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:** HE1019	**Experiment number**:
Beamline:	**Date of experiment**: from: 15/12/01 to: 18/12/01	**Date of report**: 26/02/02
Shifts:	**Local contact(s)**: Honkimaki/Buplaps	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Le Bolloc'h, Caudron, Bley, Picca, Livet, Schulli

Report:

The phase diagrams of metallic alloys which present ordered phases have been extensively investigated from an experimental point of view [1] but the electronic structure of those systems are not well understood by the theory yet (for a recent overview see for example [2]). Despite a substantial literature [3,4,5], it is still very difficult for *ab-initio* calculations to properly simulate the ground states, transition temperatures or the chemical short range order even in the case of binary alloys. We have undertaken a systematic study of the binary alloy Pt_1-V_{1-c} as a function of the concentration. The aim of this study was to determine the ordering energy from experimental data, instead of *ab initio* calculations. Indeed, a careful measurement of the chemical short range order (either by neutrons or x-ray diffuse scattering) allowed us to determine the effective interactions of an Ising model via inverse Monte Carlo simulations. Despite short range order is very sensitive to the concentration, this study showed that the effective interactions (the first nine effective pair interactions on a FCC lattice) are independent of *c*.We are able to predict the phase diagram (the Pt-rich side) with an unequalled precision from a unique set of interactions. As well as being a precious guide for electronic structure calculations [7], those interactions allow us to predict a new *A_5B phase* which should appear at c=1/6.

We have investigated this concentration on the ID15B beamline using high energy (60 keV) in transmission geometry. The (100) reciprocal plane mainly has been observed until the (300) position ($q=4\,\Pi \sin\theta/\lambda=6.22$ Å^{-1}). Thanks to the good resolution of the image plate available on id15A (150μm of resolution located at 1 meter from the sample) superstructure reflexions have been resolved ($\Delta q=0.01$ Å^{-1}) around the [100] point (see figure).
This new ordered phase is not the one expected by our theory: it is not the *A_5B phase* simulated from our interactions but an incommensurate phase displaying a superstructure at the (100) position with 4 satellites in the (100) plane.
The measurement has been done *in situ* up to 700C: The ordered phase displays 4 satellite reflexions around the (100) position at incommensurate positions. They are slightly moving with the temperature. No locking phenomena has been observed. The kinetic of the oredered phase is slow but very stable as respect to the temperature: the ordered phase disapears at 700C only.

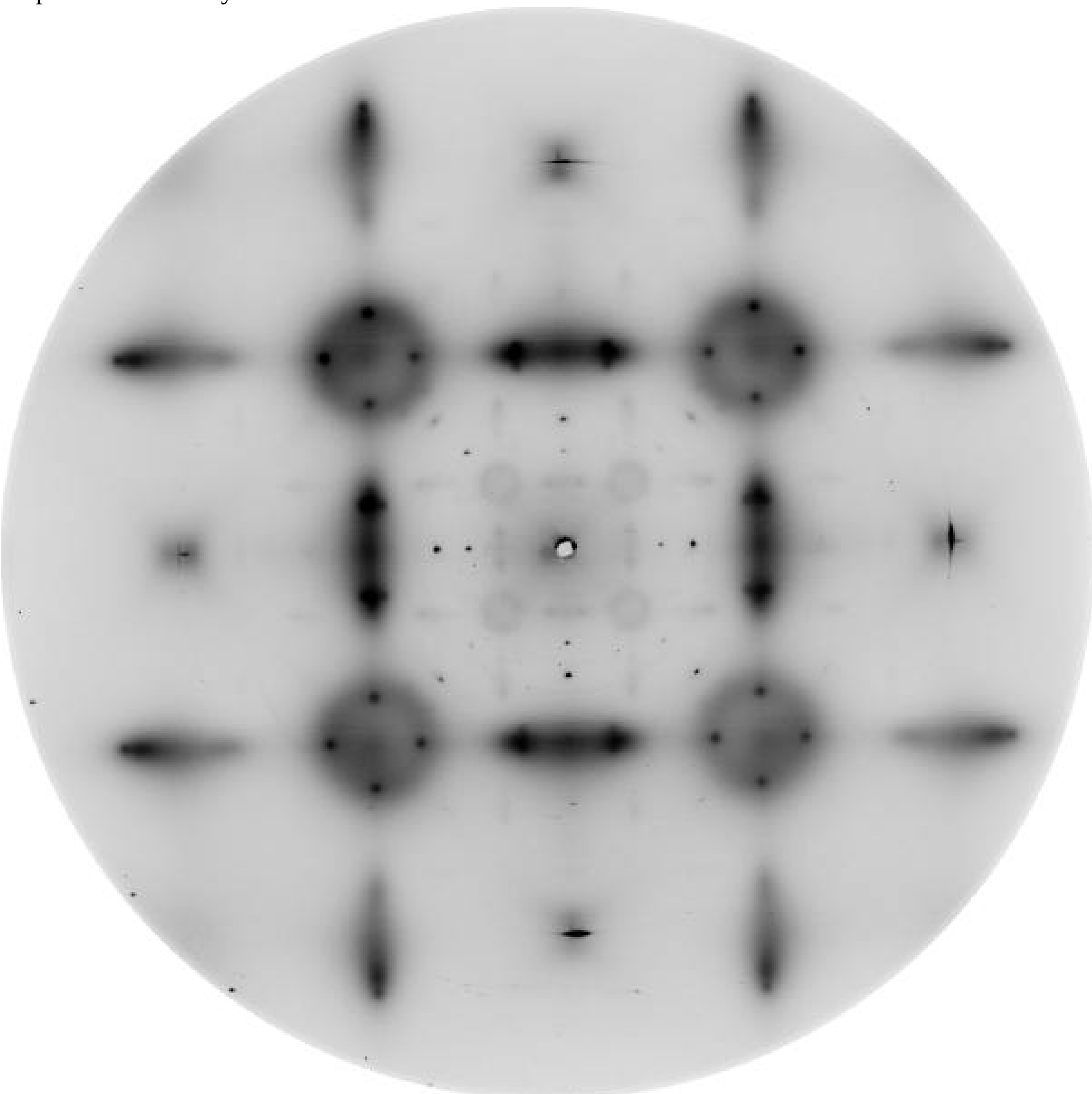

Fig 1. Short and long range order in the Pt_4V measured on ID15B

References

[1] Hansen, *Constitution of Binary Alloys*, Mc Graw Hill, New York, (1958).

[2] F. Ducastelle, *Order and Phase Stability in Alloys*, edited by F. R. de Boer and D. G. Pettifor, Cohesion and Structure **3** (North-Holland, Amsterdam, 1991).

[3] C. Wolverton, A. Zunger, Phys. Rev. B 52, 8813(1995).

[4] D.D. Johnson, J.B. Staunton, F.J. Pinski, Phys. Rev. B 50 1475 (1994).

[5] B. Schönfeld, L. Reinhardt and G. Kostorz, Phys. Status Solidi b, 147 (1988).

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[7] D. Jonhson, *private communication*.

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[9] D. Le Bolloc'h, PhD thesis, University of Rennes (1997).

[10] D. Le Bolloc'h, F. Bley, *private communication*.