MAX news

no.14 November 1998

Newsletter from the MAX-laboratory at Lund University, Sweden
National Electron Accelerator Laboratory for Nuclear Physics and Synchrotron Radiation Research

First photoemission results from I311

The undulator based beamline I311 is intended for photoelectron spectroscopy experiments on solid samples. Following the successful tests of the photon energy resolution and flux of the beamline (see results in the previous issue of MAXNEWS) the next step in the commissioning has been to mount a photoemission chamber at the beamline.

This experimental chamber has been mounted without the refocusing optics called for in the final version of the beamline. The lack of refocusing results in a quite large light spot on the sample which, in combination with the small acceptance area of the SCIENTA analyzer, reduces the countrate. Despite this reduction in efficiency, the spectra obtained so far during the commissioning demonstrate that the beamline performs excellently also for core level photoemission measurements. Here we show a few examples.

The first example demonstrates the high resolution possible in core level photoemission spectra at I311. The example is taken from the CO on Rh(111) adsorption system which we have previously studied in great detail on beamline 22 at the MAX I ring. The spectrum in Figure 1 shows the C 1s level of CO in the Rh(111)-(2x2)-3CO structure. The spectrum was measured in less than 10 min. The CO molecules in the (2x2)-3CO overlayer structure occupy both on-top and three-fold-hollow sites. These two different sites give rise to two different C 1s components; one at a binding energy of about 286 eV due to the on-top CO molecules and one at 285.3 eV due to the three-fold-hollow CO molecules. These two main C 1s components are clearly seen in Figure 1. In addition, each of these components are seen to contain fine-structure on the high binding energy side. This fine-structure is due to excitation of the internal CO stretch during the photoemission process. Figure 1 demonstrates that differences in the vibrational fine-structure between CO molecules in on-top and three-

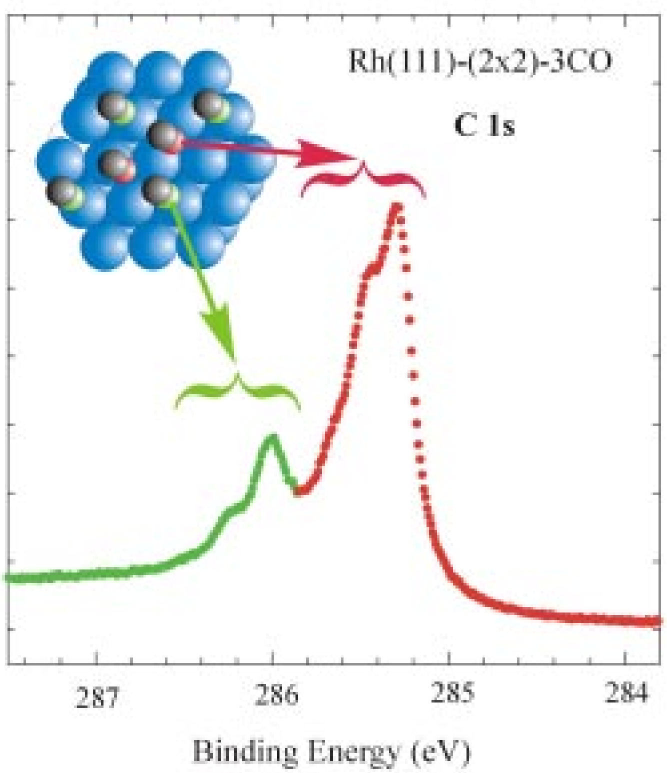


Figure 1. *Normal emission C 1s photoemission spectrum from a Rh(111)-(2x2)-3CO overlayer. Photon energy 314 eV.*

IN THIS ISSUE

fold-hollow sites are present and may be detected already with the present setup at I311. From the Fermi-edge we judge that the resolution in the spectrum of Figure 1 is better than 70 meV. Finally we note that a very good grounding of the sample seems to be a crucial requirement for reaching this high resolution.

