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*

Deadlines for submission of Experimental Reports

Experimental reports must be submitted within the period of 3 months after the end of the experiment.

Experiment Report supporting a new proposal ("relevant report")

If you are submitting a proposal for a new project, or to continue a project for which you have previously been allocated beam time, you must submit a report on each of your previous measurement(s):

- even on those carried out close to the proposal submission deadline (it can be a *"preliminary report")*,
- even for experiments whose scientific area is different form the scientific area of the new proposal,
- carried out on CRG beamlines.

You must then register the report(s) as "relevant report(s)" in the new application form for beam time.

Deadlines for submitting a report supporting a new proposal

- 1st March Proposal Round - **5th March**
- 10th September Proposal Round - **13th September**

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.

Instructions for preparing your Report

- fill in a separate form for each project or series of measurements.
- type your report in English.
- include the experiment number 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:** Probing topological instability of amorphous high entropy alloy based on the pair distribution function analysis	**Experiment number**: HC-5000
Beamline: ID31	**Date of experiment**: from: 08 November 2022 to: 09 November 2022	**Date of report**: 27/02/2023
Shifts: 3	**Local contact(s)**: Veijo Honkimaki	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Kai Zhang, Qingyu Kong, Peiyuan Su

Synchrotron SOLEIL

Report:

1. Expected results in the proposal

Our proposal is based on the crystallization and phase transition peaks observed on our DSC curve, as well as the reported hcp ground state in the reference. We believe that amorphous CrMnFeCoNi likely possesses a hcp-like local atomic structure, which would indicate that the amorphous phase should undergo successive transformations into hcp and fcc phases upon heating.

2. Results and the conclusions of the study

Thanks to the assistance of the ID31 beamline staff at ESRF, we were able to successfully conduct in-situ heating high-energy X-ray diffraction. Surprisingly, our findings show that the amorphous phase transforms firstly into a metastable bcc phase, and then into a high-temperature fcc phase, without experiencing hcp phase (as seen in Fig. 1). A updated phase diagram is shown in Fig. 2. These results are particularly inspiring, as the bcc phase has yet to be reported experimentally. Moreover, we observed that both high-temperature bcc and fcc phases can be quenched to room temperature, indicating that they have equal or similar energy levels. This motivated us to perform theoretical calculations, as depicted in Fig. 3, which revealed that a ferrimagnetic bcc phase has comparable energy to the paramagnetic fcc phase, in good agreement with our experimental findings.

