polarized absorption spectra of highly oriented films of *trans*-planar PDHG (solid line) and PDHS (dashed line) at 77 K.

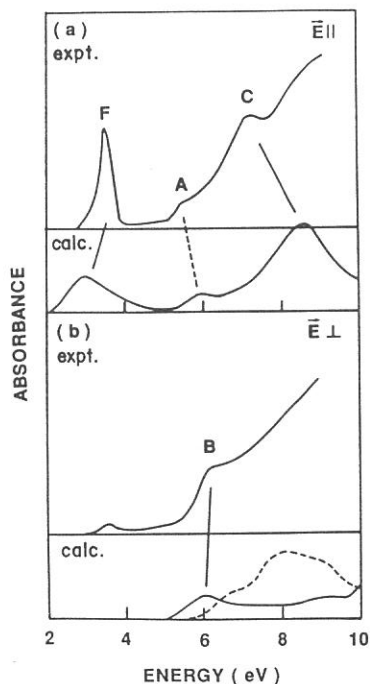


FIG. 2. Observed and calculated absorption spectra polarized parallel (a) and perpendicular (b) to the polymer chain. For the calculated spectra polarized perpendicular to the polymer chain, solid and broken line represent absorption for the polarizations parallel and perpendicular to the plane of the Si backbone, respectively.

Molecular Orientation in Thin Films of Functional Molecules by Means of Angle Resolved Photoemission

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The angular distribution of photoelectrons from thin films of organic crystals involves information on the molecular orientation in the film as well as on the wave functions of valence electrons. Therefore, the quantitative analysis of the photoelectron angular distribution from a valence state gives a detailed information on the molecular orientation in ultrathin films of functional organic molecule, when the initial-state wave function is known. An advantage of the angle-resolved ultraviolet photoelectron spectroscopy (ARUPS) in determining the molecular orientation is that it introduces much less radiation damages into the organic films than other surface sensitive techniques with electron beams. However, the quantitative analysis of the angular distribution from thin films of large organic molecules is very difficult, since the molecule consists of many atoms. Hence the analysis has been mainly performed by a symmetry consideration on the photoemission process with the dipole selection rule, and no one has performed the quantitative analysis of the angular distribution since a challenging work by Permien *et al.* [1] on thin films of lead phthalocyanine and Richardson's successful analysis [2] on their ARUPS data. In our work on ARUPS of thin films of large organic molecules, however, we found that the angular distribution calculated with the theoretical model used by Richardson [2], where the molecule was considered to be a point emitter of photoelectron, gave poor agreement with our experimental results on thin films of copper phthalocyanine [3] which showed a very sharp angular distribution.

In this talk, it is shown that the experimental ARUPS results on thin films of metal free phthalocyanine on MoS₂ crystal surface, where the molecules lie flat on the surface, can be quantitatively explained by a calculated photoelectron angular distribution using the independent atomic center (IAC) approximation [4] combined with MNDO molecular orbital calculation. The results indicate that IAC approximation combined with molecular orbital calculation is useful in the quantitative analysis of photoelectron angular distribution from thin films of large organic molecules. Further, an example of the determination of the molecular orientation with ARUPS is presented for thin films of BTQBT [bis(1,2,5-thiadiazolo)-*p*-quinobis(1,3-dithiole)] evaporated on graphite (HOPG) surface.

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Time-Resolved Spectroscopic Study on the Self-Trapped Excitons in Alkali Halide Crystals

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In the last few years, a new stage has been brought to understanding self-trapped exciton (STE) luminescence in alkali halide crystals with relation to the adiabatic instability of STE's.¹⁾ The important point made clear is that the STE emission bands are classified into three types, I, II and III, irrespective of the traditional classification into two categories (σ and π bands).²⁾ This suggests that there appear, at most, three distinct local minima in the adiabatic potential energy surface (APES) of the lowest energy, corresponding to the on-center (I) and two different off-center (II,III) configurations. One of the urgent topics to be studied is to see how the shape of the APES is, and how the population is fed into each minimum.

We have studied the origin of the short lifetime singlet σ emission band, and its relation to the longer lifetime triplet π luminescent state. Decay curves of the type I emission bands, that is, σ emission bands in NaCl, KBr, RbBr, KI and RbI and π emission bands in NaBr and NaI, were measured using TAC method at UVSOR under single-bunch operation.³⁾ Counting photons over four orders of magnitude have revealed that every σ emission band involves a phosphorescent component with a lifetime longer than 100 ns, in addition to the main fluorescent component. The phosphorescent component shows almost the same emission and excitation spectra as those of the fluorescent one. This evidences that the σ emission band originates from the lowest orbital state of the the STE. Thus, it becomes clear that type I emission results, in general, from radiative decays of nearly degenerate singlet-triplet manifolds of the on-center STE. Simultaneous detection through two different time windows discloses a split in the peak energy of the singlet and triplet components, suggesting a slight difference in the location of the minima in the APES for the singlet-triplet STE pair. Based on these results, a new scheme for the dynamics of exciton self-trapping are proposed.

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**Present and Future of Photoelectron and Photodesorption
Spectroscopic Studies at UVSOR**

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The photoelectron (UPS) experiments have been carried out at three beam lines (2B1, 6A2, and 8B2), and photodesorption (PSD) has been measured at three beam lines (3A1, 5B, and 6A2).

UPS has been applied to many materials and surfaces in order to know binding energy, p-DOS, k-dispersion, and so on. Now, UPS is recognized to be useful, standard, and powerful method for Molecular Science. Tunability and polarization of SR are very effective in UPS. Moreover, it is stressed that UPS presents new concepts to optical and PSD spectroscopies, and also it is the other way around. Therefore, new science is expected on the crossing between UPS, optical, and PSD. As an example, UPS studies of core-exciton decay on wide-band gap materials are presented.

