EUROPEAN SYNCHROTRON RADIATION FACILITY

INSTALLATION EUROPEENNE DE RAYONNEMENT SYNCHROTRON

ESRF

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: A comparative methodological analysis of the C60/Ge(111)-(V13xV13)R14 superstructure studied by SXRD.	**Experiment number**: SI-863
Beamline: ID32	**Date of experiment**: from: 2-09-02 to: 9-02-2002	**Date of report**: 27-02-2003
Shifts: 21	**Local contact(s)**: Tien-Lin Lee	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Xavier Torrelles, ICMAB-CSIC (SPAIN)

Jorg Zegenhagen , ESRF

Tien-Lin Lee, ESRF

Oier Bikondoa, Manchester (UK)

Report:

One subject of intense research is the adsorption of C60 molecules and the growth of C60 thin films on the surfaces of metals [1-3] and semiconductors [4-6]. The interaction of isolated C60 molecules with the Ge(111)-c(2x8) surface [7] causes a perturbation of the adatom arrangement of the c(2x8) structure close to the adsorbed C60 molecules. The typical defect is a shift of a part of a Ge adatom row by one surface lattice constant starting at the C60 molecule. The defective Ge adatom arrangement in the vicinity of the C60 give rise to unsaturated Ge surface atoms with a half-filled dangling bond underneath the C60 molecules and the C60 substrate bond is mediated by a charge transfer from the Ge surface to the C60 molecules. The half-filled dangling bond states play an important role by providing the needed density of filled surface states within the Ge bulk/surface state band gap.

The Ge(111) samples that were used for this experiment were new ones. The samples were cut and polished at the ESRF and introduced in UHV conditions to be prepared following repeated sputter/annealing cycles already described elsewhere [8] in the Surface Characterization Lab at the ESRF. The surface was prepared at the SCL until well defined spots intrinsic to the C60/Ge(111)r13xr13 R14º superstructure were detected by LEED. At the same time the quality and ordering of the surface were checked by STM. After preparing

the surface sample, it was transferred to a baby chamber, supplied by the Surface Characterization Lab, and mounted in the ID32 diffractometer.

During the diffraction experiment more than 2000 reflections from the superstructure were measured. This complete data set permitted the application of “3D direct methods” in order to find a reasonable model that was used as starting point to fit the experimental data.
The analysis of the data permits to arrive to a final model, which is able to fit with a rather good agreement the 50 non-equivalent fractional order rods measured. From the structural analysis of this model we are able to identify the orientation of the C60 molecule onto the Ge(111) substrate as well as to identify the C-atoms which are bonded to their closest Ge-atoms. In order to validate the model, we are planning to perform stability simulations of the whole structure as well as to simulate the density of states and electronic configuration of this surface.

References

[1] T. Hashizume et al., Phys. Rev. Lett., 71 2959, (1993).
[2] I. K. Gimzevski et al., J. Vac. Sci. Technol., B12, 1942, (1994).
[3] E. I. Eltman and R. J: Colton, Surf. Sci., 279, 49, (1992).
[4] Y. Z. Li et al, Science, 252, 547, (1991).
[5] Y. Z. Li et al, Science, 253, 429, (1991).
[6] Han Yi et al., Phys. Rev. Lett, 70, 1850, (1993).
[7] K. R. Wirth and J. Zegenhagen, Phys. Rev. B 56, 9864, (1997).
[8] K. R. Wirth and J. Zegenhagen, Surf. Sci., 351, 13, (1996).