ESRF	**Experiment title:** Lattice dynamics of Cerium at high pressure	**Experiment number**: HS-2595
Beamline: ID28	**Date of experiment**: from: 22.04.2005 to: 3.05.2005	**Date of report**: 3 August 2005
Shifts: 30	**Local contact(s)**: A. Beraud	*Received at ESRF:*

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Report:

The aim of the experiment was to study the pressure evolution of the TA and LA phonon dispersion of cerium up to and above the isostructural (fcc) γ->α transition in order to shed further light on this intriguing, and not yet fully understood phase transition. Crystals of 60-80 μm diameter and 20 μm thickness were prepared from a large ingot, obtained from Ames Lab, using laser cutting and mechano-chemical polishing techniques. In order to avoid oxidation, the surface was passivated by a thin Kapton . Three samples with a surface normal approximately oriented along the [110] direction were loaded into diamond anvil cells (DAC), using neon as a pressure transmitting medium. The crystalline quality of the samples was checked by rocking curve scans, and typical values obtained ranged between one and two degrees. The crystal quality only degraded slightly when the pressure was increased to reach the α-phase, and data could be therefore recorded as well for this phase. The spectrometer was operated at 17794 eV in Kirkpatrick-Baez focusing geometry, providing an energy resolution of 3 meV and a focal spot size at the sample position of 30 x 60 μm^2 (horizontal x vertical, FWHM).

Eight to ten IXS spectra were typically recorded per phonon branch. Figure 1 reports the pressure dependence of the LA[100] branch in the γ-phase for pressures of 1, 4 and 6 kbar, together with previous inelastic neutron scattering (INS) results [1] at ambient pressure. A clear decrease of the phonon energies with increasing pressure is observed for 1 and 4 kbar, whereas the phonon energies increase again at 6 kbar, still well within the stability field of the γ-phase. Figure 2 reports the LA dispersion along all three main symmetry directions at 6 kbar (γ-phase) and 8 kbar (α-phase), together with the INS results at ambient conditions. Besides the already discussed unusual behaviour along the [100] direction, the pressure evolution of the two other longitudinal branches in the γ-phase is quite different. The LA [110] branch shows a strong bending near the zone boundary (ZB), whereas the phonon energies at low reduced momentum transfer, q, remain close to the ones at room pressure. In contrast to this, the LA [111] branch does not display any pressure dependence. This behaviour confirms the strong anisotropy of the waves propagation of cerium under pressure.
The LA phonon energies in the α-phase at 8 kbar are systematically higher than the corresponding lower pressure phonon energies, consistent with the higher density of the α-phase and the expected larger elastic constants. We note, however, substantial changes in the lattice dynamics along the [110] direction. While the phonon energies between ξ=0.4 and 0.6 show the largest energy increase with pressure, the energy increase

at the ZB remains moderate, leading to a pronounced bending of the LA[110] branch. The shapes and intensities of the LA phonon branches in α-phase cerium are close to those measured in thorium at room conditions [2] while the γ-phase data can be better compared to fcc metastable lanthanum [3]. This behaviour might be a signature of substantial changes in the Fermi surface topology, leading to significant changes in the electron-phonon coupling mechanism. A Born-vonKarman fit to the phonon dispersion is currently being performed in order to quantify the changes in the force constant matrix.

The present study was limited to the longitudinal dynamics. This was partly due to the limited time, but as well due to the fact that the samples had a miscut of about 15 degrees (angle between the surface normal and the [110] direction). In conjunction with the limited angular opening of the DAC, this prevented us from measuring the TA phonons. We are confident that the next batch of samples can be prepared, reducing the miscut angle to less than two degrees, thus allowing to focus on the pressure evolution of the transverse dynamics, most notably the TA[111] branch (see proposal).

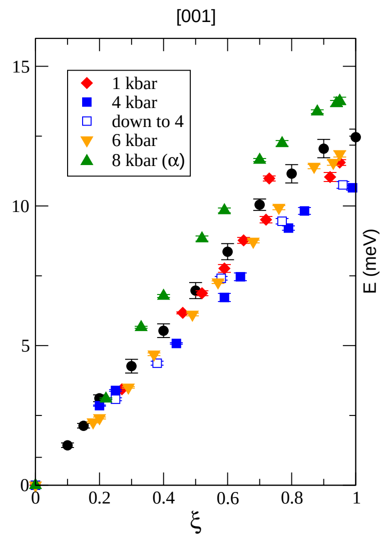

Figure 1

Evolution of the LA [001] branch with pressure.

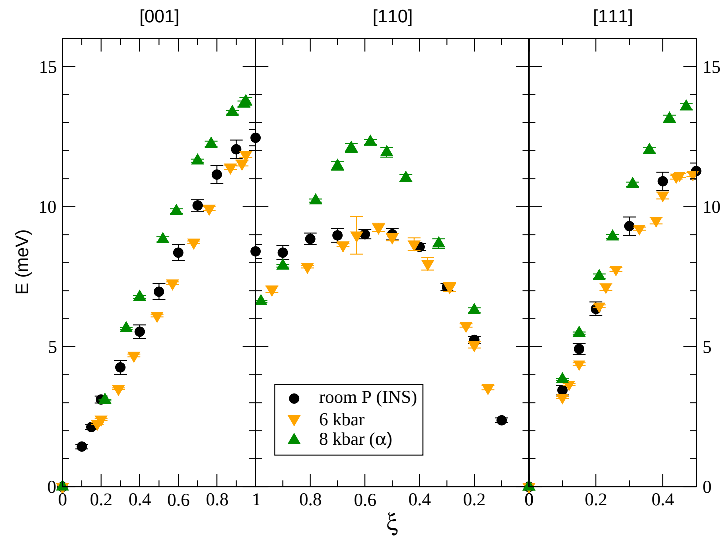

Figure 2

Full sets of LA phonon branches at room conditions, 6 kbar and 8 kbar.

References:

[1] C. Stassis et al.; Phys. Rev. B 19, 5746 (1979), C. Stassis et al.; Phys. Rev. B 25, 6485 (1982).
[2] R.A. Reese et al.; Phys. Rev. B 8, 1332 (1973).
[3] C. Stassis et al.; Phys. Rev. B 31, 6298 (1985).