

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://www.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: Direct observation of atomic-scale shear band dynamics in metallic glasses	Experiment number: HC-4479
Beamline:	Date of experiment: from: 9 june 2021 to: 14 june 2021	Date of report: 13/09/2021
Shifts:	Local contact(s): Yuriy Chushkin	<i>Received at ESRF:</i>
Names and affiliations of applicants (* indicates experimentalists): Eloi Pineda* Departament de Física, Universitat Politècnica de Catalunya, Barcelona Max Frey* and Nico Neuber* Universität des Saarlandes, Lehrstuhl für Metallische Werkstoffe Beatrice Ruta* CNRS Researcher, Light Matter Institute, UMR5306, Lyon 1 University		

Report:

We measured samples of Pd-based and Au-based metallic glasses while applying continuous heating/cooling ramps. The main objectives of the experiment were: 1) to prove that the supercooled liquid dynamics of metallic glass-forming melts can be resolved during constant heating experiments and, taking profit of this strategy, 2) to investigate the liquid-liquid transition of $\text{Au}_{51.6}\text{Ag}_{5.8}\text{Pd}_{2.4}\text{Cu}_{20.2}\text{Ga}_{6.7}\text{Si}_{13.3}$ (NGL6) and related alloys.

The experiment was successful. The intensity time correlation function $g_2(q, t) = 1 + a|g_1(q, t)|^2$ while applying temperature ramps at constant rate can be modelled taking into account two contributions. Firstly the decorrelation due to the thermal expansion of the furnace-sample system. This decorrelation is similar to the one expected for a drift (or collective velocity) of the scattering particles: $|g_1(q, t)|^2 \propto \exp[-(\dot{\epsilon}t)^2]$, with $\dot{\epsilon}$ proportional to the collective velocity. This type of decorrelation is clearly observed in the time correlation functions obtained at low temperatures. Applying the usual analysis of fitting to a KWW function: $|g_1(q, t)|^2 = \exp[-2(t/\tau)^\beta]$, the collective drift due to the movement of the whole system during the temperature ramp is characterized by an exponent $\beta=2$. Fig. 1 shows this type of response at low temperatures, where the intrinsic dynamics of the material are much longer than the decorrelation produced by thermal expansion, and only this latter contribution can be observed.

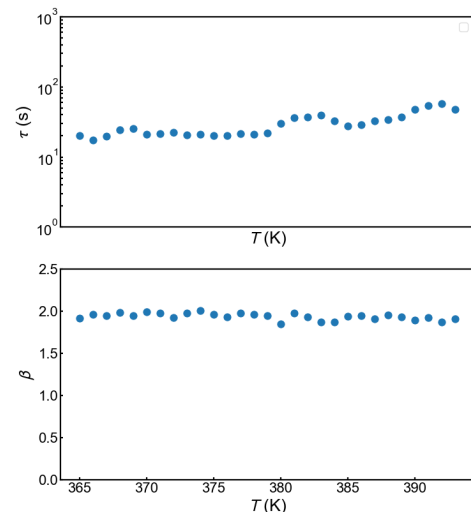


Fig. 1. Relaxation time and stretching KWW exponent of the $\text{Pt}_{42.5}\text{Cu}_{27}\text{Ni}_{9.5}\text{P}_{21}$ glass at low temperatures.

At higher temperatures, as soon as the intrinsic dynamics become of the same timescale (or shorter) than the experimental decorrelation, they start to be visible and the XPCS signal can be modelled considering $|g_1(q, t)|^2 \propto \exp[-2(t/\tau')^{\beta'}] \exp[-(\dot{\epsilon}t)^2]$, where τ' and β' are now describing the timescale and shape of the microscopic relaxation dynamics. Fig. 2 shows the evolution of temperature in the supercooled liquid region of one of the tested samples.

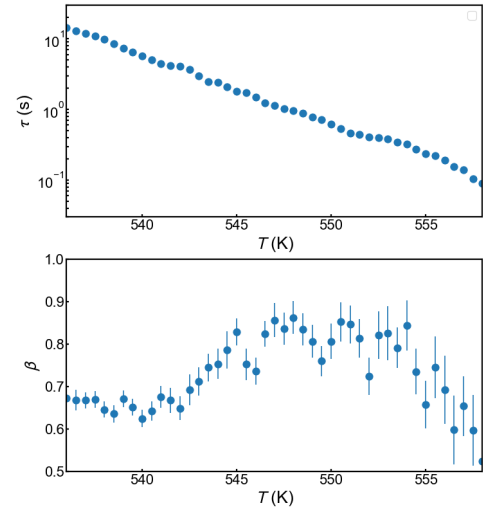


Fig. 2. Relaxation time and stretching KWW exponent of the $\text{Pt}_{42.5}\text{Cu}_{27}\text{Ni}_{9.5}\text{P}_{21}$ supercooled liquid.

The data of the different metallic melts measured in the experiment is still under analysis. For the NGL6 alloy, preliminary analysis show that the supercooled liquid relaxation dynamics can be well resolved showing a change in fragility, presumably associated to a fragile-strong viscous behaviour, at the expected temperature range as seen in Fig. 3.

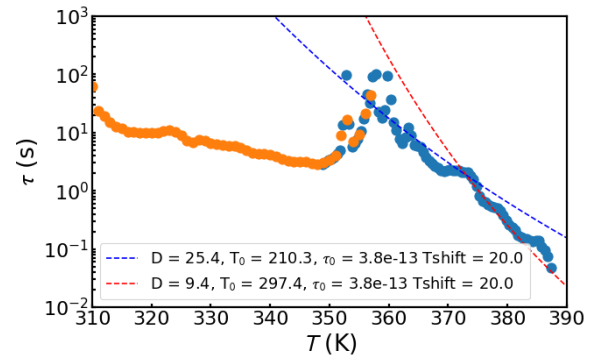


Fig. 3. Dynamics during glass transition and supercooled liquid regions of the NGL6 alloy obtained from XPCS and VFT behaviours (dashed lines) considering two different fragilities.

The amount of data collected using this strategy of measuring XPCS signal during temperature ramps is very large, the analysis is challenging and new python routines are being developed to make the procedures more automatic. This report will be updated in the future with further results.