EUROPEAN SYNCHROTRON RADIATION FACILITY

INSTALLATION EUROPEENNE DE RAYONNEMENT SYNCHROTRON

Experiment Report Form

The double page inside this form is to be filled in by all users or groups of users who have had access to beam time for measurements at the ESRF.

Once completed, the report should be submitted electronically to the User Office using the **Electronic Report Submission Application:**

http://193.49.43.2:8080/smis/servlet/UserUtils?start

Reports supporting requests for additional beam time

Reports can now be submitted independently of new proposals – it is necessary simply to indicate the number of the report(s) supporting a new proposal on the proposal form.

The Review Committees reserve the right to reject new proposals from groups who have not reported on the use of beam time allocated previously.

Reports on experiments relating to long term projects

Proposers awarded beam time for a long term project are required to submit an interim report at the end of each year, irrespective of the number of shifts of beam time they have used.

Published papers

All users must give proper credit to ESRF staff members and proper mention to ESRF facilities which were essential for the results described in any ensuing publication. Further, they are obliged to send to the Joint ESRF/ ILL library the complete reference and the abstract of all papers appearing in print, and resulting from the use of the ESRF.

Should you wish to make more general comments on the experiment, please note them on the User Evaluation Form, and send both the Report and the Evaluation Form to the User Office.

Deadlines for submission of Experimental Reports

- 1st March for experiments carried out up until June of the previous year;
- 1st September for experiments carried out up until January of the same year.

Instructions for preparing your Report

- fill in a separate form for each project or series of measurements.
- type your report, in English.
- include the reference number of the proposal to which the report refers.
- make sure that the text, tables and figures fit into the space available.
- if your work is published or is in press, you may prefer to paste in the abstract, and add full reference details. If the abstract is in a language other than English, please include an English translation.

ESRF	**Experiment title:** High energy angle resolved photoemission	**Experiment number**: HE-1009
Beamline: ID08	**Date of experiment**: from: 2000 to: 2002	**Date of report**: 2002-09-01
Shifts:	**Local contact(s)**: Nick Brookes, Celine de Nadai, Federica Venturini	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Oscar Tjernberg, Claudia Dallera, Lamberto Duo, Marco Finazzi, Martin Månsson, Hao Tjeng, Nicholas Brookes, Sarnjeet Dhesi, Alberto Tagliaferri

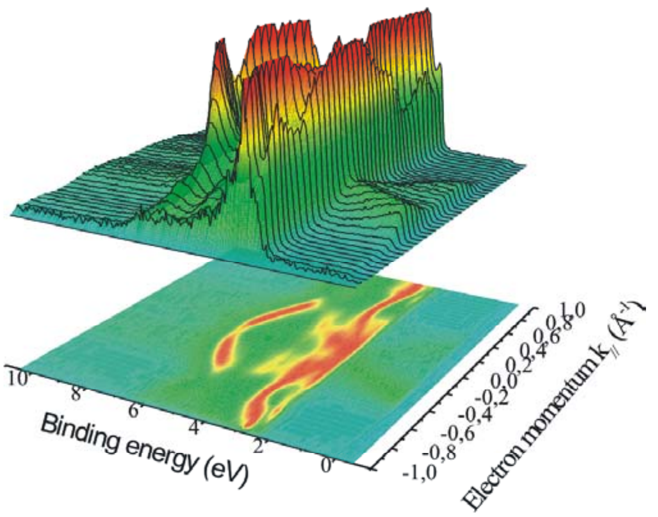
Report:

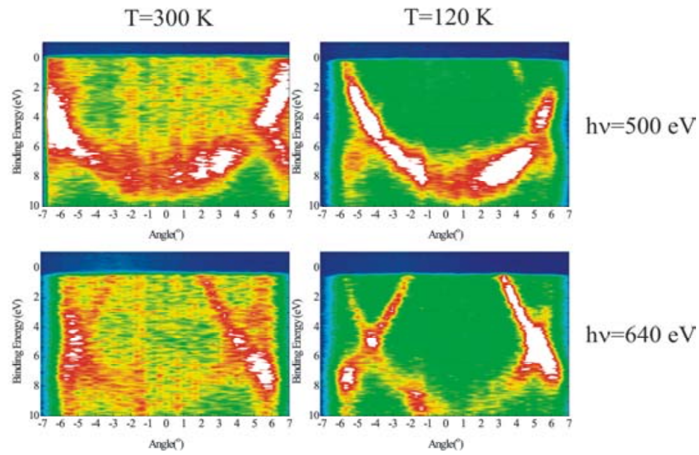
Background

The long term project on high energy angle resolved photoemission (HARPES) that was approved by the beam time review committee in 2000 is the continuation of in-house work that was conducted at ID12B from the fall of 1997 and onwards. The aim of the project is to develop an experimental setup capable of performing angle resolved photoemission spectroscopy in the 400-1000 eV range with sufficient angular and energy resolution to study valence band dispersion. This requires very high photon flux because of the low cross-sections, angular resolution on the order of 0.1° and an energy resolution on the order of 100 meV. The main interests for going to high photon energies are increased bulk sensitivity, a free electron like photoelectron decoupled from the rest of the system and an approximately linear relation between electron momentum and emission angle. All of these properties make HARPES an excellent experimental tool in the study of strongly correlated 3D system as well as systems were the surface electronic structure is expected to differ from the bulk.