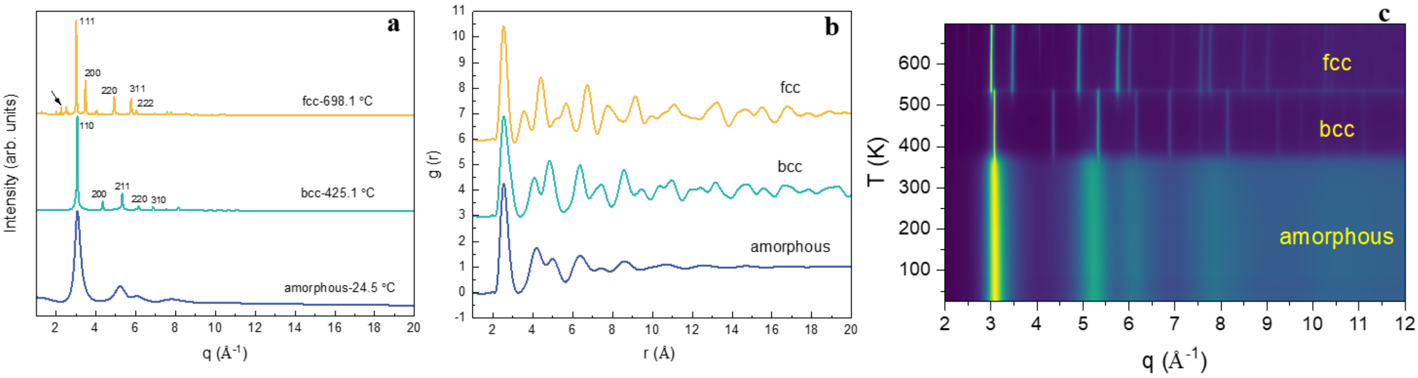

Fig. 1 in-situ heating high-energy X-ray diffraction of amorphous CrMnFeCoNi high-entropy alloy. (a) representative XRD patterns corresponding to amorphous, bcc, and fcc phases. (b) the corresponding pair distribution function. (c) structur factor during heating

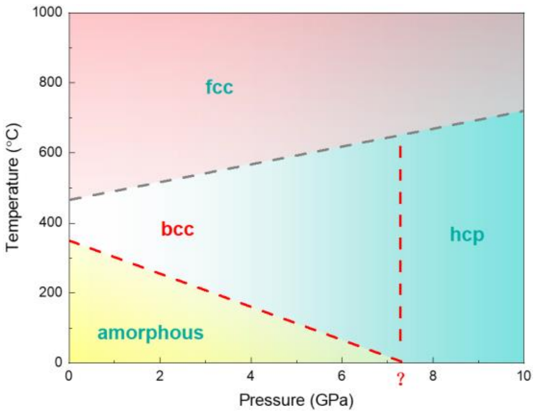

Fig. 2 A updated diagram based on the in-situ high-energy X-ray diffraction conducted at ID31 beamline.

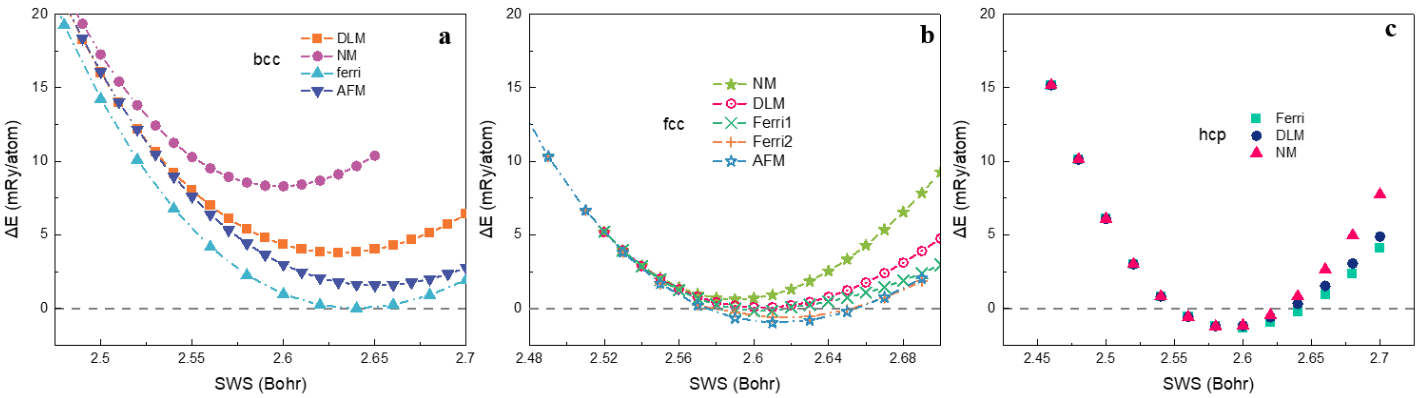

Fig. 3 Total energy comparison in bcc (a), fcc (b), and hcp (c) phases with different magnetic states. For clarity, the total energy of ferrimagnetic bcc was set as the reference (horizontal dashed line)

3. Publication

Currently, our work is still in progress as we plan to measure high-pressure XMCD to reveal the crucial role of magnetism in amorphous and bcc CrMnFeCoNi HEA. We are eager to submit our paper in the near future and share our findings with the scientific community.