Among lots of attractive subjects for future of UPS, spin-resolved UPS with circular polarized SR on non-magnetic materials is interesting and promising, since the spin-resolved electronic states and the spin-dependent decay processes can be clearly understood. The planning of the spin-resolved UPS studies is presented with the design of a spin detector.

PSD is also a young and attractive spectroscopy, since it is related with basic science and engineering. Tunability, high intensity, and pulsive nature of SR are very powerful to PSD. The interesting results of time-response of the excited-state alkali desorption are shown on SR-irradiated sodium halides. The planning of the high-sensitive detection system is proposed for one of the future PSD experiments.

High Resolution Photoelectron Spectroscopy on Solids: Past, Present and Future

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ABSTRACT

In 1964 electron spectroscopy of inner core levels had reached sufficiently high energy resolution that chemical shifts [1] were detected for the first time for sulphur in some sodium compounds: the technique of electron spectroscopy for chemical analysis (ESCA) was born. About ten years later, Gelius et al [2] published a paper where monochromatized Al K α radiation made it possible to resolve vibrational levels in the carbon 1s level of CH₄. Since the mid-1970's, synchrotron radiation has played an increasingly important role in high resolution core-level spectroscopy. The instrumental resolution has been improved to well below 100 meV for core levels with binding energies below about 200 eV. In this talk, we will review some recent high resolution core level work at MAX-Lab, Lund University, Sweden, and we will discuss future opportunities with the next generation of synchrotron radiation sources.

From an instrumental point of view it is argued that it is extremely important to have an optimal match between the synchrotron radiation source, the monochromator/optical system, the electron spectrometer and the detector. The system in its entirety will not perform better than its weakest component. The centerpiece of MAX-Lab is a 550 MeV storage ring, with fairly low emittance: 40 nm-rad horizontally. The beam current is typically 100-200 mA and the lifetime 3-4 hours. The work reported here was done on a bending magnet beamline, equipped with a modified SX-700 plane grating monochromator [3]. With a typical source size of 100 microns (vertical) x 400 microns (horizontal), the photon spot on the sample is about 0.5 mm x 3 mm. This spot size is well matched to the acceptance of the energy analyzer which is of the hemispherical type, developed and manufactured at the Institute of Physics at Uppsala University (under the leadership of Prof. N. Mårtensson) in close collaboration with Scienta [4,5].

The beam line covers the spectral region from 20 eV to 1000 eV. The resolving power of the monochromator at for instance 240 eV is 4000. For core levels with binding energies below 100 eV extremely good resolution and intensity can be achieved, as demonstrated by the 2p core level spectra from a single crystal of Al(100). With a total instrumental resolution of 50 meV and a data accumulation time of less than 20 minutes, a surface core-level shifted peak can be determined with high accuracy, -96 ± 5 meV [6]. On the (111) surface, no core-level shifted peak is observed to within 15 meV. These observations are state-of-the-art experimentally and pose challenges for future theoretical calculations.

Measurements of surface core level shifts play an important role in the understanding of both the electronic and structural properties of surface layers. Furthermore, surface core level shifts can be correlated with thermodynamical properties of the surface, like solution, segregation, and adhesion energies. With the new experimental capabilities at MAX-Lab, it has been possible to study the 3d core levels of the 4d transition metals with high resolution: 0.2-0.3 eV

total instrumental resolution for photon energies 380-450 eV [7]. For a Pd (100) single crystal, a surface core-level shift of 0.44 ± 0.03 eV towards lower energy has been determined for the Pd 3d core level (binding energy 335 eV). Adsorption of CO on the very same surface results in three different ordered structures dependent on the CO coverage. High resolution spectra of the Pd 3d and C 1s core levels (instrumental resolution of 270 meV and 220 meV, respectively) make it possible to establish a direct relation between the detailed geometry of the CO overlayer and differently shifted peaks in the Pd 3d spectra [8]. From the C 1s spectra, it is furthermore possible to establish and confirm earlier reports that CO only occupies bridge sites on Pd (100).

It has been commonly assumed that no intermixing occurs for alkali metal chemisorption onto free-electron like metals: in all models, the alkali atoms have been thought to reside on top of the surface. Recent work at MAX-Lab on the Al 2p [instrumental resolution $\Delta E = 40$ meV] and Na 2p [$\Delta E = 60$ meV] core levels for different ordered structures of Na/Al (111) clearly demonstrates that intermixing does occur [9]. All previous models must therefore be discarded, and a new picture is emerging for the surface structures of these prototypical systems.

A final example of high resolution core-level spectra is illustrated with recent work by Landemark et al [10] on the clean Si(001) surface. Judged from the Si 2p core-level spectra (total instrumental resolution better than 70 meV) the local structure appears very similar for the two reconstructions 2×1 and $c(4 \times 2)$, respectively. Surface core-level components from both the up and down Si surface atoms in the asymmetric dimers as well as the second-layer Si atoms can be identified, removing some ambiguity in earlier work. The large chemical shift (0.55 eV) between the two dimer-atom components further points to a substantial charge transfer within the dimers.

Based on core-level spectroscopy with a total instrumental resolution of 40-250 meV, as illustrated with a few examples above, it is argued that it makes sense to improve the resolution another order of magnitude for the instrumentation being planned for the third generation of synchrotron radiation sources. Even if the instrumental response function can be deconvoluted (if it is known accurately enough) from the recorded core-line, it is highly advantageous if it is sufficiently small, so that it can be neglected compared to other broadening mechanisms. For investigations of small chemical shifts and subtle changes in line-shapes it can be advantageous to have a total instrumental resolution which is only a small fraction of the inherent line-width.

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Can We Obtain X-Ray Absorption Spectra beyond the Core-Hole Lifetime Broadening?

