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:** Correlation between structural relaxation and high-entropy effect in metallic glasses	**Experiment number**: HC-5108
Beamline: ID-10	**Date of experiment**: from: 26 January 2023 to: 01 February 2023	**Date of report**: 04 March 2023
Shifts: 15	**Local contact(s)**: ZONTONE Federico	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

*Xin Zhang, Center for High Pressure Science and Technology Advanced Research

*Hongbo Lou, Center for High Pressure Science and Technology Advanced Research

*Qiaoshi Zeng, Center for High Pressure Science and Technology Advanced Research

*Fujun Lan, Center for High Pressure Science and Technology Advanced Research

*Dazhe Xu, Center for High Pressure Science and Technology Advanced Research

Report:

In the experiment HC-5108, we studied a HEMG system, $Zr_{20}Nb_{20}Cu_{20}Ni_{20}Ti_{20}$, with highly tunable configurational entropy. The HE-MG exhibits irreversible structural crossover upon heating, specifically, from a relatively disordered high-energy glass state to a more ordered low-energy glass state in the supercooled liquid region. The pair distribution function (PDF) derived from XRD data , shown in **Fig.1**, suggests that the unique role of short-range order associated with the high-entropy effect in HEMGs.

According to the studies in high-entropy alloys, it is well recognized that high chemical disorder (configurational entropy) naturally raises local atomic distortion, thus, the energy barrier for atomic diffusion (sluggish diffusion effect), leading to slower dynamics. But our XPCS results of $Zr_{20}Nb_{20}Cu_{20}Ni_{20}Ti_{20}$, shown in right plane of **Fig.2**, reveal that the relaxation behavior of the disordered state (high configurational entropy) is significantly faster than that of the ordered state (low configurational entropy). Moreover, to get quantitative information of the relaxation process, the time average intensity autocorrelation functions, $g_2(q,t)$ are calculated, shown in left plane of **Fig.2**, by averaging each TTCF along the tw axis. In order to get the relaxation time and shape parameters, we use a modulated Kohlrausch-Williams-Watts (KWW) model function: $g_2(q,t) = 1 + a + c[\exp(-2(t/\tau)\,\beta\,)]$ to fit the $g_2\,(q,t)$ functions. However, through the comparison of $g_2(q,0)$ (the value of $g_2(q,t)$ when t=0, parameter regarded as a reflection of the strength of β relaxation), we found that the β relaxation of the disordered state is significantly stronger than that of the ordered state.

Our preliminary findings have led us to realize that the impact of the high-entropy effect on the dynamics of MGs is more complex than a simply expectation of sluggish diffusion, and its impact on glasses is more intricate than anticipated before. Furthermore, conventional techniques relying on the relaxation of macroscopic physical parameters are inadequate in accurately reflecting the effect of high-entropy at the atomic structural level in MGs. Therefore, we need more time to conduct a further XPCS experiment to systematically investigate these abnormal dynamic behaviors of the HEMG systems from multiple aspects, such as q-dependence of steady relaxation and aging (at temperatures close to the glass transition temperature) behavior, dynamics feature change through the glass transition into supercooled liquid. These results will provide a more complete picture of the entropy effect on the dynamics of HEMGs and guide our future efforts to regulate dynamics in MGs by adjusting the configurational entropy.

Figures:

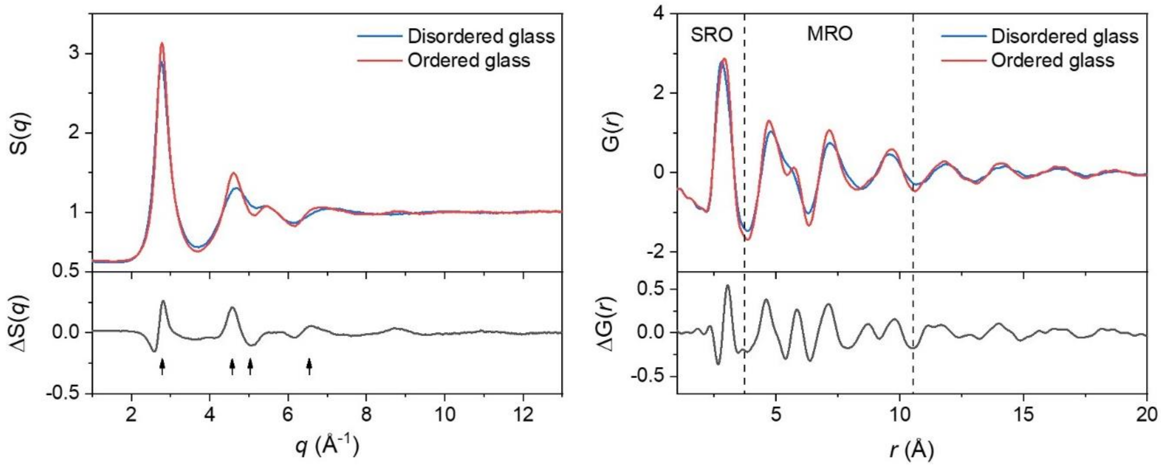

Fig. 1 Structural characterization of metallic glass, $Zr_{20}Nb_{20}Cu_{20}Ni_{20}Ti_{20}$ by structure factors (left plane) and paired distribution functions (right plane).

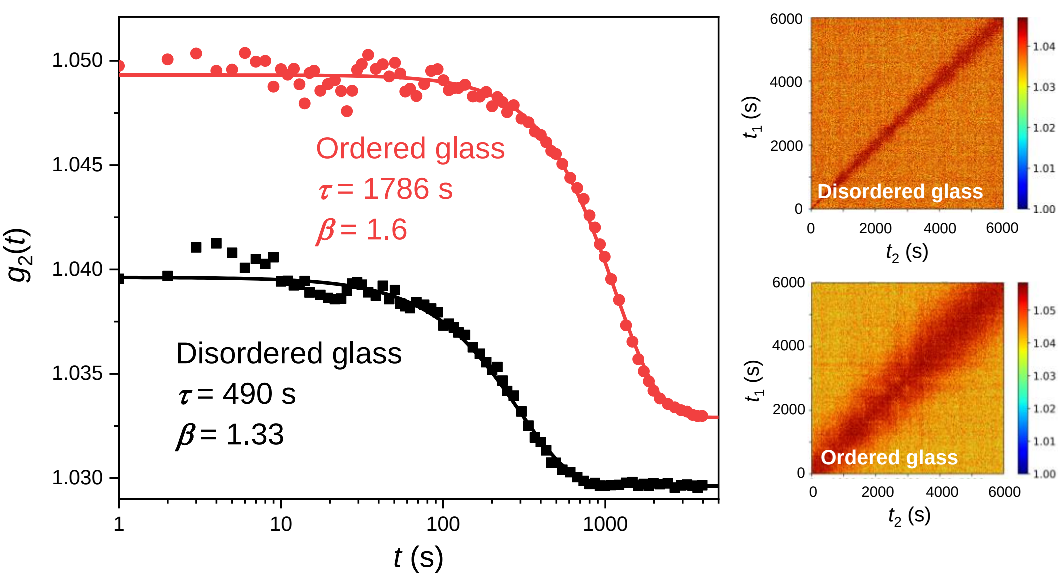

Fig. 2 Correlation functions of disordered and relatively more ordered glassy states measured at q_p and 573 K (left plane); Two-time correlation functions corresponding to these $g_2(t)$ curves (right plane).