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.

ESRF	**Experiment title:** Direct investigation of collective modes in liquid and supercritical CO_2	**Experiment number**: SC-4361
Beamline: ID28	**Date of experiment**: from: 20/07/2017 to: 26/07/2017	**Date of report**: 17/10/2017
Shifts: 18	**Local contact(s)**: Alexei Bossak	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Martin Dove*, Ling Wang*, Guanqun Cai*

Queen Mary University of London, UK

Report:

Introduction: There have been many studies of acoustic modes in fluids, including supercritical fluids, which have established the existence of the longitudinal acoustic modes and also of some transverse acoustic modes. Most of these have focussed on the shape of the excitation spectrum including the dependence of peak width on temperature [1]. The qualitatively new aspect of this experiment is the idea that the transverse acoustic modes exist over a range of frequencies, with the lower-limit of this range increasing with temperature so that the range becomes narrower on heating [2]. This experiment was aimed specifically at trying to observe this effect.

Experimental: $\mathbf{P_1}$=30 bar, $\mathbf{T_1}$=223, 233 K; $\mathbf{P_2}$=70bar, $\mathbf{T_2}$=223, 233, 243, 253, 263, 273, 283, 293 K. Each map collected with 8 analysers. The range of frequencies up to 15 meV and wave vectors Q up to 25 nm^{-1}.

Results:

No transverse acoustic modes found.

Although CO_2 has the perfect critical pressure and temperature (72.9 atm, 304.2 K) and very safe for experiment, it turns out CO_2 is different and complicated in the way to detect transverse and longitudinal acoustic modes.

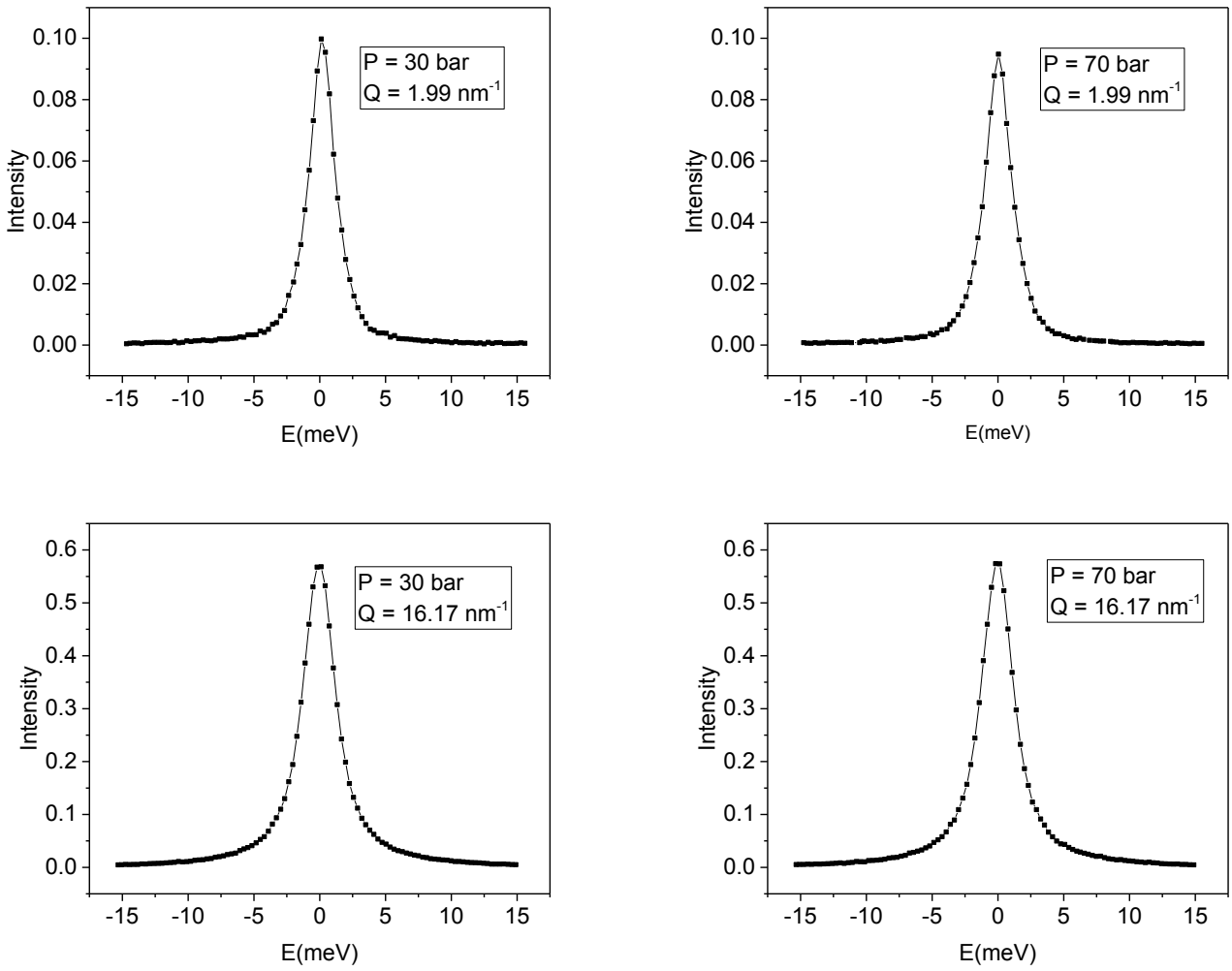

Fig 1. IXS spectra of liquid and supercritical CO_2

Future Plan:

1. **MD simulation.** We have begun supporting molecular dynamics simulations based on a new model for the intermolecular forces. Our plan is to simulate the inelastic scattering spectrum, and to identify the contributions to the scattering from rotational motions and the acoustic modes which is the objective of our experimental study. Then we will compare MD simulation results with experiment data.

2. **Liquid Ga.** We propose to measure a simple liquid -- liquid Ga instead of CO_2, because this is a well-documented liquid where transverse modes have been measured [3]. Moreover, the boiling point of Ga is very high, enabling us to span a wide range of the liquid state in this system.

References:

1. S Hosokawa, M Inui, Y Kajihara, S Tsutsui & AQR. Baron, *J. Phys. Condens. Matt.* **27**, 194104 (2015)
2. C Yang, MT Dove, VV Brazhkin & K Trachenko, *Phys. Rev. Letters* **118**, 215502 (2017)
3. VM Giordano & G Monaco, *Phys. Rev. B* **84**, 052201 (2011)