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Recently, Hämäläinen *et al.*¹⁾ observed experimentally the excitation spectrum of L_3M_5 X-ray emission of Dy compounds in the region of Dy L_3 absorption edge, and found a dramatic improvement in resolution far beyond the limit of the L_3 core-hole lifetime width. We analyze theoretically this excitation spectrum on the basis of the coherent second order optical formula with multiplet coupling effect.²⁾ The width of the calculated spectrum is determined by the M_5 core-hole lifetime, instead of the shorter L_3 lifetime. A fine pre-edge structure of L_3 edge due to $L_3N_{6,7}$ quadrupole transition can be seen in the excitation spectrum, while this structure is quite invisible in the conventional XAS. We discuss the relationship between the excitation spectrum and the conventional XAS, and possible applications of this new technique.

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Magnetic Circular Dichroism in Core-Level Absorption of Magnetic Materials

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Magnetic circular dichroism (MCD) in core-level absorption is element specific and site selective. Thus it can provide valuable information about local magnetic states in compounds and alloys as well as in metals. We present the results of MCD studies around the Fe, Co, and Ni $M_{2,3}$ core edge and Pt $N_{6,7}$ and $O_{2,3}$ edges for Ni and Fe metals, and an $Fe_{50}Pt_{50}$ alloy, and two ferrites (Fe_3O_4 and $CoFe_2O_4$).

The experiments were performed with a bulk-sensitive reflection method^{1,2)} by utilizing circularly polarized synchrotron radiation from both a bending-magnet source (BL-11D) and a helical undulator (BL-28U) at the Photon Factory. The direction of the magnetic field was reversed with the photon helicity fixed.

The MCD spectrum of Ni showed a large negative peak followed by a small positive one with photon energy around the $M_{2,3}$ edge.^{1,2)} A satellite feature in MCD was also observed several eV above the edge. The MCD spectrum of Fe exhibited a nearly antisymmetric shape at the $M_{2,3}$ edge with no satellite structure; this is in contrast to the MCD of Ni. The result for Ni could be favorably compared with the calculations by Yoshida and Jo³⁾ and van der Laan and Thole.⁴⁾

The MCD spectrum of an ordered $Fe_{50}Pt_{50}$ alloy showed a clear negative peak at the Fe $M_{2,3}$ and Pt N_6 edges and a positive peak at the Pt N_7 edge. Positive and negative MCD signals were also observed at the Pt O_2 and O_3 edges, respectively. The observation of MCD at the Pt core edges indicates induced magnetic moment in the 5d electron states in Pt. Comparison with theoretical consideration of MCD for the $p \rightarrow d$ and $f \rightarrow d$ transitions shows that the magnetic moment in Pt is parallel to that in Fe; i.e., the interaction between the 3d electrons in Fe and the 5d electrons in Pt is ferromagnetic. Two causes can be responsible for no observation of a positive MCD peak at the $M_{2,3}$ edge. First, the negative broad MCD signal due to the Pt O_3 edge spreads over this region, resulting in a cancellation of the possible positive MCD at the $M_{2,3}$ edge. Second, the Fe 3d orbital angular momentum in the alloy could be less quenched than in metal Fe.

For Fe_3O_4 and $CoFe_2O_4$, the MCD of multiplet structures in the Fe $M_{2,3}$ prethreshold region was studied in detail using circularly polarized undulator radiation. Three high-lying MCD peaks are common to two compounds while two low-lying MCD features are seen only in Fe_3O_4 . This observation leads to the assignment that the former is attributed to multiplet transitions in the Fe^{3+} ions and the latter is due to transitions in the Fe^{2+} ions. Abundance of features observed in the MCD spectra of Fe_3O_4 and $CoFe_2O_4$ in the Fe $M_{2,3}$ prethreshold region demonstrates the capability of MCD to reveal structures obscured in unpolarized spectra.

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Far Infrared Spectroscopy of Rare Earth Hexaborides

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Reflectivity spectra of trivalent rare earth (R=La, Ce, Pr, Nd, Gd, Dy and Ho) hexaborides were systematically measured in the wide energy region from 1meV to 40 eV. Optical conductivity spectrum was obtained from the reflectivity spectrum by a Kramers-Kronig transformation. A broad infrared absorption band was found at 0.5-0.7 eV in common with the rare earth elements except La which exhibits a normal metallic property. The energy position of the infrared absorption band was almost independent of the kind of the rare earth element but its intensity strongly depended on it. We found that the intensities are nearly proportional to the occupied 4f electron numbers of the rare earth element. This means that the infrared absorption is strongly correlated with the total 4f-angular momentum of these materials.

Up to now, some models on the origin of the infrared absorption have been proposed by other group. The first model was a so-called "f-d model" which suggests that the infrared absorption band originates from the absorption due to the optical excitation between the 4f and the 5d states of the rare earth element. According to the XPS data of the some trivalent rare earth hexaborides, however, the position of the occupied 4f level of the rare earth element below the Fermi level changes with the element although the 5d state is almost unchangeable. This result means that if the "f-d model" holds the energy position of the infrared absorption should change with the element. But this is strictly in contrast with the present results.

The other is the excitonic model. In this model the infrared absorption was considered to be due to the optical transition between the bonding and the antibonding states which are composed of the boron 2p and 2s electrons. This prediction, however, can not explain that the intensity is proportional to the occupied 4f electron numbers of the rare earth element.

Then, considering our experimental results and also the results of the recent band calculation on LaB₆ [1], we propose that the infrared absorption is due to the optical excitation between the saddle points, 1 of the valence band and 25 of the conduction band of which transition is mediated by the exchange interaction between the 4f-conduction electrons. The energy separation between these points in the B.Z. coincides with the energy of the observed infrared absorption.