The second example is also taken from the CO on Rh(111) adsorption system. It demonstrates the high intensity capability of beamline I311 and how this can be used for dynamic real-time measurements of, for example, adsorption phenomena. Figure 2 shows how the C 1s binding energy region develops as a Rh(111) crystal kept at 150 K is exposed to an ambient CO pressure of $6*10^{-9}$ torr. The measuring time for each of the spectra in the figure is only 10 seconds. At present, the overhead needed for setting up and saving each spectrum is quite high, about 8 seconds. Thus a C 1s spectrum is measured every 18 seconds. As demonstrated by Figure 2, this timescale still allows us to follow the adsorption of CO on Rh(111) in great detail from such C 1s spectra. The spectra in Figure 2 show how the on-top site is the first site to become occupied by CO molecules at low CO exposures and that the three-fold-hollow site only becomes occupied at higher coverages. Although it may be difficult to see from the plot in Figure 2, the spectra actually clearly show that the beginning occupation of the three-fold-hollow site is accompanied by a decrease of the on-top occupation. It may also be noted that fine-structure is visible on the high binding energy side of the peaks in Figure 2. This structure is the aforementioned vibrational fine-structure. The fact that it is visible in the spectra of Figure 2 indicates that the resolution is still rather high. Clearly, this high resolution could be traded for higher intensity which would translate into even shorter measuring times. At present we feel confident that once the refocusing optics is installed it should become possible to follow real-time processes on surfaces with time-constants on the order of one second or in favorable cases even below. This will necessarily also involve modifications of the detector system of the electron energy analyzer as saturation effects of the present system is a limiting factor already now.

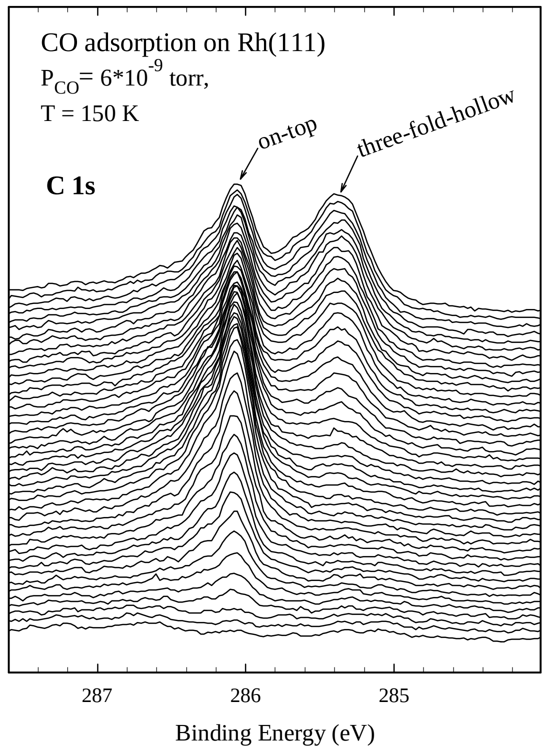


Figure 2. *Normal emission C 1s photoemission spectra from a Rh(111) surface as it is exposed to an ambient CO pressure of $6*10^{-9}$ torr. Photon energy 314 eV. Time between spectra is 18 seconds, each spectrum is measured in 10 seconds.*

For the near future, we still need to get more experience concerning the behavior of the beamline for photoemission experiments. E.g. a lot of tedious measurements to check for long term stability of the photon energy and flux etc. are facing us in the next months. However, the present results are quite encouraging.
(see also: http://www.maxlab.lu.se/beamline/max-ii/i311/i311.htm)

Ralf Nyholm, Ulf Johansson.
and Jesper Andersen.

User meeting 1998 at MAX-lab

The eleventh user meeting at MAX took place september 24-25 1998 at the Conference hall at Sparta in Lund. 112 researchers attended the meeting. 90 from Sweden and 22 from other countries.

The director of MAX-lab, Nils Mårtensson, gave his annual report where he, in addition to a description of the status of the MAX I and MAX II facilities, discussed the future perspectives for the laboratory. One important isssue is the funding of a new injector system.

Mikael Eriksson, MAX-lab, reported on the performance of the MAX II facility, which has reached the design values of current, emittance etc. Of a special interest was the results concerning the implementation of Landau cavities in order to increase the performance of the undulator beamlines, especially at higher harmonics. Very encouraging results have been obtained.

