UVSOR
ACTIVITY REPORT
2001

edited by
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PREFACE

This Activity Report covers the research activities done at the UVSOR facility in the Institute for Molecular Science (IMS) in FY2001. This is the eighth volume in the red-covered activity report series for the second 10 years in UVSOR. For these years the total beamtime, beamlines, and users are in a steady state; that is, ~40 weeks/year (~2,500 hours/year), ~20 beamlines, and ~800 users/year (with ~180 projects/year). However, some of the equipment is gradually being behind the times in comparison with undulator-based highly brilliant synchrotron facilities in the world. In recent three years, we discussed with our Ministry (MEXT) an additional budget for the upgrade of the light source of UVSOR to enhance our activities even for the third 10 years. Finally we have succeeded in getting it for FY2002. We hope that the UVSOR will begin supplying low-emittance ~27 nmrad photons and 2 or 3 additional undulator beamlines from the autumn in 2003.

In FY2001 one associate professor of three, one research associate of four and one technical associate of six left the UVSOR facility. Dr. Masao Kamada and Dr. Shigeru Kouda moved to the Synchrotron Light Application Center, Saga University, as professor and research associate, respectively, in October and July in 2001. Mr. Toshio Kinoshita retires upon completion of 19 years of service and support this March. These changes are our great loss, but fortunately we succeeded in having two new members. In August 2001 Dr. Akira Mochihashi came as a new research associate from the Photon Factory, the Institute of Material Structures Science. He belongs to the light source division. In April 2002, Dr. Shin-ichi Kimura comes back as associate professor from Kobe University. He will reinforce infrared spectroscopy and high-resolution photoemission of correlated materials in UVSOR.

I attach herewith a report by Dr. A. M. Bradshaw. He is one of the two distinguished foreign councilors of the IMS during FY2001-02. We are very grateful to him for a valuable report to evaluate the present status and future of the UVSOR facility. After receiving his report, we received great news about the approval of the upgrade plan from MEXT. We will further elaborate our future programs by taking into account his comments.

March, 2002

N. Kosugi

Nobuhiro Kosugi
Director of UVSOR

THE UVSOR FACILITY: A SHORT APPRAISAL

INTRODUCTORY REMARKS

UVSOR is known mainly in the international community for its fine work in molecular photoionisation, photochemistry and macromolecular physics. The author of this brief survey, a former scientific director of BESSY with research interests in molecular photoionisation and surface science, has been familiar with the research carried out at UVSOR for many years, but visited the facility itself for the first time during his stay at IMS from 21st – 24th October 2001.

STATUS OF THE BEAM LINES

The machine has four straight sections two of which are used for insertion devices - a linear undulator (BL3A) and an undulator for circularly polarised light (BL5A), which is also used as an optical klystron for a free electron laser experiment. BL3A is equipped with an irradiation facility as well as with a constant deviation SGM used for the study of dissociative multiple photoionisation, unique among synchrotron radiation facilities. On BL5A there is a highly flexible SGM with an energy range of 5 - 250 eV which is used for high resolution spin- and angle-resolved photoemission studies of solids and surfaces. More insertion device beam lines are planned following an upgrade of the machine which is discussed below. There is also an impressive mono-chromator park on the bending magnet beam lines, including a further eight grazing-incidence monochromators and two crystal monochromators. A variable line spacing PGM has just finished trials on a bending magnet beamline (BL4B). Altogether there is a total of twenty measuring stations, including normal-incidence monochromators and beam lines for white light and IR. Eleven of these stations are used by outside users, i.e. by scientists from institutions other than IMS.

A BRIEF OVERVIEW OF THE RESEARCH PROGRAMME

It is not possible in such a brief account to do justice to the extensive research programme. The examples of world-class research work chosen by the author in the following are necessarily subjective and certainly influenced by his own research interests, as well as by some of the very fine talks he heard at a symposium held during his visit.

Both fluorescent decay and laser-induced fluorescence have been used to study the photofragmentation of molecules such as H_2O, OCS and CH_3CN following excitation with UV synchrotron radiation as well as to characterise the frag-ments. Similarly, the coincidence techniques PIPICO and AEPIPICO have been employed to study fragmentation in core-ionised CF_4, CD_3OH and CH_3CO, CD_3CN, respectively. The latter study was particularly interesting in that two-body dissociation with rearrangement was found to accompany N 1s resonant Auger decay to give CD_2^+ and DCN^+ alongside the "normal" products ($C_2D_3^+$ and N^+) and (CD_3^++ and CN^+). Similarly exciting is the increased level of understanding of core level photoabsorption of diatomic molecules achieved by both new experiments and theory. In particular, a very simple experiment has recently been conceived for the new variable line-spacing PGM in which two identical detectors register the photoion current at 0° and 90° to the **E** vector of the incident synchrotron radiation. Since the absorption cross section will be largest when the transition dipole is aligned parallel to the **E** vector the aniso-tropy in the ion distribution will reflect the symmetry of the excited states. Thus for a linear molecule it is possible to distinguish between final states of π and σ symmetry. In the case of core level excitation of N_2 a previously unidentified state of π symmetry was found at 419 eV in the region of the σ shape resonance. Recent calculations by the same group show that this could be a bound state involving a triple excitation. Combined synchrotron radiation and laser experiments are likely to play a more important role at UVSOR in the future: The technique has already been used to study the time dependence of photo-induced phase transitions in inorganic systems as well as of the surface photovoltage (SPV) effect in semi-conductors. It was found, for example, that both for the GaAs(100) surface and for a GaAs-GaAsP superlattice that the laser-induced photoelectron core level shift is due to the SPV and that its decay can be observed on a microsecond timescale. Beamline BL6A2 has been upgraded for experiments of this kind and combined with a facility for photoemission investigations on surfaces with a spatial resolution in the micron range. A deeper understanding of the preparation and properties of Si surfaces has also been obtained, in particular of the hydrogen adlayers resulting from etching techniques. Infrared reflection-absorption spectroscopy played an important role in these measurements. Single crystal surface science studies at UVSOR have also shed new light on the chemisorption of simple molecules on metal surfaces. For example, it was shown that N_2O adopts a lying-down geometry on the Pd(110) surface and already dissociates at about 120 K, giving rise to several N_2 desorption states and leaving oxygen on the surface. Studies of the electronic structure and molecular orientation of polymer films continue at UVSOR, if not with the same intensity as in the past. Recently, angle-resolved photoemission and NEXAFS have been used to show that the heterocyclic pendant group in poly(9-vinylcarbazole) exhibits a larger average tilt angle at the surface than that expected on the basis of random orientation.