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A Future Direction of Synchrotron-Radiation Photoemission Study of Solid Surfaces

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It is known that the binding energies of core-levels in the selvedge region of solid surfaces are shifted slightly from those of the bulk atoms (called surface core-level shift; SCLS). This SCLS can be best detected by synchrotron-radiation photoemission in the photoelectron energy region for the shortest mean-free-path, which can be attained by tuning the energy of synchrotron-radiation. Both clean and alkali-metal saturated Si(001) surfaces were chosen as examples. For the clean Si(001)2×1 surface, the situation was quite controversial until a recent high-resolution photoemission study of Landemark et al.[1] appeared. Recent and unpublished results of synchrotron-radiation photoemission study of the author's group for both the clean and potassium-saturated Si(001)2×1 surfaces were introduced[2]. It was indicated that an interpretation of the our results following the result by Landemark et al. [1] shows that the photoelectron intensity for the upper dimer Si atoms is dependent on photoelectron emission-angle. This angular dependence is indicative of photoelectron diffraction effect for the SCLS component. A future direction of synchrotron-radiation photoemission study of solid surface was raised, i.e., photoelectron diffraction of SCLS for semiconductor surfaces.

There have been several studies of SCLS photoelectron diffraction for metal surfaces but only a few attempts have been made for semiconductor surfaces. An recent example by Gota et al.[3] was introduced. In their work, azimuthal photoelectron diffraction patterns for In 4d SCLS of an InP(110)1×1 surface were measured and analyzed based on the well-understood zigzag relaxation of the (110) surface of III-V semiconductors. The analysis showed a promising feature of the SCLS photoelectron diffraction as a means of surface structure-analysis although it was too premature to be conclusive.

The key factors of SCLS photoelectron diffraction in future would be the following.

- (1) High photon flux and/or high efficiency in photoelectron detection.
- (2) How easy or how difficult is the analysis of SCLS photoelectron diffraction?

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XAFS Studies of Molecular Adsorbates on Metals

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The adsorption behaviors of S-containing molecules, thiophenol (C_6H_5SH), and thiophene (C_4H_4S) on clean Ni(100) have been studied by polarization dependent S K-edge XANES and EXAFS at BL 11B soft X-ray double crystal monochromator station in the Photon Factory. Clean Ni(100) surface was dosed with each molecule at 100 K and heated up to some temperatures subsequently. S K-edge absorption spectra were measured by the fluorescence and total electron yields at each stage.

(1) Thiophenol on Ni(100)

Heating up to 200 K, physisorbed molecules desorb and the surface is covered by only monolayer, judging from the signal to background ratio. From the polarization dependence of the XANES peak characteristic of the $\sigma^*(S-C)$ transition, we found that the S-H bond is cleaved and the remained phenyl thiolate ($C_6H_5S^-$) stands on the surface almost perpendicularly. Polarization dependence of S K-edge EXAFS shows that sulfur atom of phenyl thiolate sits on the 4-fold hollow site. Heating the sample further, phenyl rings are removed from the surface and S atoms remained on the 4-fold hollow sites.

On the other hand, it turned out that thiophenol at very low coverage (0.075 ML) lies down flat on the surface and heating induced dissociation and left S atoms at the hollow site without passing the process of phenyl thiolate formation.

(2) Thiophene on Ni(100)

Heating up to 145-160 K, physisorbed molecules desorb and monolayer species remain on the surface, which consist of thiophene and atomic S. Further increase of the temperature induces the gradual dissociation and only atomic S exists on the surface at 180 K. On the other hand, remarkable polarization dependence appears in the XANES spectra of submonolayer species at 100 K, suggesting the thiophene molecule lying parallel to the surface.

High resolution spectra of S K-edge XANES from thiophene on O precovered Ni(100) and clean Ni(100) were measured at the undulator beamline BL 2A in the Photon Factory. It was revealed that the first prominent peak consists of π^* and σ^* transitions with 0.6 eV splitting for thiophene on O-precovered surface, while the splitting is 1.4 eV for thiophene on clean surface at low coverage (0.05 ML). The σ^* peak remains at the same energy, and the π^* peak shifts lower by 0.8 eV. This indicates that the charge transfer occurs from nickel substrate to S in thiophene. At the slightly higher coverage (0.1 ML), additional peak appears at the grazing incidence spectrum, whose position is almost same as that of π^* peak from thiophene on O precovered Ni(100). This result suggests the second layer begins to adsorb at this coverage.

Above results demonstrate the usefulness of the XAFS technique for the investigation of adsorption behavior of molecules on metal surfaces.

New Directions in the Study of Electronic Structure using Synchrotron Radiation.

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A brief review will be given of some of the opportunities for the study of electronic structure which are opening up as a result of recent and future developments in synchrotron radiation. Of primary importance is the construction of new sources of synchrotron radiation and an account will be given of the new beamline constructed on the Daresbury Synchrotron by the UK IRC in Surface Science. The construction of the beamline is being organised by Dr G. Thornton of the Chemistry Department of the University of Manchester in close collaboration with staff at the SERC Daresbury Laboratory. The beamline will have two stations; 4.1 with an energy range of 15 eV to 250 eV and which is scheduled for completion in February 1993 and 4.3 covering the energy range 640 eV to 1 keV and which is currently being commissioned.

Improvements in the resolution and sensitivity of monochromators of synchrotron radiation offer obvious ways in which the study of electronic structure will be advanced. It is suggested that the development of monochromators capable of matching the resolution and sensitivity of the best of current laboratory instruments should be a high priority. Current commercial x-ray photoelectron spectrometers (XPS) have the sensitivity to measure core level spectra with good signal to noise from significantly less than 1% of a monolayer of adsorbates using monochromated Al K α radiation with a resolution of ~ 0.25 eV. The development of monochromators of synchrotron radiation with equivalent performance in the energy range of ~ 1 keV to 2 keV offers the possibility of obtaining important new information on local electronic structure from the linewidths and lineshapes of photoelectron lines. This would be particularly important in the study of "shallow buried interfaces" which are of technological importance in the semiconductor and magnetic

recording industries and are difficult to study with other techniques. The results of a recent study [1] of Cooper minimum photoemission from Ag impurities in Cd and Al will be used to illustrate the potential of improvements in sensitivity for the study of the wavefunctions of adsorbates.