Results and current status

During the 15 days of beam-time that the project has had so far, there has been a considerable amount of progress. The valence band dispersions of Al, Cu, $TaSe_2$ and NiO have been measured with success and some of the results are included in this report

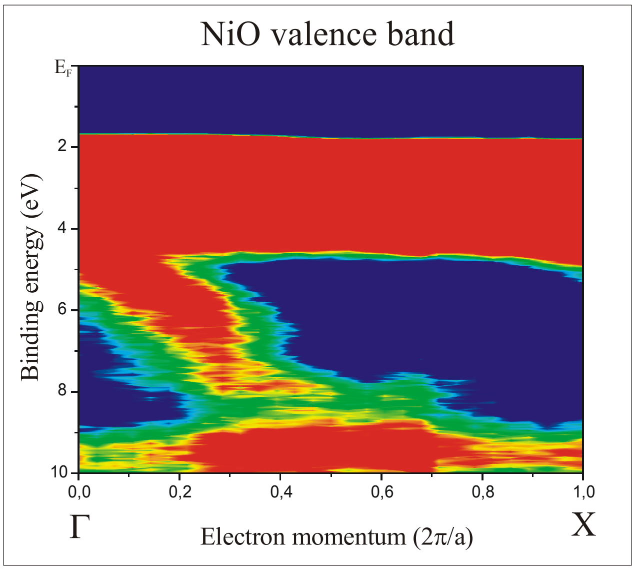




In the figure on the left, Cu valence band data measured at a photon energy of 580 eV are presented. Due to analyzer problems discussed below, the relative intensities are not correct and the spectrum has been normalized to equal maximum intensity. Irrespective of this, the Cu d band dispersion can be clearly seen between 2 and 8 eV binding energy as can the Cu s-p band with its parabolic dispersion crossing the Fermi level at a parallel momentum of approximately 0.4 $Å^{-1}$.

In the figure on the right, Al valence band data for two different temperatures and photon energies are presented. Both the parabolic in plane dispersion as well as dispersion in the normal direction as a function of photon energy is clearly seen. Another prominent feature in these data is the temperature dependence of the signal to background ratio. A more detailed study of the signal to background ratio as well as momentum broadening as a function of photon energy and temperature is planned for the next beam time.

From the physics point of view, there have also been some unexpected results. While the bulk dispersion in samples such as Al, Cu, $TaSe_2$ and NiO can be measured in the 400-650 eV range, there has been no success whatsoever in observing the valence band dispersion in the 1D system $(TaSe_4)_2I$. We are currently planning further experiments in order to investigate whether this result is due to a stronger phonon coupling in the photoemission process for a low dimensional material, an apparent destruction of momentum conservation due to the increased photon momentum or some other mechanism. The general problem of establishing the role of phonons in the photoemission process also needs further studies.



As an example of the direct application of the HARPES technique, we have measured the prototypical Mott-Hubbard system NiO. A color topological plot of the NiO valence band, recorded with hν=610 eV, is shown on the left. Blue color indicates low intensity and green, yellow and red indicate increasingly higher intensities. A very high intensity is seen in the 2-4 eV region. This intensity is according to calculations due to Ni $t2_g$ bands[i]. At 9-10 eV binding energy there is a feature that dispersis to lower binding energy and back as one goes from Γ to X. This feature is most likely Ni e_g related. Apart from these features, there is also a highly dispersive feature crosses over from the upper

to the lower part of the valence band as the momentum increases. The interesting point here is that band structure calculations that take into account the antiferromagnetic nature of NiO show one or two additional flat bands in the region between 5 and 8 eV[i]. Low energy ARPES also display additional peaks in this region and they have been interpreted as proof of antiferromagnetic influence on the band structure[ii,iii]. The data presented here do, on the other hand, not show any sign of an extra flat band due to the antiferromagnetic ordering. In our opinion, the difference between our high-energy data and the low energy data stems from the assumption of a free electron like final state in the analysis of the low energy data. This assumption is highly questionable in a strongly correlated system such as NiO and is therefore likely to introduce erroneous features in the experimentally derived dispersion relations.
In view of the presented results, it is clear that the aim of the project is well within reach. At the same time, there have been some severe hardware and software problems with the SES-2002 analyzer that have hampered the progress and delayed the project schedule. As a result of these problems, the analyzer was sent back to Gammadata for repairs and modifications during the spring of 2002. The analyzer now seems to be working correctly and there is also hopes for future software upgrades that will allow an even higher angular resolution to be achieved. It should be noted that the lost shifts will be recuperated in the schedulling period 2003/1 so a final report will not be avialable until September 2003.
The data obtained so far have also shown that sample alignment is crucial (as expected) and a new sample manipulation system is under development. This new system is necessary in order to be able to measure samples that can not be carefully pre-aligned to the sample holder i.e. small samples and/or samples where the orientation of the crystallographic axis are not known with high enough accuracy. New software that enables automation of the data taking to a much higher extent has also been developed and will be tested during the next beam-time. Unfortunately the beam line can still not use both undulators in the lower part of the energy range. This means a factor of 2-3 lower intensity and correspondingly longer collection times.

Future plans

Further work is expected to be done on the sample handling and alignment system. Discussions with Gammadata on the possibility to develop specially designed lens tables that better utilize the small beam spot available at ID08 are also under way.

Now that the viability of the technique has been proven we will focus on characterizing the effects of phonons and photon momentum on momentum broadening as well as the study of a few physically interesting systems. Close at hand are studies of surface effects and interlayer coupling in high T_c superconductors, interference effects in angular resolved resonant photoemission from antiferromagnetic compounds and attempts to detect dynamic stripe ordering in cuprates.

---

[i] O. Bengone et al. Phys. Rev. B **62**, 16392 (2000)
[ii] Z.-X. Shen et al. Phys. Rev. Lett. **64**, 2442 (1990), Phys. Rev. B **42**, 1817 (1990), *ibid*. **44**, 3604 (1991)
[iii] H. Kuhlenbeck et al. Phys. Rev. B 43, 1969 (1991)