Planned upgrade and future emphasis

As is now widely known, an undulator is a periodic magnetic structure, or insertion device, which is inserted into the straight section of a storage ring, causing the electron (or positron) beam to oscillate transversally about its prescribed orbit. The intense beam of radiation produced in the forward direction is strongly peaked at one wavelength on account of the quasi-coherent addition of the radiation emitted from the points of maximum excursion. UVSOR is a so-called second-generation synchrotron radiation source which was planned and constructed at a time when the principle of the undulator was already known, but essentially untested. Third generation sources built in the last ten years are those which contain a large number of straight sections for undulators and wigglers. These, rather than the bending magnets, then provide the most important sources of synchrotron radiation on the storage ring. (The periodic excursions from the orbit are larger in the wiggler due to a stronger magnetic field and there is no quasi-coherent addition of the emitted radiation.) UVSOR has currently two undulators and a short wiggler with superconducting magnets which is intended as a "wavelength shifter".

A modification to the lattice of the storage ring ("upgrade") is currently in the planning stage. This will create – without changing the circumference – four new short straight sections which can also be used for insertion devices. The new lattice can be created by replacing all the separate quadrupole and sextupole magnets of the old lattice with "combined function" magnets which have both quadrupole and sextupole fields. The bending magnets would remain un-changed. A further attractive feature of the upgrade would be the lower emittance (27 nm-rad as opposed to 165 nm-rad) which is an important factor in obtaining high spectral resolution and high photon flux on the various mono-chromators installed on the beam lines. The use of specially constructed *in vacuo* undulators with gaps as narrow as 10 mm will give access to the photon energy range up to 500 eV with the first and third harmonics. The short length available (1.5 m) for the undulators in the new straight sections means that the flux and pseudo-monochromaticity will be somewhat lower at these photon energies than on storage rings with electron energies in the 1–2 GeV range. However, UVSOR will still become competitive in this important soft x-ray region where very exciting work is currently being performed at facilities such as MAX II (Lund), ALS (Berkeley), ELETTRA (Trieste) and BESSY II (Berlin).

At the same time, the author of this report is of the opinion that it is very important to maintain, and to expand, the undulator capacity for photon energies from 10 to 100 eV. Storage rings with electron energies of the order of 750 MeV optimally provide first-harmonic undulator radiation in this photon energy range. The last few years has seen a reduction in the number of such facilities available worldwide. BESSY I has been closed; Super-ACO in Orsay will suffer the same fate when the construction of SOLEIL begins; MAX I is used as part of the injection system for MAX II; the ISSP ring in Tokyo has been dismantled; further, it is not clear how long the UV ring in Brookhaven will remain in operation. UVSOR has the unique opportunity – particularly with the upgrade – of becoming the prime facility world-wide offering undulator radiation of very high spectral brilliance in the far UV up to 100 eV primarily for experiments in surface and solid state physics, for fundamental photoionisation studies (e.g. in the inner valence region) and for photochemistry.

The scientific programme already has many highlights, a few of which have been described briefly above. In line with the mission of IMS the main thrust of these activities lies in photochemistry (including surface photochemistry), molecular photoionisation and polymer science. However, there are several areas, particularly in surface and solid state physics, which are not as strongly represented as they could be, even though UVSOR has a very good monochromator park. (After the upgrade it will no doubt improve further!) This imbalance is all the more surprising since the ISSP ring is no longer in operation and one might have expected that outside users particularly in the area of solid state physics would have shown greater interest in coming to Okazaki. It therefore seems necessary – parallel to the implementation of the upgrade – to recruit new users or to initiate new activities at IMS itself in areas such as high energy and high angular resolution photoemission, spin-polarised photoemission, high spatial resolution photoelectron microscopy and photoelectron diffraction. This would establish UVSOR as an important multi-disciplinary, and internationally unique, facility with its most important areas of research focussed on the far UV.

A. M. Bradshaw
Garching, November 2001