It will be argued that important advances in the study of electronic structure are also likely to come from coordinated studies combining a variety of synchrotron and laboratory based techniques. This will be illustrated by a case study of a decade of research on the link between the physical and electronic structure of CuPd alloys [2,3].

Finally it will be argued that there is always scope for the development of new theoretical approaches which can advance the understanding of electronic structure by offering new ways of interpreting the results of standard experimental techniques. An example will be given of a new approach to the interpretation of Auger parameter shifts which offers insight into mechanisms of charge transfer and electron screening in alloys [4], semiconductors [5] and interfaces [6].

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PHOTON STIMULATED DESORPTION BY CORE ELECTRON EXCITATION

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The photon stimulated ion desorption (PSID) from the adsorption system of H₂O on the Si(100) surface has been studied in the range 500–700 eV. Experiments have been carried out at the Photon Factory of the National Laboratory for High Energy Physics using the grasshopper monochromator beamline (BL11A). Ions were detected and analyzed by a time of flight (TOF) spectrometer utilizing pulsed synchrotron radiation (turn time: 624ns, width: 100ps) from the Photon Factory storage ring in single bunch mode operation.

H⁺ ion is dominant in all investigated region and O⁺ ion is also observed in the TOF spectrum which is strongly energy-dependent. The relative ion yield curves of these ions indicate characteristic behavior near and above the O K-edge (539.7 eV); H⁺ ion exhibits sharp rises at ca. 530 eV and two broad peaks below (ca. 535 eV) and above (ca. 555 eV) the O K-edge, O⁺ exhibits a delayed threshold at ca. 570 eV and gradual increase up to 700 eV.

To explain these experimental results and to elucidate the mechanism of PSID, the O_{KLL} auger electron yield (AEY) spectrum and the photoion-photoion coincidence (PIPICO) spectrum between H⁺ and O⁺ in this energy region have also been obtained. The results are discussed in terms of the primary excitation followed by the Auger decay and the modification of charge state of desorbing species. Our experimental results are consistent with a mechanism of formation of multiple charged OH^{m+} (m≥3) ions followed by reneutralization of the excess of charge with strong interactions with the substrate and finally desorption as single charged H⁺ and O⁺ ions.

Science and Engineering in Synchrotron Radiation-Excited Semiconductor Process

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Abstract

Recent results of the Synchrotron Radiation excited Semiconductor process experiments are reviewed. Unique material selectivity is observed both in the etching and CVD reactions. As a possible explanation for these material selectivity, a generation of reactive centers with certain lifetime is proposed.

1. Introduction

It can be said that the surface photochemical reaction induced by the vacuum ultraviolet light is started by the appearance of the synchrotron radiation (SR). Since the first experiment of the SR etching(1) and CVD(2) are reported, studies of this field have become more active year by year. The study of the SR semiconductor process contains not only engineering interests of exploring the future new process technologies, but also scientific interests of developing a new scientific field of VUV surface photochemistry. In the present report, several interesting phenomena as a problem of photochemistry observed in the SR etching and CVD experiments are introduced and the reaction mechanisms are briefly discussed.

2. Material selectivity observed in SR etching and CVD.

Under the reaction gas SF_6+O_2 , or without reaction gases, SiO_2 , Si_3N_4 and poly- or amorphous Si can be etched (or evaporated) by electronically exciting the substrate surface by SR irradiations. In this etching, the unique difference of the etching rate among materials were found (1,3). The tendency of the material selectivity is roughly similar between etching (with reaction gas) and evaporations (without reaction gas). In a detailed comparison, however, it has been found that the etching rate is significantly enhanced by the existence of the reaction gas in the case of Si_3N_4 and poly-Si. The temperature dependence is also quite different between etching and evaporations. The evaporation rate increases with increasing temperature. But, the etching rate decreases with increasing temperature.

Concerning to the CVD, similar kind of material selectivity is observed.(4) Silicon nitride film is deposited from the mixture gas $SiH_4 + NH_3$ by the SR irradiation. In this system, it has been found that while the film composition (N/Si) increases in proportion to the partial pressure ratio of NH_3/SiH_4 (P) initially, it rapidly increases nonlinearly at around 1 of P. The position (value of P) of this sharp increase is slightly lower in insulating substrate than in c-Si substrate. This phenomena indicates that the incorporation efficiency of nitrogen is larger in insulating materials than in c-Si.

At the present stage, the reaction mechanisms for these etching and CVD reactions are not explained clearly yet. A possible explanation is that a reactive center resulting in the fluorination reaction or nitridation reaction is generated by the SR irradiation on the substrate surface, and the material selectivity is due to the difference of the lifetime of the reactive center.

