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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: Determination of the local structure of amorphous InSe films by EXAFS**	**Experiment number**: HS-1391
Beamline: BM32	**Date of experiment**: from: 23/09/2000 to: 28/09/2000	**Date of report**: 27/02/2001
Shifts: 9	**Local contact(s)**: Dr. Olivier Proux	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

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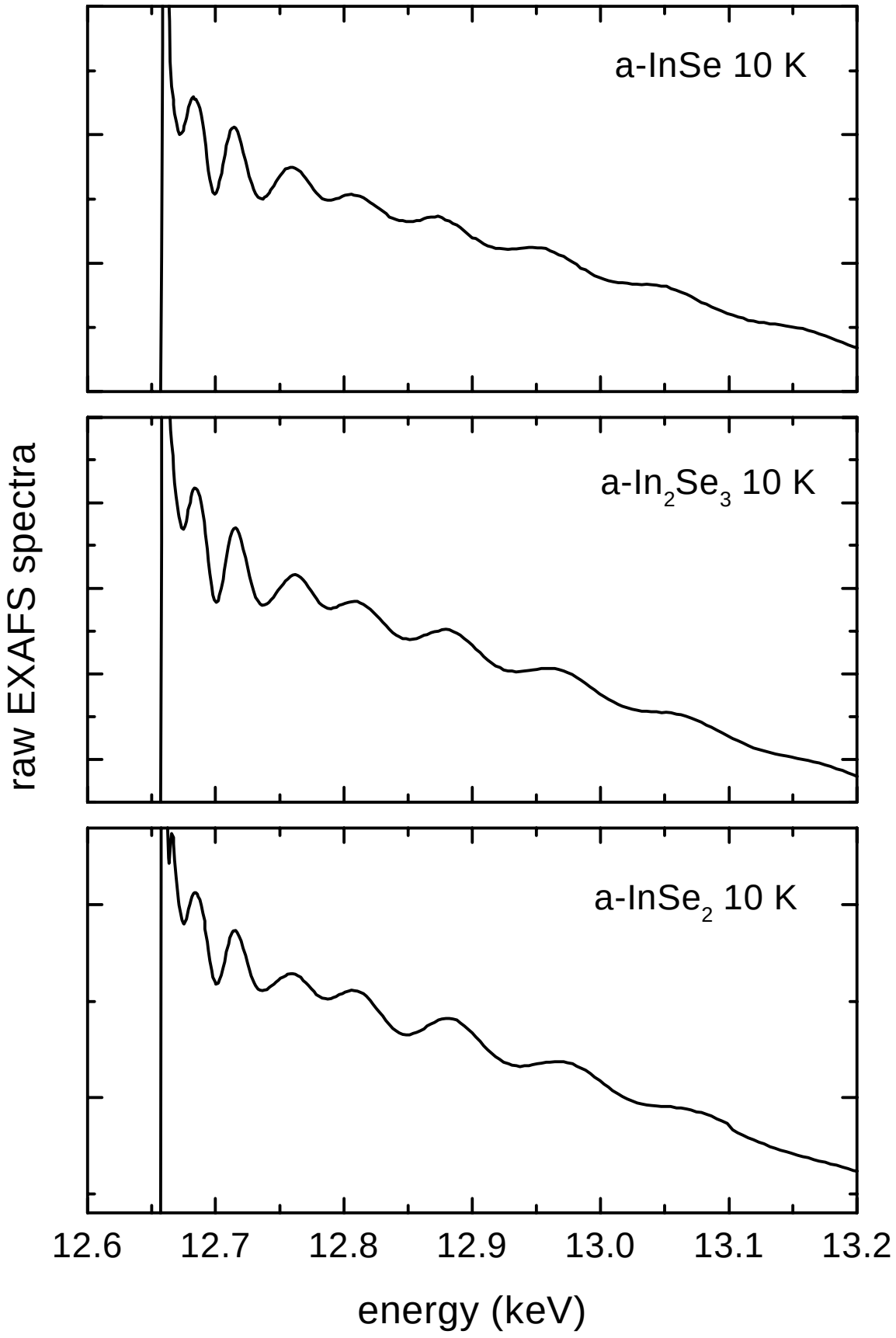
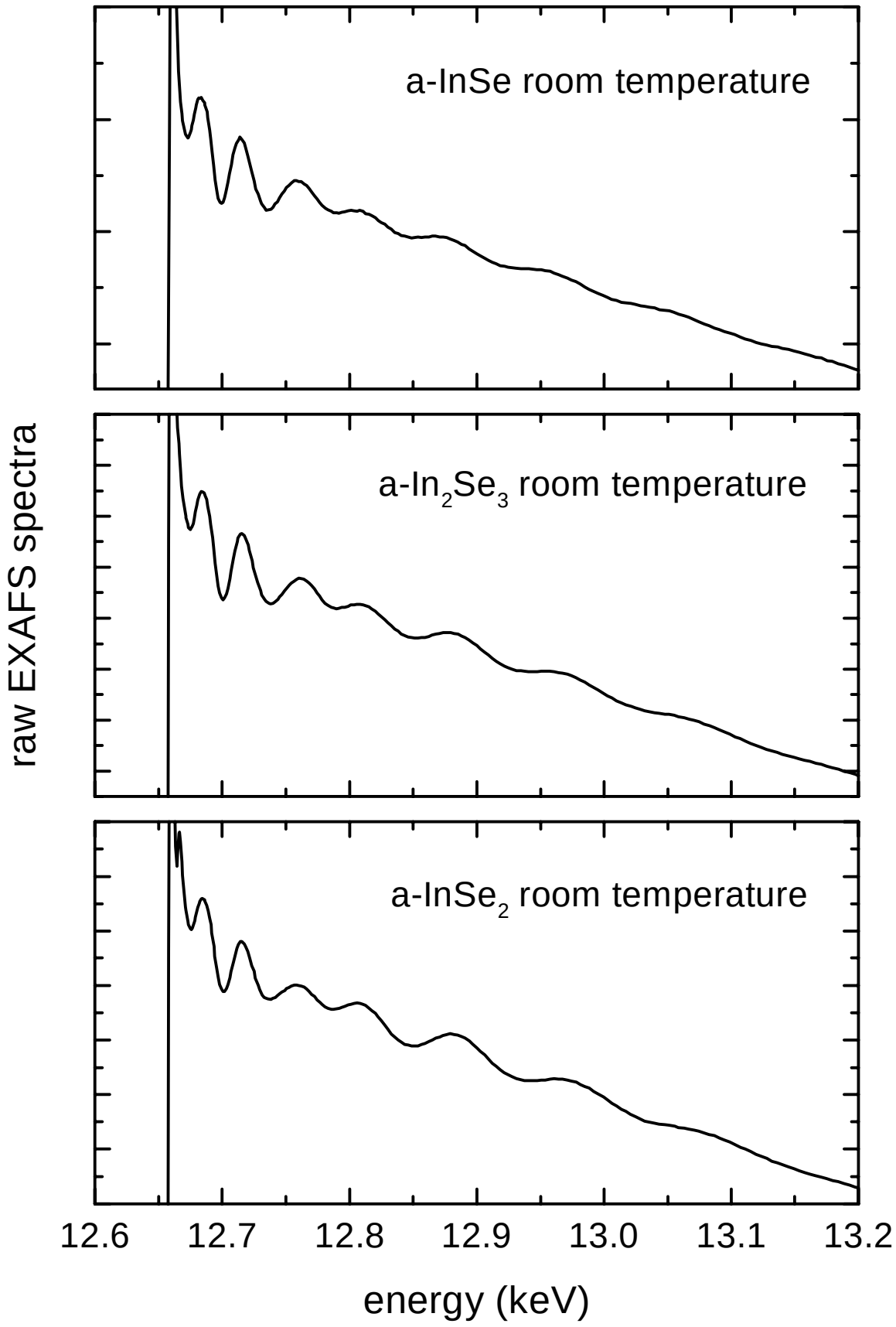
Report:

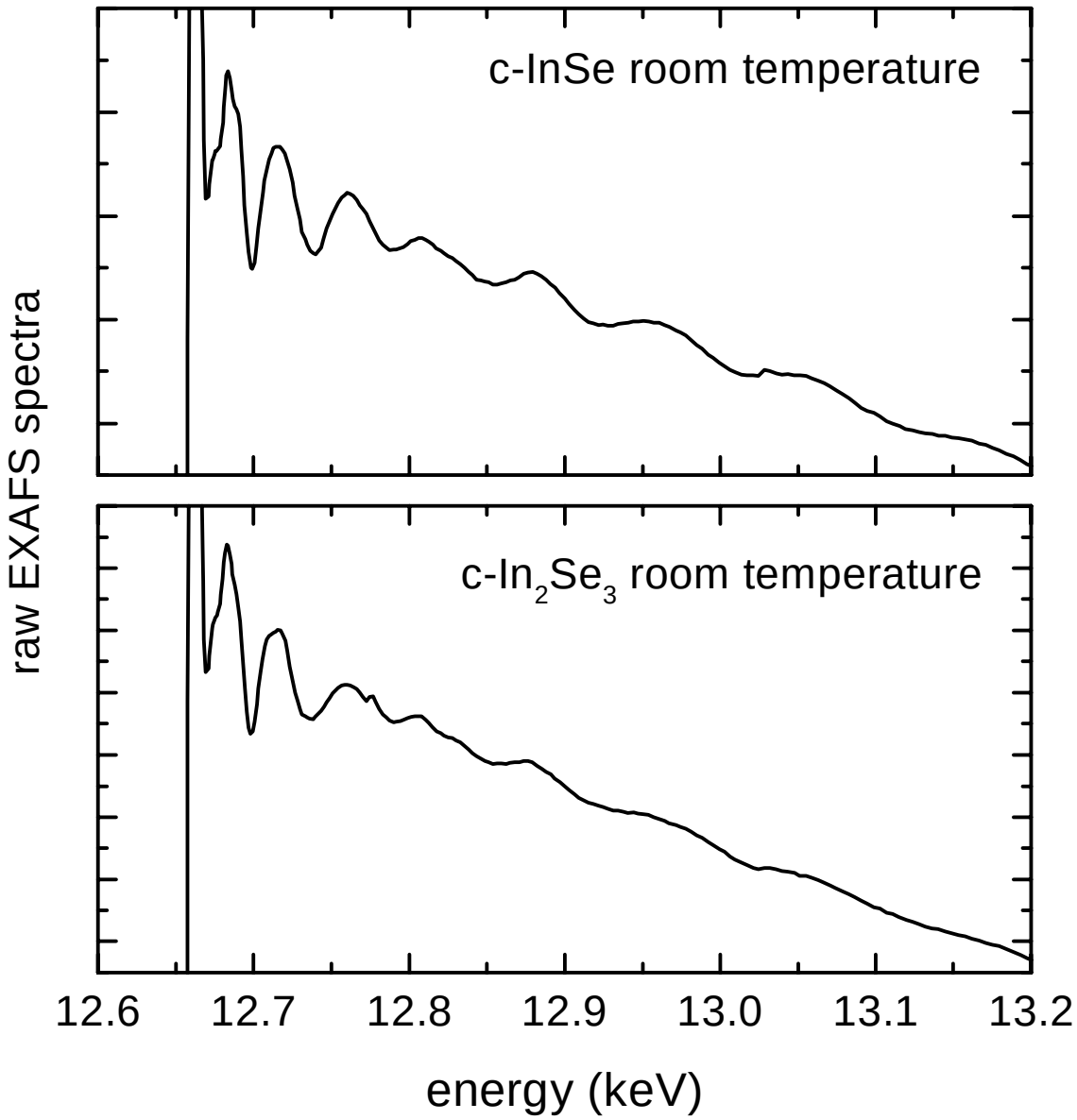
Semiconducting amorphous In-Se films, produced by thermal evaporation in vacuum, containing 50, 60 and 66 at.% Se have been studied by Se K-edge X-ray absorption fine structure (EXAFS). The deposition was carried out at a pressure of 10 mPa. The final thickness of 40-50 μm was achieved after series (usually about 10) of 5-min. evaporation runs. Compositional analysis performed by the microprobe and XPS methods showed that the composition of the investigated films are exactly the same as the source materials due to a high deposition rate, not less than 15 nm/s. The most important characteristic of these compounds is that they form strong covalent bonds within layer and have weak interlayer interaction of the Van der Waals type. In thin film form, both crystalline and amorphous, indium selenide compounds have suitable electrical and optical properties for applications as solar cells and switching elements for memory applications. The layered structure of the In-Se films make them attractive material for intercalation and a potential application in lithium batteries. Owing to the layered structure a low density of dangling bonds is expected which makes it possible to produce heterojunction devices with a low interface density of states.