Ralf Nyholm, MAX-lab, reported on the status of the beamlines. All the beamlines at MAX I have operated very satisfactorily during the last year. The first beamline (I711) at MAX II has been operative since a year, and the research at this BL is very successful. Around 70 new users have started to work here during a very short period.

Reports were given from spectroscopy beamlines I311, I411 and I511 by Jesper Andersen (Lund University), Margit Bässler (Uppsala University and MAX-lab)) and Reinhard Denecke (Uppsala University and MAX-lab), respectively. All these beamlines have the monochromators installed and absorption measurements to characterize the light hav been performed. The first electron spectroscopy results have been obtained at I311, showing very high performance. Very high resolution results were presented from the absorption measurements.

There were four invited talks. Two of these were given in the main sessions.

Prof. Janos Hajdu from the Department of Biochemistry at Uppsala University gave an inspiring overview of future possibilities in crystallography, notably protein studies, where the possibility of studying the structure of a single molecule was discussed.

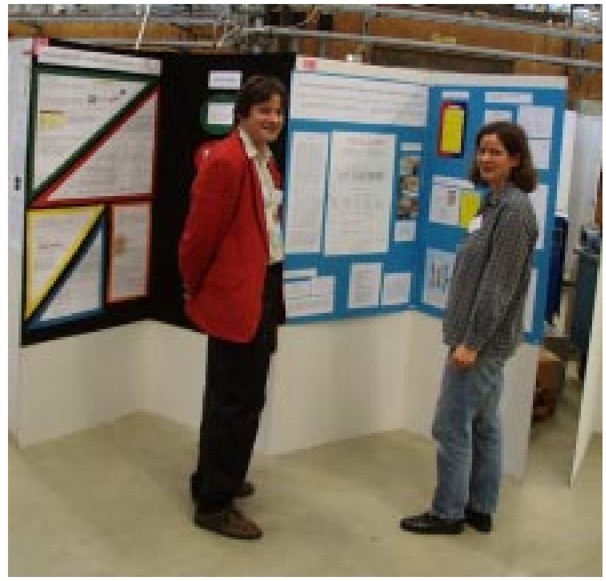
Prof. Surrendra Saxena from the Department of Theoretical Geochemistry in Uppsala made an intellectually fascinating review of how crystallography in high pressure cells can be used to unveil the properties of materials in the very inner core of the earth itself.

A happy gang from 7-eleven.
Surrendra Saxena, Yngve Cerenius and Maria Johansson.

Five oral presentations from results during the last year were presented.

Mika Kivilompolo, Univ of Oulu, reported on a fundamental study of the Auger Resonant Raman effect. Among the interesting points it was shown that the envelope of the Resonant Auger lines for exitation to successively higher and higher core excited Rydberg states below the threshold develops into the post collision normal Auger line profile above the threshold.

Henrik Oskarsson, Chalmers University, showed interestning results on a thickness dependent bandwidth in MBE grown InAs layers on GaAS(111) surface. The method used included high performance photoemission.



Drs. Reinhard Denecke and Margit Bässler
at the poster session.

Paul Bruhwiler, Uppsala University, reported on linear magnetic dichroism of C60 covered films of Co on Cu(100).

Balasubramanian Thiagarajan, University of Linköping, gave a talk on valence band and core level studies of beryllium surfaces.

Finally Andreas Beutler, Lund University, presented results concerning mobile precursor states from C O adsorption.

In the last afternoon there was a miniconference on Crystallography at MAX II. There were two invited lectures. The first was given by Hans. D. Bartunik from DESY, who gave a broad review of how MAD phasing is used in protein crystallography in order to solve the phase problem.

The second invited lecture was given by Inger Andersson, Dept. of Molecular Biology in Uppsala, who reported on a recent study structural study at I711 that has given insights into the penicillin and cephalosporin biosynthesis. It was shown that the structural biology plays a key role in the possible development of new antibiotics.