Acknowledgement

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DESIGN AND DEVELOPMENT OF SPECTROSCOPY BEAM LINES AT INDUS-1

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ABSTRACT: INDUS-1 IS THE FIRST SYNCHROTRON RADIATION SOURCE BEING BUILT AT CENTRE FOR ADVANCED TECHNOLOGY (CAT), INDORE, INDIA. THIS SOURCE, A STORAGE RING, OPERATES AT 450 M eV ENERGY AND HAS A CRITICAL WAVELENGTH OF 61 Å. THE CRITICAL WAVE LENGTH WILL BE 30 Å WITH THE USE OF A WIGGLER. THUS INDUS-1 IS AN INTENSE SOURCE OF PHOTONS, THEIR ENERGIES RANGING FROM SOFT X-RAYS TO INFRARED. SEVERAL BEAM LINES ARE PLANNED AT INDUS-1 TO CARRY OUT STUDIES OF INTERACTION OF RADIATION WITH MATTER. SPECTROSCOPY DIVISION OF BARC, IS DESIGNING AND FABRICATING THREE OF THE BEAM LINES AND THE REQUIRED EXPERIMENTAL FACILITIES. ALL THE BEAM LINES OPERATE UNDER UHV CONDITIONS (PRESSURE < 10⁻⁹ TORR). A BRIEF DESCRIPTION OF THE WORK IS GIVEN BELOW.

1. PHOTOPHYSICS BEAM LINE: THIS BEAM LINE MAKES USE OF PRE AND POST FOCUSING TOROIDAL MIRRORS AND A 1 METRE SEYA-NAMIOKA TYPE MONOCHROMATOR AS EXCITING MONOCHROMATOR AND 0.5 - 1 METRE MONOCHROMATORS AS ANALYSING MONOCHROMATORS. THIS BEAM LINE IS DESIGNED TO CARRY OUT STUDIES ON PHOTO ABSORPTION, PHOTO DISSOCIATION AND FRAGMENTATION, CLUSTERS ETC. MOST OF THE BEAM LINE COMPONENTS, BARRING UHV SLITS, MIRRORS AND GRATINGS, ARE INDEGENOUSLY BUILT.

2. HIGH RESOLUTION VUV BEAM LINE: THIS BEAM LINE HAS A FORE OPTICS CONSISTING OF THREE CYLINDRICAL MIRRORS. THE HIGH RESOLUTION INSTRUMENT IS A 6.65 METRE CONCAVE GRATING SPECTROGRAPH/SPECTROMETER IN OFF-PLANE EAGLE MOUNT. A HIGH TEMPERATURE FURNACE AND ABSORPTION CELL ARE BEING FABRICATED TO CARRY OUT EXPERIMENTS ON SPECTRA OF ATOMS AND MOLECULES INVOLVING RYDBERG STATES, MULTIPLY EXCITED STATES AUTO IONIZING LEVELS ETC. MOST OF THE BEAM LINE COMPONENTS INCLUDING THE 6.65 M SPECTROGRAPH/SPECTROMETER IS BEING BUILT INDEGENOUSLY. HOWEVER, THE GRATINGS, MIRRORS AND UHV SLITS WILL BE IMPORTED.

3. PHOTO ELECTRON SPECTROSCOPY BEAM LINE: THIS BEAM LINE MAKES USE OF PRE AND POST FOCUSING TOROIDAL MIRRORS, A TOROIDAL GRATING MONOCHROMATOR (TGM 1400) AND A SPHERICAL SECTOR ANALSER ELECTRON SPECTROMETER AND A SAMPLE CHAMBER. THIS BEAM LINE IS DESIGNED TO CARRY OUT EXPERIMENTS ON HIGH T_c MATERIALS, PARTIAL PHOTOIONIZATION CROSS SECTIONS ETC. THE BEAM LINE COMPONENTS ARE BEING DESIGNED.

*CENTRAL WORK SHOPS

Present Status and Future Perspective of Synchrotron Radiation Research Center

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The Synchrotron Radiation Research Center (SRRC) is the name of new institute in Taiwan, R.O.C. for collaborative research center for scientific community in Taiwan area. Presently, the main facility of this center is, of course, a dedicated electron storage ring for synchrotron radiation researches.

The project of the SRRC was initiated and proposed by a feasibility study group in 1982. It was approved by authority in July, 1983, and a task organization for the construction of main facility was organized and the construction has been started.

The detailed parameters are shown in the table shown below.

The booster has been purchased from the Scantronix company and has been put in operation recently. The transport line has been constructed successfully. The main ring is almost having its shape. All magnet systems are placed and pre-aligned. All aluminum vacuum chambers will be installed by the end of this year. RF cavity has been installed and those high frequency power station and power transmission circuits are on construction.

We expect to commission the system by the middle of next year and three beam lines will be assembled by the end of next and start for research. By that time our organization will be a National facility of our scientific community. It will be welcomed international research collaborations in these variety application of the synchrotron light.

Nominal energy	1.3 GeV
Nominal circulating current	200 mA
Number of stored electron	5×10^{11}
Horizontal natural emittance	1.92×10^{-8} m-rad
Circumference	120 m
Revolution frequency	2498.27 kHz
Radio frequency	499.654 MHz
Harmonic number	200
Number of superperiods	6
Free long straight section length	6 m
Bending field	1.24 T
Bending radius	3.495 m
Horizontal tune	7.18
Vertical tune	4.13
Synchrotron tune	1.15×10^{-2}
Max. horizontal beta	18.43 m
Max. vertical beta	12.06 m
Bunch length (rms)	0.74 cm
Bending Magnet Beam size	
Horizontal σ_H	0.14 mm
Vertical σ_V	0.131 mm
Critical photon wavelength (dipole)	8.89 Å

Present Status of HESYRL

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The Hefei synchrotron radiation laboratory (HESYRL) was completed and passed a technical examination organized by the Chinese Academy in October 1991. The current intensity has got to over 200 mA under 800 MeV and the beam lifetime has been 6 hours at keeping the current intensity over 10 mA each injecting. Now the HESYRL operates on schedule and 5 beamlines with stations are available to users to do experiments.

The HESYRL facility consists of three major systems: the 200 MeV electron Linac, the 800 MeV electron storage ring and photon beamlines with corresponding experimental stations. Fig.1 shows the general layout of the facility and Table 1 summarized its main parameters.^[1]

There are twelve dipoles, thirty two quadrupoles, fourteen sextupoles and four long straight sections in the storage ring.

