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

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.

	Experiment title: Porperties of the Quartz A-B transition at high pressure	**Experiment number**: 1211
Beamline: ID06	**Date of experiment**: from: 14/02/2023 to: 19/02/2023	**Date of report**: 13/03/2023
Shifts: 15	**Local contact(s)**: Dmitrii Druzhbin	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

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Report:

This was a continuation of proposal ES910, during which we had investigated the nature of the alpha-beta transition of quartz at various pressure and temperature (PT) conditions in the Large Volume Press (LVP) of ID06. Experiments were performed in a 6-6 configuration (i.e., using a cubic cell assembly). The XRD data were collected using monochromatic beam and a Pilatus 2D detector. The data were processed by sequential Rietveld refinement. At low pressures (< 1 GPa), results show, as previously documented, that the lattice parameters of quartz increase dramatically when approaching the transition in the alpha field, then remain constant despite increasing T in the beta field. At high pressures however, the results show a much smoother transition.

The main result from that first round of investigation was therefore the successful and accurate monitoring of the transition across a range of PT conditions. The aim of the present proposal was thus to combine these high PT XRD data with measurements of sound velocities to provide full constraints on the effect of this transition on seismic velocities in the conditions of the Earth's lower crust (Sheehan et al., 2014). The approach was to use an already established acoustic setup that uses a 6-8 configuration of the LVP (octahedron cell), where an acoustic transducer is used to collect pulse-echo waveforms and determine travel times of P and S-waves in the sample (Thomson et al., 2019).

The experimenters benefitted from invaluable user support from Dmitrii Druzhbin and Wilson Crichton for both sample preparation and data collection. Three attempts were made over the course of 15 shifts in this beamtime. The first two were unsuccessful due to failures of the acoustic sensor and of the heater. The third attempt was successful and allowed us to collect both XRD and acoustic data. This sample was cycled multiple times across the A-B transition by varying either P or T up and down during a total of 8 shifts. Preliminary data reduction shows a very good correlation between phase change and both compressional and shear wave velocities (Vp and Vs), which, as expected, decrease with increasing temperature in the alpha field, then increase to higher values in the beta field upon further heating (Moarefvand et al., 2021). Subsequent refinements, in particular regarding the evolution of the sample length observed by X-ray absorption images, will allow quantifying accurately

the relations between P, T, Vp and Vs (Figure 1). It is the first time such data are collected in the actual conditions of the Earth's deep crust. In the future (proposal ES1364), we plan to round off this dataset by collecting similar data in a 6-6 configuration where the effects of stress can be assessed and quantified by performing azimuthal XRD scans with the detector, as also successfully achieved during ES910.

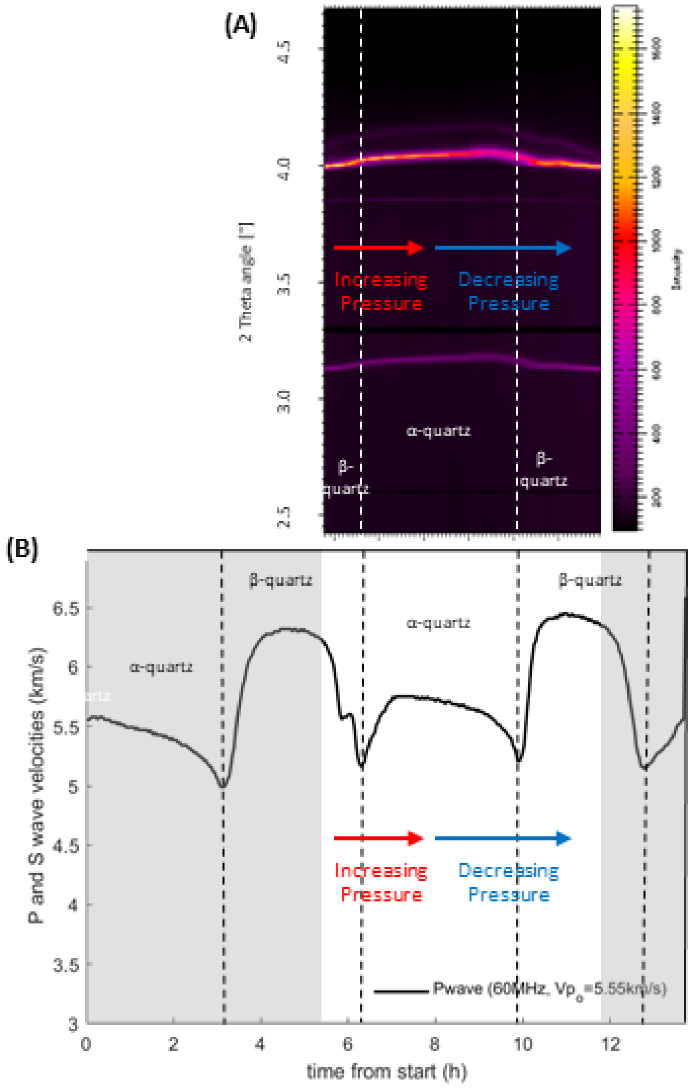

Fig. 1 Results from ES-1211 showing (A) evolution of the two main reflections of quartz (100 and 011) and (B) p-wave velocity while the pressure was ramped up and down at constant rates. The transition is evidenced in the former data by pronounced peak position shifts (dashed lines) and also clearly identified in the latter on both the up- and down-pressure paths by a minimum in velocity. Velocity is here approximated assuming a constant sample length equal to that of the initial length and a reference velocity of quartz, Vp_0, calculated for given PT conditions.

Moarefvand, A., Gasc, J., Fauconnier, J., Baïsset, M., Burdette, E., Labrousse, L., Schubnel, A., 2021. A new generation Griggs apparatus with active acoustic monitoring. Tectonophysics 816, 229032.

Sheehan, A.F., de la Torre, T.L., Monsalve, G., Abers, G.A., Hacker, B.R., 2014. Physical state of Himalayan crust and uppermost mantle: Constraints from seismic attenuation and velocity tomography. Journal of Geophysical Research-Solid Earth 119, 567-580.

Thomson, A.R., Crichton, W.A., Brodholt, J.P., Wood, I.G., Siersch, N.C., Muir, J.M.R., Dobson, D.P., Hunt, S.A., 2019. Seismic velocities of CaSiO3 perovskite can explain LLSVPs in Earth's lower mantle. Nature 572, 643-+.