Elin Grahn from Uppsala University reported on structure studies of an RNA hairpin and Kenny Ståhl from DTU, Lyngby, gave a review of powder diffraction and showed results from I711.

In the Poster Session 42 posters presented results from MAX during the last year. In connection to this session there was a commercial exhibition with 8 firms represented.

The yearly meating of the user organisation FASM at MAX was held, where different problems concerning the work of the users at MAX were discussed. A future research school organized by the laboratory during 1999 was presented, and also an advertisment for the European Synchrotron Radiation Society, ESRS, was made.

The traditional dinner was held at "Löddeköpinge Gästgifvaregård", a traditional regional restaurant. The chairman of the FASM, Svante Svensson, adressed the researchers and the staff of the MAX laboratory. He expressed a special thank to the staff for their enthousiastic support for the external users of the facility.

Svante Svensson, Uppsala University

Beamline I511

The new undulator beamline I511 at MAX-lab, now under commissioning, has been optimized for x-ray emission and photoelectron spectroscopies. It will house two endstations, one for surface science and the other for solids and gas phase experiments. Using an SX-700 high flux monochromator the accessible photon energy ranges from 90eV to about 1500 eV. The performance of the undulator and the monochromator agree very well with the specifications. Beamlines I511 and I411 will be the first synchrotron beamlines making use of a so-called beam waist phenomenon, known from laser physics.

The present situation at BL I511 is such that the test measurements to determine the performance of the beamline are almost completed. One of the two endstations is being installed and tested. The remaining optical parts, like the flip mirror to choose the branchline and the refocusing mirrors are being manufactured and will be installed within the next weeks. In this contribution we want to summarize the results of the test measurements.

In order to check the resolution of the monochromator, absorption measurements using a gas phase absorption cell have been performed. As already mentioned in the last issue of MAX news (no. 13, May 1998) the resolution determined by these measurements agrees quite

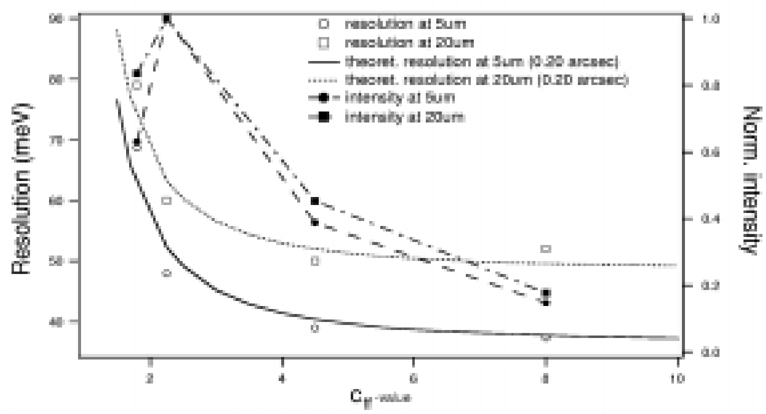


Fig. 1. Resolution (left scale) and intensity (right) as a function of C_{ff}-value, deduced from N_2 absorption measurements.

well with expectations. We would like to summarize the results in Fig.1, where we show both typical (not optimal!) resolution and relative intensity as a function of the so-called fix-focus constant c_{ff} for N_2 absorption at about 400.8 eV. The resolution has been determined by a least-squares fitting routine using a convolution of Lorentz and Gauss curves to model the life time and experimental contributions respectively. This procedure is, of course, only a rough approximation. In fact, in order to obtain meaningful Gaussian widths one has to adopt Lorentzian life times from other measurements. For the N_2 measurements in Fig.1 we used a Lorentzian of 122 meV. It can be seen that the change in resolution with c_{ff} -value is quite distinct for low c_{ff} -values, but very little change can be observed for c_{ff} larger than 4. This behavior is due to the dominance of the mirror slope error contribution to the overall resolution for large c_{ff}-