Three long straight sections will be used in the future for the installation of wigglers, undulators and free electron lasers. The Linac injector consists of four accelerating sectors and a preinjector. Each sector is composed of two 3 m long accelerating sections and is powered by a klystron of 15 MW. The preinjector is composed of a triode gun, a prebuncher and a 3 m long accelerating section and is powered by a klystron of 10 MW.^[2]

The storage ring is installed in a hall 50 m in diameter and the experimental area is the floor that surrounds it as shown in Fig.1. The Hefei synchrotron radiation facility can produce a wide spectrum of radiation from the infrared to the soft X-ray region. Every bending magnet has two beam ports whose opening angles are 85 and 120 mrad in the horizontal direction, respectively. Therefore light from 24 ports in total can be extracted from the storage ring. Each beamline will be split two branch lines, so the storage ring can be equipped with about 50 beamlines, including ones from insertion devices, and corresponding stations.

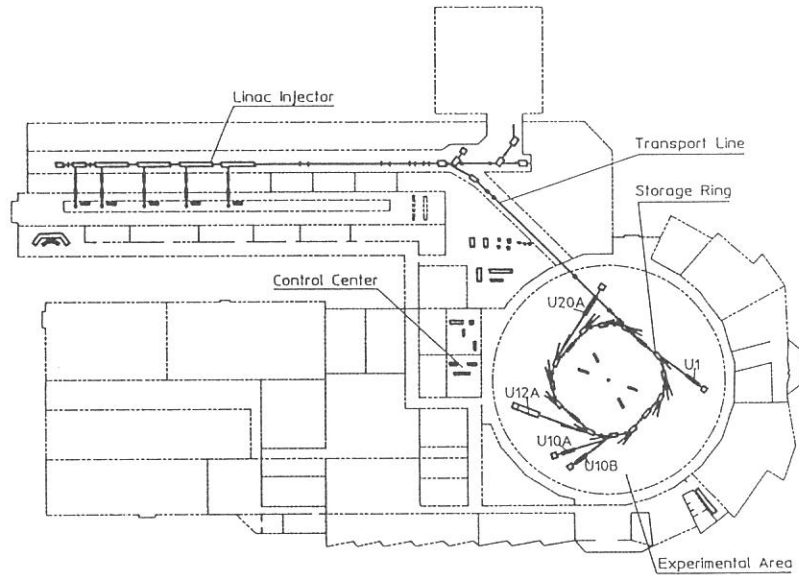


Fig.1 Layout of Hefei synchrotron radiation facility.

Table 1 Parameters of Hefei synchrotron radiation facility

Storage ring	
Energy	800 MeV
Current intensity	100-300 mA
Circumference	66.13 m
bending magnets	12
Bending field	1.2T
Bending radius	2.222 m
Critical wavelength	24 Å
Total radiation power	4.89 kW
Energy loss per turn	16.3 keV
Working pressure	2×10^{-9} Torr
Linac injector	
Energy	200 MeV
Peak current	130 mA
Total length	35 m

Five beamlines and corresponding stations were constructed at the first stage. All of them were installed in the experimental hall and open to users to do experiments on X-ray lithography, photochemistry, time-resolved spectroscopy, soft X-ray microscopy and photoelectron spectroscopy since the end of last year. Fig.2 and Table 2 show their optical design and the main parameters.[3]

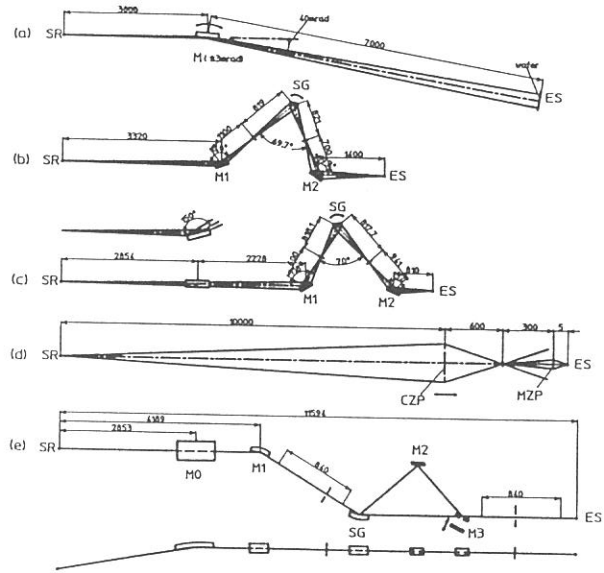


Fig.2 Optical layout of the beamlines.

Table 2 Main optical parameters of the beamlines

Beamline	U1	U10A	U10B	U12A	U20A
Monochromator	none	1m Seya	1m Seya	linear	SGM
Grating(l/mm)		2400 1200 600	2400 1200 600	n=1506 1082 770	1100 600 500 200
Resolution(nm)		0.1 at 35 nm	0.1 at 35 nm	0.03	$\lambda/\delta\lambda=10^3$
Wavelength range(nm)	0.5-2	35-600	35-600	2-5.4	1-110
Pre-mirror		toroidal	spherical		spherical
Post-mirror		toroidal	ellipsoidal		cylindrical
Accept. h _{xv} (mrad)	15×0.6	25×5	25×5	0.27×0.27	20×2.5
Spot at sample h _{xv} (mm)		2×1	3×0.2	0.2μm	3×1
Flux at sample(phs/s)	0.1W/cm ²	5×10^{11}	2×10^{11}	5×10^5	10^{10}

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BSRF Status and Research Opportunities

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The Beijing Synchrotron Radiation Facility (BSRF) is a partly dedicated Synchrotron Radiation (SR) facility whose construction was started in 1985 and affiliated with the Beijing Electron Positron Collider National Laboratory (BEPC). It is located at the Institute of High Energy Physics (IHEP) in the west suburb of Beijing. BSRF is one of four constituents of BEPC. The other three are a 1.55 GeV linac injector, a 1.55-2.8 GeV storage ring (BEPC) and a particle spectrometer for high energy physics research. At present, most shifts are run for high energy physics research. The dedicated mode was commissioned at the end of 1989 and the storage ring energy is 2.2 GeV, and a horizontal emittance of 70 nm-rad was achieved[1]. The construction project of BSRF is divided into two phases. First phase was from 1985 to 1990. The second one is from 1991 to 1995.

