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 via the User Portal:

https://wwws.esrf.fr/misapps/SMISWebClient/protected/welcome.do

Reports supporting requests for additional beam time

Reports can 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:** Structural behavior of BeH2 under pressure	**Experiment number**: HC1074
Beamline: ID09a	**Date of experiment**: from: 02/22/2014 to: 02/24/2014	**Date of report**: 03/02/2014 *Received at ESRF:*
Shifts: 9	**Local contact(s)**: Michael Hanfland	

Names and affiliations of applicants (* indicates experimentalists):

Charles Pépin*

Thomas Plisson*

Report:

Scientific background

There is currently a great interest for the synthesis of novel hydrides, driven by their potential applications for hydrogen and energy storage and by their possible high-temperature superconductivity. BeH2 is part of these promising hydrides and the application of pressure is a way to tune its properties. However experimental studies on crystalline BeH2 under pressure are non-existent because its synthesis is very challenging. Moreover theoretical do not agree on the high pressure behavior of this compound[1,2,3], calling for a detailled experimental study of BeH2.

Experimental technique

Pristine beryllium powder has been loaded in the high pressure chamber of diamonds anvil cells with hydrogen as pressure medium and heated at several pressures using two differents methods: (i) using an external heater at low pressure (~2-5 GPa) and (ii) heating the sample unsing a YAG-laser at higher pressures (5 GPa and 80 GPa). The conditions reached in 5 experimental runs are summarized in table 1. X-Ray diffraction characterization was performed *in situ* with wavelength λ=0.415Å. Diamond anvils were thermally insulated using KCl or c-BN grains. Pure crystalline BeH2 was succesfully synthesized in every run.

Run	**Anvil culet size (µm)**	**Heating**	**P range (GPa)**	**Comment**
THT5	300	External heater	2.4 to 40	
CDMX21	300	External heater	5 to 45	
CDMX23	300	YAG-laser	15 to 45	Laser heated at 15 GPa
CDMX18	70*300	YAG-laser acting	82 to 102	Laser heated at 80 GPa. Weak diffraction signal.

CDMX22	100*300	YAG-laser	75- nan	Sample lost due to a quick pressure variation

Table 1 - Experimental conditions for HC-1074

Results

- At low pressure the known ambient-pressure *Ibam* phase of BeH2 forms (fig. 1a), along with another phase. Structural determination of this second phase is undergoing.
- Above 30 GPa the *Ibam* phase seems to dissociate into the elements.
- This very exciting observation needs to be reproduced in independent experimental runs; the electronic properties of these materials will be characterized with infrared spectroscopy which will complement the structural information provided by X-ray diffraction.
- At 82 GPa the predicted[2,3] *P-3m1* structure is synthesized (fig. 1b).

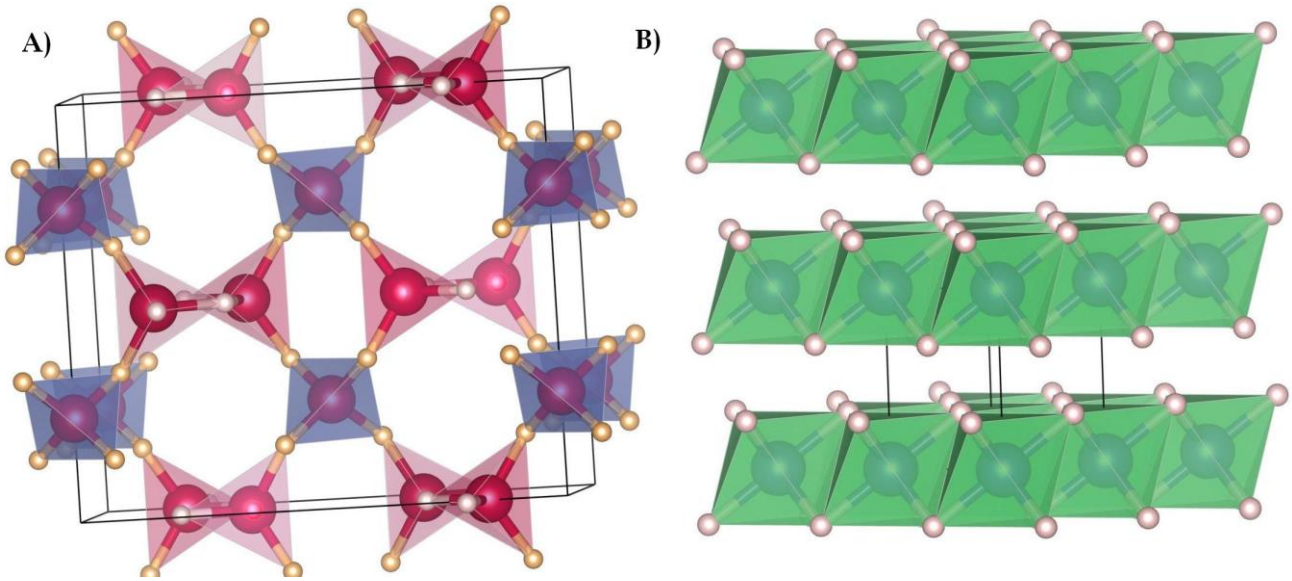

Figure 1: structures of BeH2 obtained under pressure. A) Ibam phase B) P-3m1 phase

References

[1] Vajeeston *et al.*, Appl. Phys. Lett. 84, 34, 2004
[2] Wang *et al.*, J. Chem. Phys., 140, 124707, 2014
[3] Yu *et al.*, AIP Advances, 4, 107118, 2014