



## 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.



	<b>Experiment title:</b> Crystal structure of the light hydrides AlH <sub>3</sub> , MgH <sub>2</sub> and CaH <sub>2</sub> under high pressures.	<b>Experiment number:</b> HS3002
<b>Beamline:</b> ID09A	<b>Date of experiment:</b> from: 10/03/2006 to: 13/03/2006	<b>Date of report:</b> 28/02/2007
<b>Shifts:</b> 9	<b>Local contact(s):</b> M. Amboage and M. Hanfland	<i>Received at ESRF:</i>
<b>Names and affiliations of applicants</b> (* indicates experimentalists): Igor Goncharenko, <i>Laboratoire Léon Brillouin C.E.A.-C.N.R.S.*</i> Michael Hanfland, <i>ESRF*</i>		

## Report:

It is well known that dense monoatomic hydrogen, if ever it would be obtained experimentally, would be probably a room temperature superconductor. The high value of  $T_c$ , which had been calculated in the standard BCS model, comes from very high phonon frequencies in the dense lattice made from light atoms (i.e. hydrogens). Despite enormous experimental efforts, until now metallic hydrogen has been never observed experimentally, even at pressures as high as 300-350 GPa. Some recent calculations put onset of metallization in solid hydrogen at pressures as high as 600 GPa, far away from the current experimental limit for static pressures. There is another possibility to create a dense net of light elements which would have metallic conductivity. It was noticed recently [1,2] that "light" hydrides (such as CH<sub>4</sub>, SiH<sub>4</sub>, AlH<sub>3</sub>, or MgH<sub>2</sub>) might indeed be high- $T_c$  superconductors, if they would be transformed into metallic state by pressure (at ambient pressure these hydrides are insulators). Until now, there are no published data on pressure-induced metallization in these systems. In 2006, we had studied crystal structure of  $\alpha$ -AlH<sub>3</sub> in the wide pressure range 0-110 GPa, aiming to find new structural modifications with dense hydrogen sublattice and possible metallic conductivity. Taking into account limited amount of allocated beamtime, we focused on AlH<sub>3</sub>, whereas study of others hydrides (MgH<sub>2</sub>) will be subject of new proposal. We had measured more than 100 pressure points and discovered two new structural modifications: monoclinic phase II, at pressures above 60 GPa, and cubic phase III, at pressures above 100 GPa [3]. Whereas exact atomic positions in the low-symmetry phase II are not determined yet, the cubic phase III is remarkably simple.

We had determined positions of Al atoms in the structure and, using molecular dynamics calculations, were able to select possible locations of H-atoms in the unit cell. Final structure of the phase III is highly interesting. The shortest allowed H-H distances are only 0.15 nm, and considerably shorter than the shortest Al-H distances (0.17 nm; notice that at P=0 in AlH<sub>3</sub> and all other “light” hydrides the situation is just opposite, i.e. the Me-H distances are always the shortest ones), which means that H-H interactions and electronic hybridisation becomes very important in the phase III. Moreover, these distances are shorter than the expected H<sub>2</sub>-H<sub>2</sub> intermolecular distances in molecular hydrogen at the highest ever reached static pressure, 350 GPa [4,5]. Indeed, our preliminary results on transport properties of AlH<sub>3</sub> under pressures up to 160 GPa, carried out in collaboration with Max Plank Institute, show that the phase III of AlH<sub>3</sub> is metallic [3]. So we conclude that the predicted by theory “hydrogen dominant metals alloy” is finally found in our experiment.

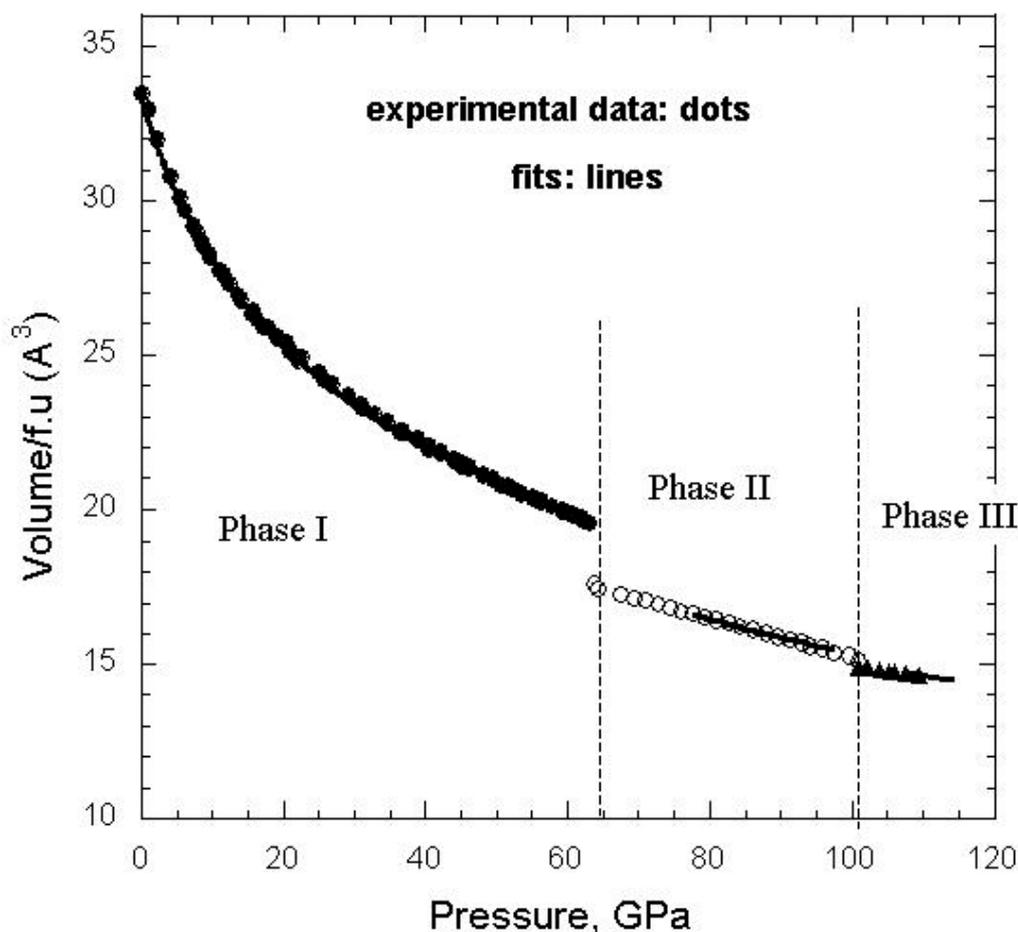


Fig. Equation of state of  $\alpha$ -AlH<sub>3</sub> measured at the ID9A in the ESRF

### References

- [1] N. Ashcroft, Phys. Rev. Lett. 92, 187002 (2004)
- [2] J. Feng et al., Phys. Rev. Lett. 96, 017006 (2006)
- [3] Goncharenko, Erements, Tse, Hanfland, to be submitted to *Nature*
- [4] C. Narayana et al., Nature 393, 46 (1998)
- [5] P. Loubeyre, Nature 416, 613 (2002)