The Se K-edge absorption spectra were recorded on the BM32 beam line at 10 K and at room temperature. The spectra were measured in transmission mode for free-standing samples in the energy range from 12400 to 15000 eV or in the wave vector range from 0 to about 22 1/Å. The crystalline counterparts In_2Se_3 and InSe were also measured at room temperature as the reference materials. The raw results are

shown in the included figures in the reduced energy range from 12600 to 13200 eV in order to emphasise the evolution of the spectra. Influence of temperature for all the measured compositions can be clearly seen from comparison of the plots for the amorphous films (a-InSe, a- In_2Se_3 and a-$InSe_2$) at 10 K and room temperature. At 10 K the EXAFS oscillations are much more pronounced, which is the result of freezing the thermal vibrations. In fact, at this temperature disorder in atomic arrangement is related only to static disorder, resulting from changes in the interatomic distances and the valence angles. Comparison of the spectra for the amorphous films, recorded at the same temperature, shows clearly visible peak shifts towards higher values of the wave vector going from a-InSe to a-$InSe_2$. This observation is in agreement with the proposed structural model, deduced from the X-ray scattering data. In the proposed model it has been assumed that the local structure of crystalline InSe is retained in the amorphous state. In the InSe structure each Se is coordinated by 3 In. When the Se content is increased the statistical occupancy of the Se position by In and Se is suggested to account for the increased Se content. The Se-Se distance (2.49 Å) is shorter than the Se-In (2.62 Å) and the observed shifts of the peaks can be explained by the presence of the shorter interatomic distances in the Se rich samples. Moreover the spectra recorded for amorphous films are much more like as that of crystalline InSe, which also support the proposed models. But in order to precise description of the local structure in the investigated amorphous films additional studies (EXAFS at the In K-edge, anomalous scattering) and more profound analysis of the data are necessary.


a-InSe 10 K
a-In2Se3 10 K
a-InSe2 10 K
raw EXAFS spectra
12.6
12.7
12.8
12.9
13.0
13.1
13.2
energy (keV)


a-InSe room temperature
a-In2Se3 room temperature
a-InSe2 room temperature
raw EXAFS spectra
12.6
12.7
12.8
12.9
13.0
13.1
13.2
energy (keV)


c-InSe room temperature
c-In2Se3 room temperature
raw EXAFS spectra
12.6
12.7
12.8
12.9
13.0
13.1
13.2
energy (keV)