Experimental report

17/02/2020

Proposal: **7-01-498** **Council:** 4/2019

Title: Modelling the lattice dynamics of the lower mantle, an INS study on CaTiO3

Research area: Other...

This proposal is a new proposal

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Samples: CaTiO3

Instrument	Requested days	Allocated days	From	To
IN8	7	7	03/02/2020	10/02/2020
IN3	2	2	24/01/2020 02/02/2020	25/01/2020 03/02/2020

Abstract:

The travel times of seismic waves through the Earth's interior provide one of the only direct constraints of the chemistry and properties of the deep mantle. Calcium perovskite is the third most abundant mineral throughout the lower mantle (~ 700 - 3000 km depth in Earth), but because it is not stable under ambient conditions the speed that sound travels through this phase is almost completely unconstrained. We will perform inelastic neutron scattering measurements on IN8 to measure the acoustic velocities of the titanium end member of calcium perovskite between room temperature and 1500 Celsius, revealing whether its presence in the deep Earth may explain heterogeneous seismic signals that are currently not understood.

Experimental report 7-01-498: Modelling the lattice dynamics of the lower mantle, an INS study on $CaTiO_3$

D.J. Voneshen, A. Piovano, A. Thomson

The aim of this experiment was to measure the transverse and longitudinal acoustic velocities of $CaTiO_3$ through its structural phase transitions. These experimental velocities would be used to test first principles calculations of the thermoelastic properties of the calcium perovskites which make up 10-30 % of the lower mantle.

A 1 g synthetic single crystal of single domain $CaTiO_3$ was aligned in the cubic *hhl* scattering plane (orthorhombic *h0l*) using orient-express and IN3 on a Nb mount with Ta wire. IN8 was set up with the pyrolytic graphite monochromator and analyser and 30' of collimation was used throughout. The temperature was controlled with a standard ILL high temperature furnace using Nb elements.

Full datasets were collected at room temperature, 800, 1000, 1275, 1375 and 1500 °C with a limited set collected at 300 °C on cooling back down. So far we have extracted the velocities of both longitudinal and transverse modes along the cubic 00*l* direction and these are shown in figure 1. Both modes soften dramatically on approaching the orthorhombic to tetragonal phase transition, unexpectedly however the longitudinal softens much more relative to the transverse.

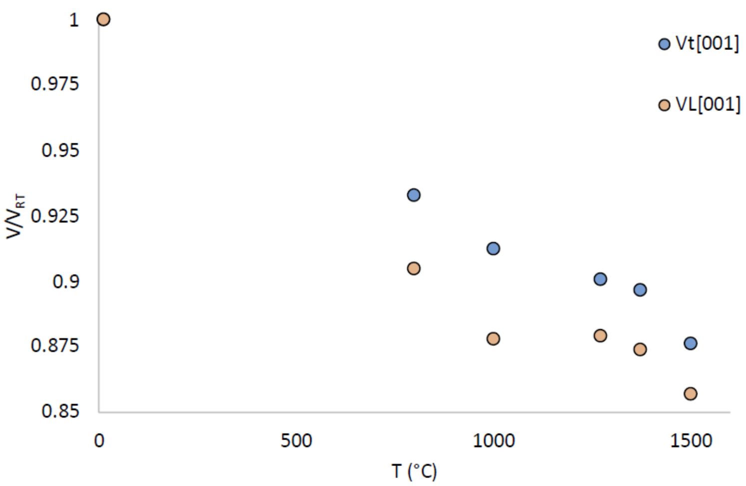

Figure 1: the relative speeds of sound obtained by fitting the acoustic dispersion. Both modes soften significantly but, unexpectedly the longitudinal mode softens even more than the transverse. From elastic measurements the first phase transition is at 1225 °C and the second between 14 and 1500°C

Initial work suggests that the longitudinal softening along *hh*0 is even more pronounced as the tetragonal to orthorhombic transition is approached. This is unexpected as previous work on polycrystalline $CaSi_{0.6}Ti_{0.4}O_3$ under pressure found that the transverse velocity softened significantly more than the longitudinal [1]. In $SrTiO_3$ changes in the acoustic velocity are driven by soft optic phonons [2,3] and it is possible that that similar physics underlies the changes seen here.

[1] A.R. Thomson *et al.*, *Nature*, **572**, 643-647 (2019)

[2] R.A. Cowley, *Phys. Rev.*, **134** A981 (1964)

[3] Y. Yamada and G. Shirane, J. Phys. Soc. Jpn. **26**, 396-403 (1969)