The first phase of BSRF construction project consists of three beam ports, seven beamlines and nine stations[2]. one beam port is a wiggler port and the other two are bending magnet ports. The nine stations are the topography and microprobe fluorescence station with white beamline (4W1A), XAFS station with monochromatic beamline (4W1B), general purpose diffraction station with monochromatic and focusing beamline (4W1C), the diffraction and small angle scattering station with a monochromatic and focusing beamline (4B9A), photoelectron spectroscopy station with VUV/soft X-ray compatible beamline (4B9B), lithography studies station with soft X-ray beamline (3B1A) and biology spectroscopy station with monochromatic and focusing beamline (3B1B).

The second phase of construction project of BSRF has being designed[3]. It consists of two insertion devices, and four experiment stations. The first beam port is the wiggler port 1W1. The permanent magnet wiggler in designing is a 16 pole wiggler (17 kG). Two beamline 1W1A and 1W1B will be from this port. The beamline 1W1A is a unfocusing white and monochromatic beamline providing for diffraction at ultra-high pressure and microprobe X-ray fluorescence station. The beamline 1W1B is planned to be designed for nuclear resonance scattering station. The second is the undulator beam port 3U1. The insertion device is a 34 pole permanent magnetic undulator (5.2 kG). The preliminary design of the optical system of beamline 3U1 includes a horizontal focus mirror and a SX-700 type plane grating monochromator. The two stations will exploit this beamline. One is the atomic and molecular physics station. The other is the soft X-ray optics station. The third is a bending magnet beam port. The beamline 3B7 is a general purpose beamline which will be used for synchrotron radiation diagnostics and calibration of detectors etc.

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Current Status of the PLS Project

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The Pohang Light Source (PLS) project, which was started on April 1, 1988, is progressing smoothly. The PLS consists of a 2 GeV electron linear accelerator and an electron storage ring optimized at 2 GeV. The synchrotron radiation will cover from VUV to soft X-rays. The major parameters and the current status for the storage ring and the linear accelerator are described below:

Storage Ring

The nominal electron energy is 2 GeV, and the initial goal for the electron beam current is 100 mA for the multi-bunch mode and 7 mA for the single-bunch mode. The circumference of the ring is 280.56 m and the natural beam emittance is 12×10^{-9} m-rad. The ring has 12 straight sections. Ten of them are for insertion devices and other two sections are for injection system and RF system.

The prototype dipole and quadrupole magnets have been tested and approved for production. All magnets including sextupoles and correctors are scheduled to be completed by the end of 1993. Also, the test for the second prototype vacuum chamber have been completed.

Initially there will be two bending magnet beam lines, one for VUV and another for X-ray users. The monochromator for the VUV beam line will cover the energy range of 12-1230 eV and will be used for ARUPS, XPS and XAS. The X-ray beam line will provide the photons of energy 3-12 keV and will be used for X-ray diffraction, XAFS and X-ray standing wave experiments.

Linear Accelerator

The 2 GeV full energy linear accelerator, which is 150 m long, has 42 accelerating columns and are powered by 11 klystrons. The maximum output power of the each klystron is 80 MW. A 200 MW modulator will be installed to operate these klystrons.

The 60 MeV preinjector for the linac was commissioned in February, 1992. Eight accelerating columns for the second and third modules were installed. The second module was tested successfully at 200 MeV in December, 1992 and it is expected that the test for the third module will be done by the end of February, 1993. The installation of the linac system will be completed by the end of 1993.

Synchrotron Radiation Sources in Japan

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Table I is a list of the synchrotron radiation sources in Japan operated and under construction. The total number is 17. They are classified into two, one of which is belonging to the public institutes widely opened for scientific research (upper 6)¹⁾ and the other, to the private companies used closely for industrial purposes (lower 11)²⁾(with one exception). The sources in the planning stage are not given.

Table I Existing Synchrotron Radiation Sources in Japan

<u>Machine</u>	<u>Location</u>	<u>Institution</u>	<u>E(GeV)</u>	<u>ϵ_c(keV)</u>
TERAS	Tsukuba	ETL	0.8	0.57
PF	Tsukuba	KEK	2.5	4.0
AR	Tsukuba	KEK	6.5	26.4
SOR-RING	Tanashi	Univ.Tokyo	0.38	0.11
UVSOR	Okazaki	IMS	0.75	0.43
Spring-8*	Nishiharima	JAREI-RIKEN	8	28.3
HITACHI-I	Hitachi	HITACHI	0.2	0.026
JSR	Tokai	JAERI	0.3	0.072
NIJI-II	Tsukuba	ETL-SEI	0.6	0.342
NIJI-III	Tsukuba	SEI-ETL	0.62	1.057
NIJI-IV	Tsukuba	ETL-KHI	0.5	0.231
LUNA	Tsukuba	IHI	0.8	0.568
SORTEC	Tsukuba	SORTEC-ETL	1.0	0.792
AURORA	Tanashi	SHI	0.65	1.218
NAR	Atsugi	NTT-TOSHIBA	0.8	0.614
Super-ALIS	Atsugi	NTT-HITACHI	0.6	0.715
MELCO-II	Itami	MELCO	0.8	1.893

*Under construction

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