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 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.

	Experiment title: Crystal structure of the non-centrosymmetric superconductor AuBe	**Experiment number:** HC-2726
Beamline: BM20	**Date of experiment:** from: Sept. 15, 2016 to: Sept. 20, 2016	**Date of report:** Dec. 6, 2016
Shifts: 12	**Local contact(s):** Christoph Hennig	*Received at ESRF:*

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Report:

High resolution powder X-ray diffraction patterns of AuBe have been successfully recorded at the BM20 Rossendorf beamline with a wavelength of $\lambda = 0.459317(1)$ Å.
The diffractograms could be indexed with a primitive cubic unit cell with the lattice parameter $a = 4.6667(2)$ Å at 300 K (Fig. 2, left panel). On cooling, the lattice parameter decreases by 0.2 % down to $a = 4.6556(2)$ Å at 100 K. We found no indication of a phase transition in this temperature range. From the precisely determined peak positions it was possible to exclude the previously observed small impurity peaks and ascertain that they don't belong to the AuBe pattern, but to a so far unreported secondary phase.
The data were used to solve the crystal structure of AuBe in the cubic space group type $P2_13$ and refine the lattice parameters, atomic positions, atomic displacement parameters and site occupation factors (Tab. 1). The obtained model for AuBe is of the FeSi-structure type and the high-resolution data allowed even the precise determination of the Be position next to the heavy Au atoms. In this structure the Au and Be atoms form a distorted cubic arrangement (Fig. 1a). The obtained data will furthermore serve as input for electronic structure calculations of AuBe.

We were also able to record powder X-ray diffraction patterns of a new Pt-Be binary phase. The pattern of the single phase sample was indexed with a large, face centered cubic unit cell of lattice parameter $a = 15.90302(3)$ Å at 300 K (Fig. 2, right panel). Also here, we found no indication of a phase transition in the investigated temperature range. Based on the extinction conditions we found the possible space group types $Fd\bar{3}m$ or $F\bar{4}3m$. The structure was then

solved in the latter by direct methods. Consequently not only the Pt positions but also a large part of the Be positions could be determined by difference Fourier synthesis. The remaining Be positions were found in an iterative process by using the partial structure model as input for neutron powder diffraction data, collected recently at the ECHIDNA high-resolution diffractometer of the OPAL reactor (ANSTO, Lucas Heights, Australia). With both datasets combined we were able to solve and refine the structure of the cubic γ-phase with the corrected composition Pt_5Be_{21}. This compound contains 416 atoms in its unit cell and is part of the family of large unit cell complex metallic alloys. It is an ordered variant of the $Cu_{41}Sn_{11}$ structure type and can be described as an arrangement of nested polyhedral clusters (Fig. 1 b,c). It is the first Be containing large unit cell γ-phase where the complete structure determination could be achieved solely by powder diffraction data.

Tab. 1: Atomic parameters for AuBe at 300 K.

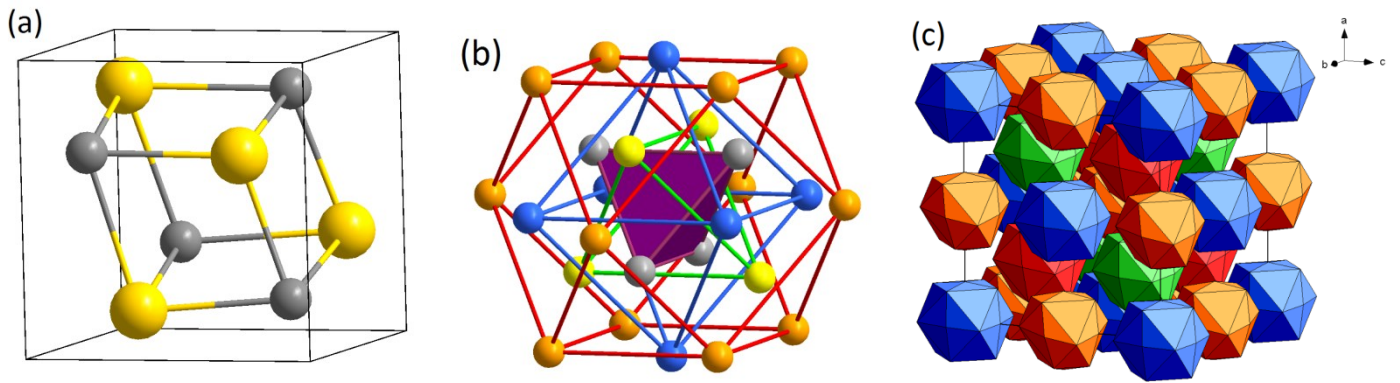| Atom	Wyck. Pos.	x/a	y/b	z/c	B_{iso} / Å^2
Au1	4a	0.35006(4)	-x+1/2	x+1/2	0.411(3)
Be1	4a	0.826(2)	-x+1	-x+1/2	0.67(2)

Fig. 1: (a) Crystal structure of AuBe (FeSi-type) showing the distorted cubic arrangement of Au (yellow) and Be (gray) atoms in the cubic unit cell.(b) Nested polyhedral structure of the Pt-Be clusters in Pt$_5$Be$_{21}$. Right panel: Arrangement of the clusters in the crystal structure of Pt$_5$Be$_{21}$.

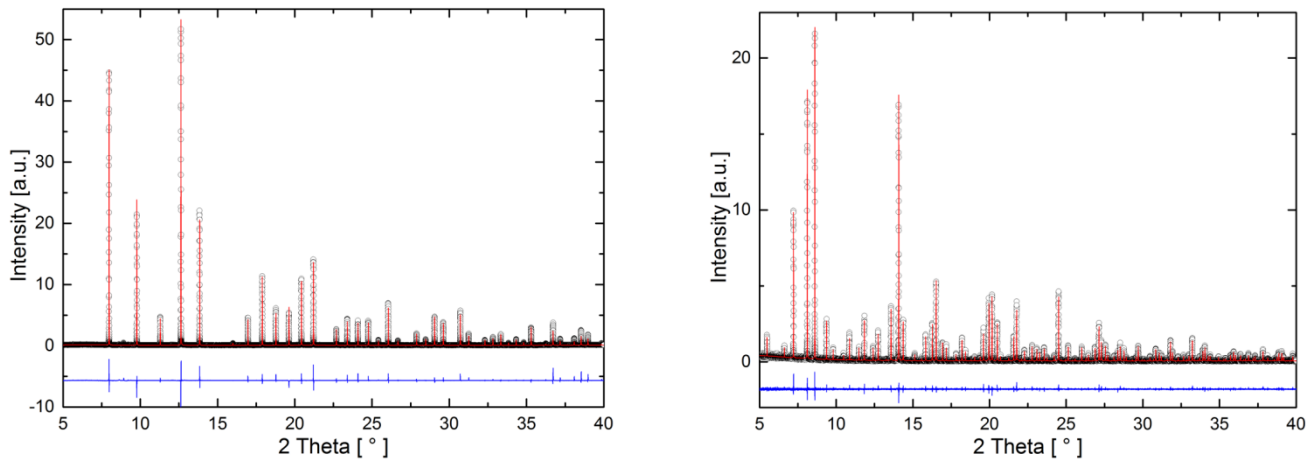*Fig. 2: Synchrotron powder diffraction patterns of AuBe (left panel) and Pt$_5$Be$_{21}$ (right panel). Experimental points (black circles), Rietveld model (red line), Difference plot (blue line).*