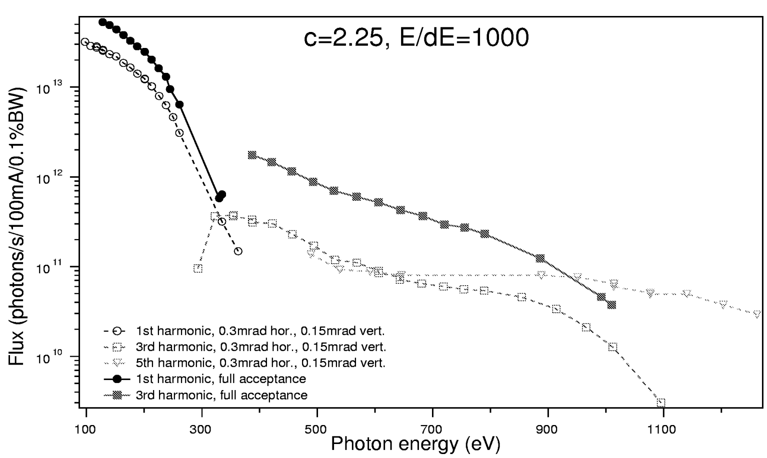


Fig. 2. Photon flux for C_{ff}=2.25 and a fixed resolution of E/dE=1000 as a function of photon energy.

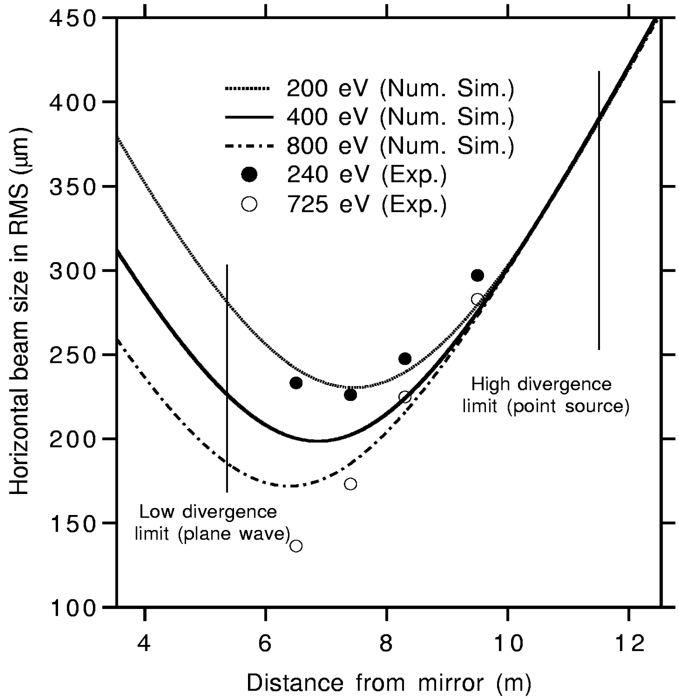


Fig. 3. Comparison betwen numerical simulations and experimental findings for the horisontal beamsize as a function of distance from the focusing mirror.

values. On the other hand, the intensity decreases for larger c_{ff} -values, as expected from the geometrical effect of the finite grating size. However, for very small c_{ff} -values the intensity decreases after a maximum around c_{ff} =2.25. Here the reduced reflectivity of the plane mirror rules the scene. These findings are also depending on the photon energy considered. From curves like the ones in Fig.1 one has to find the optimum parameters for a given experiment, trading resolution for flux and vice versa.

As a second point we want to show measurements of the photon flux as obtained using a GaAsP photodiode. This diode has been calibrated for quantum efficiency and is mounted directly after the exit slit. In Fig.2 we plot the photon flux as a function of energy for a fixed resolution of 1000 and c_{ff} =2.25, achieved by varying the exit slit width for each data point. Shown are results for two different acceptance angles, with the full acceptance angle being the most interesting one. We obtain a maximum photon flux for the lowest energies of about $5*10^{13}$ photons/s/100mA/0.1% BW. These values place the beamline close to beamline 8 at the ALS in Berkeley where the surface science endstation was used before.

As a final point in this discussion here we want to focus on the beam waist phenomenon, known from laser physics and observed at BL I511 for the first time at a synchrotron beamline. The underlying physical argument is based on the horizontal beam parameters in an undulator source. Since the divergence of the photon source is quite small compared to the source size (in our case the divergence is about 0.026 mrad, and the beam size is about 0.34 mm), the source is in fact better described as a plane wave, as opposed to the normally assumed point source characteristics. Therefore, the smallest beam diameter in horizontal direction behind the focusing pre-mirror (called the beam waist) is not found close to the image plane, but rather close to the focal plane. This concept has been experimentally tested at BL I511. Measuring the beam profiles at four points along the beamline we find a very good agreement with predictions from ray-tracing calculations, as shown in Fig.3. One can clearly see the shift of the beam waist towards the focal plane. The phenomenon is photon energy dependent since the divergence of the source is energy dependent. BL I411 and I511 use these findings and put the source point for the refocusing mirrors at the beam waist position rather than at the exit slit position. That way, we should be able to gain a smaller light spot on the sample without a loss in intensity. Especially for the x-ray emission experiment this small spot is important for increasing the signal.

Reinhard Denecke, MAX-lab

Status of beam line I411 at MAX II

Beam line (BL) I411 is one of the three beam lines at MAX II for the VUV and soft x-ray region being close to normal operation. It is outlined for high resolution electron spectroscopy and houses a rotatable SES200 Scienta analyser. Solid, liquid and gaseous samples can be handled. All the beam line components including refocusing optics and the experimental chamber are in place, aligned and roughly tested. The SX700-monochromator delivers good results concerning resolution and flux. The first tests of the electron spectrometer with synchrotron light took place right now and showed that everything is working in principle.

BL I411 consists mainly of parts being relocated and rebuilt from BL 51 at MAX I. The SX700 monochromator containing a plane elliptical mirror for the focusing got water cooling for the first two optical elements. The experimental station was directly transferred. The undulator is new, a 2.65 m long hybrid undulator providing light from around 50-1500 eV. The refocusing optics was completely changed to allow for an extra meter in front of the main experiment for exchangeable set-ups. Despite this ‘recycling’ of beam line components BL I411 will be far away from getting a environmental prize here at MAX-lab. It is especially equipped to handle gas phase experiments with a comparatively high throughput of material. Moreover it is one of the few stations where ‘nasty’ molecules, this means highly reactive and therefore often poisonous but also chemically very interesting molecules or molecules incompatible with UHV-conditions can be studied. The beam line is a result of Swedish-Finnish collaboration. Further details can be found on the web-site (http://www.maxlab.lu.se)

At present all the beam line components are in place, aligned and under vacuum. The monochromator resolution tests show good results. In Fig. 1 an N_2 absorption spectrum is presented. A resolving power E/ΔE of around 7000 can be deduced at 400 eV. The ratio between the first valley and the third peak is 0.8. The resolution compared to BL51 is increased due to the small vertical eletron beam size in MAX II. At normal conditions (coupling of 10%) the vertical electron beam size is 45 µm. The tangential errors of the plane elliptical mirror are now limiting the resolution. But we reach a much better resolution than calculated with a nominal tangential error of 0.4 arcsec. The mirror must be obviously much better, which was already recognized on BL51. A new mirror with a tangential error of 0.2 arcsec is ordered from Zeiss. Taking this together with an even smaller electron beam (1% coupling, 14 µm size) at 400 eV a resolving power of 9500 can be calculated.

An other big improvement compared to BL51 is the increased flux. In Fig. 2 two undulator spectra taken at 29 mm and 27 mm gap respectively show peak maxima of around 2*10^{12} photons and still sufficient flux up to high energies. They were taken with the SX700 monochromator and the same settings as the resolution measurements above.

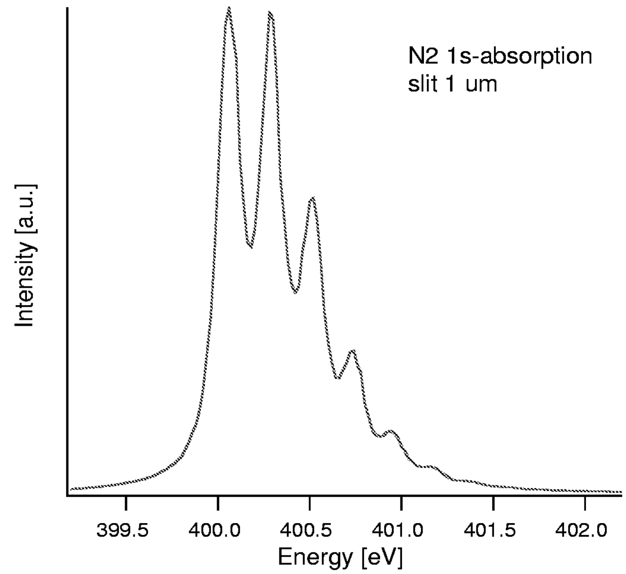


Fig. 1. Vibrationally resolved gasphase absorption at the nitrogen edge.

The first electron spectrometer tests with the synchrotron light and a gas cell took place right now and showed, that everything is aligned and working in principle. After further work on the monochromator and especially the spectrometer performance the beam line will be soon open for users!

Margit Bässler, MAX-lab

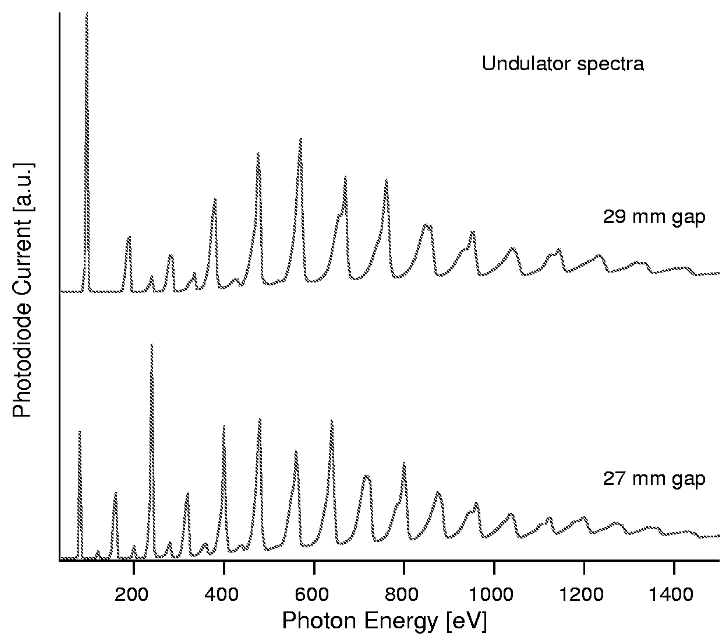


Fig. 2 Undulator spectra taken with the SX700-monochromator at different gaps.

Mid-term review of TMR-LSF projects

A number of leaders for EU-projects in the TMR (Training and Mobility of Researchers) and LSF (Large Scale Facility) programmes came to Lund between the 18 and 20 of October to meet with an Expert panel and Dr. Marco Malacarne from the European Commission to discuss their projects. The panel was chaired by Prof. P. Papon with the members Mme M. Crance, Prof. D. Loyd, Prof I. McGovern, Prof R. Scherm and Prof. I Veretennicoff. 16 projects from around ten European laboratories were scrutinised.

(see also: http://www.maxlab.lu.se/maxlab/conference/roundtable/tmr-lsf.htm)

Meeting of The European Round Table for Synchrotron Radiation and Free Electron Laser

As a new recruit in the Large Scale Facility program MAX-lab could prodly house the annual meeting of the European Round Table for Synchrotron Radiation and Free Electron Laser in Lund on October 19-20 this year. Representatives from the different Round Table member laboratories (ELETTRA - Trieste, BESSY - Berlin, LURE and CLIO - Paris, SRS - Daresbury, DESY-HASYLAB - Hamburg, EMBL - Hamburg and Grenoble, FOM - Utrecht and MAX-lab - Lund) and their users joined in the old Bishops house. During the meeting overviews of the development at the laboratories were given. Discussions followed regarding sponsoring of workshops and schools and practicalities with the TMR-LSF programmes and the continuation into the 5th Framework program. The announcement of 110 M£ for the Diamond project given by the Wellcome Foundation was a moment of great joy.

The European Round Table for Synchrotron Radiation and Free Electron Laser is an initiative supported by the European Commission. Its main purpose is to encourage the exchange of information between large-scale SR and FEL facilities and European researchers on subjects of common interest, complementing national and international efforts in this area.

(see also: http://www.maxlab.lu.se/maxlab/conference/roundtable/roundtable.htm)

The workshop Current Development of Free Electron Lasers

***DESY and MAX-lab jointly organised a workshop on Current development of Free Electron Lasers in connection to the Round Table meeting in Lund. The workshop was sponsored by The European Round Table for Synchrotron Radiation and Free Electron Laser*.**

Jochen Schneider started the workshop with an odyssey over LINAC driven FELs as the next generation of Lightsources. Jörg Rossbach elaborated on the production of the necessary electron beams for X-ray and VUV-FELs. Steve Milton from the APS and Josef Feldhaus from DESY made an overview over their VUV FEL projects. Marie-Emanuelle Couprie from LURE made a summary of Storage ring based FELs and the Infrared region was described by Jean-Michel Ortega, also from LURE.

In a short session there were contributions from existing european FEL activities such as FELIX, Darmstadt and CLIO as well as ideas about hard X-ray FEL applications in Biology.
Roger Carr from SSRL/SLAC described the LCLS X-ray project and Jochen Schneider and Jörg Rossbach introduced the TESLA X-FEL project. All the diffeent wavelength regions had their own discussion session where a variety of subjects were treated.
A report from the workshop will soon be available from MAX-lab.

(see also: http://www.maxlab.lu.se/maxlab/conference/roundtable/workshop.htm

Ingolf Lindau - Sweden's most cited physicist

The Institute for Scientific Information (ISI) has produced a list over the most cited physicists between 1981 and 1997 (http://www.isinet.com). Around 500.000 authors are represented more than once over this period. The first Swede, Ingolf Lindau, is found on place 44. Ingolf Lindau is

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professor em at Stanford University, California and since 1990 professor in Synchrotron radiation physics at Lund University. His research, which has resulted in 570 scientific works, has mainly been focused on electronic and structural properties of surfaces and interfaces. During 1980-90 he was the technical director for SSRL at Stanford and between 1991 and 97 the director of MAX-lab in Lund. Professor Lindau is a member of the Royal Academy of Sciencies since 1995.

"What a Friend We have in MAX-lab"

We Swedes do sing a lot when we are having a party (but sometimes we need british help with the texts). A while ago Mikael Johansson successfully defended his dissertation, which naturally was celebrated by a party. At that occasion he was honoured by this description of the daily life at MAX-lab.

Tune: *What a friend we have in Jesus*
Text by: *Struan Gray*

Chorus:
Oh how we love to work at MAX-lab
Joy-filled week by joy-filled week
'Cos every time we finish bakeing
The beamline springs another leak.

Well STM was getting boreing
Taking data every day
We were writing lots of Phys. Rev. Letters
By Johansson, Johansson and Gray
But then Lars suggested time at Max-lab
And like fools we said ' Well, yes, OK'
And since then it-s all been going downhill
To the sad state that you see today

Oh how we …

So we turned up early Monday morning
Hoping for a rapid start
But the venting piece had gone to Stockholm
And the Turbo needed a new part
The manipulator'd lost it's feedthroughs
All the windows were obscured with soot
And our samples fell into the ion pump
And the beamline PC wouldn't boot

Oh how we ---

We started pumping Tuesday evening
Down to ten to the minus six
It was only half way through the bakeout
That the pressure started playing tricks
Small clouds of smoke came from the system
And the lab filled with an acrid smell
Could it be that viton gasket
With the six heating tapes in parallel?

Oh how we …

The second bakeout went like clockwork
On the third I would prefer not to dwell
By the forth we were calling ourselves experts
And the fifth one really went quite well
So we started taking our first spectrum
Surely nothing could go wrong?
Then the ring dumped all it's cooling water
And shorted out the microtron

Oh how we …

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