	Experiment title: Determination of the pressure dependence of elastic constants of hcp-cobalt	**Experiment number:** HS-2046
Beamline: ID28	**Date of experiment:** from: 11.06.2003 to: 24.06.2003	**Date of report:** 1 September 2003
Shifts: 36	**Local contact(s):** M. Krisch	*Received at ESRF:*

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Report:

Based on the measured dispersions of longitudinal and transverse acoustic phonon branches in single crystalline hcp-Cobalt, we have derived the five independent elastic moduli C_{11}, C_{33}, C_{44}, C_{12} and C_{13} for pressures of 31.5 and 39 GPa at room temperature, extending the previously investigated range.
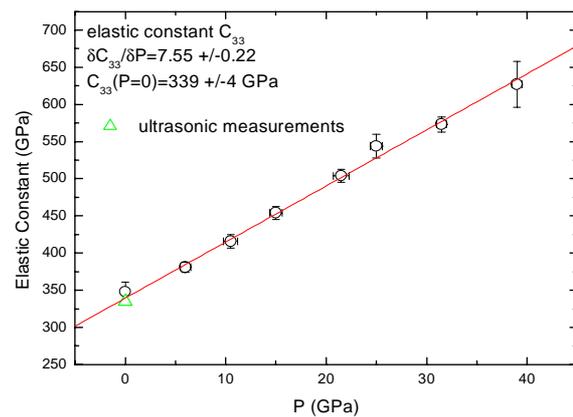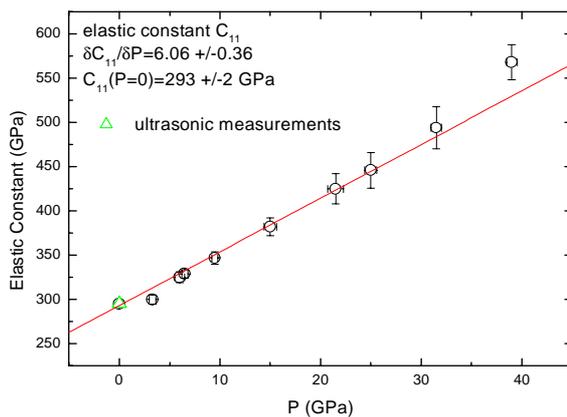

Figure 1: Evolution of the elastic moduli C_{11} and C_{33} with pressure. The red lines are linear fits to the data. The determined pressure derivative and the extrapolation to room pressure are reported as well. Ultrasound measurements at room pressure are indicated as green triangles.

High quality single crystals (45 μm diameter and 20 μm thickness with their surface normal parallel to the [110] direction) were loaded in a Rhenium gasket and pressurized in a diamond anvil cell (DAC) with helium as pressure transmitting medium. The pressures were determined *in situ* by the conventional ruby fluorescence technique and crosschecked with x-ray diffraction, making use of the known equation of state of cobalt [1,2]. The experiment was performed with an overall energy resolution of 3 meV and a momentum resolution of 0.3 nm^{-1}. Tree to four points were recorded in the linear part of the dispersion branch in order

to derive the sound velocities from the slope of the linear fit made to these data. The elastic moduli were then determined solving the Christoffel equation for each of the five phonon branches. Representative results are shown in *Figure 1* for C_{11} and C_{33}. All five Cij's show a linear behaviour in the explored pressure range as witnessed by the fit to the data points, thus allowing robust estimates of their pressure derivatives. Moreover, extrapolation of the Cij(P) curves towards room pressure yields an excellent agreement with the values obtained by ultrasound measurements [3].

Further, the knowledge of the elastic moduli allows the derivation of the anisotropy of the longitudinal and transverse sound velocity in the meridian (a-c) plane for each pressure and thus comparisons with the anisotropy estimated from first principle calculations [4].
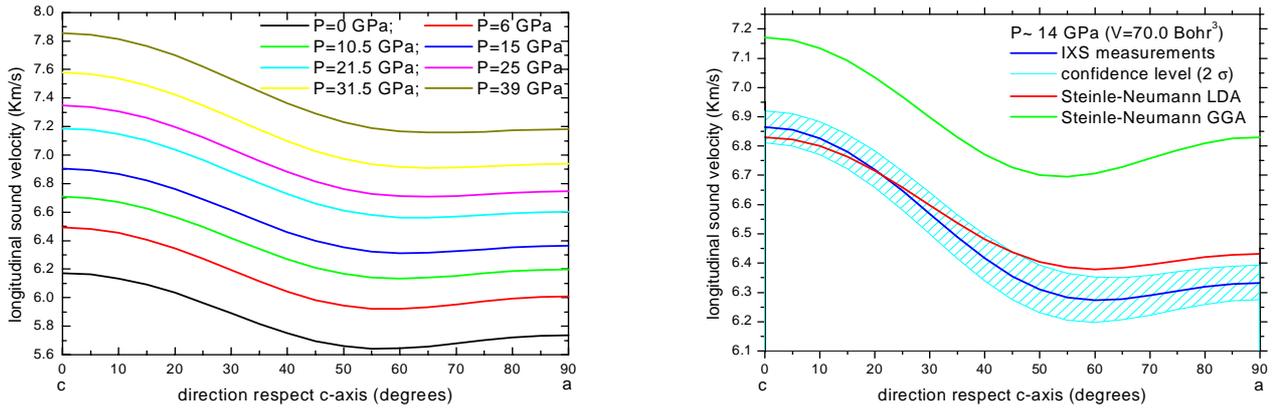

Figure 2: (left panel) Anisotropy of the longitudinal sound velocity in the meridian a-c plane as a function of pressure; (right panel) Comparison between IXS results and first principle calculations performed in the general gradient approximation (GGA) and in the local density approximation (LDA) at 14 GPa.

The main feature of Figure 2 is the stronger increase of the sound velocity along the c-axis compared to the a-axis. As a consequence, the anisotropy, already present at room pressure, becomes more pronounced with pressure, leading to the progressive vanishing of the minimum around 55°. The overall shape of both computational methods in Figure 2 is in good agreement with the IXS data. The LDA calculation yields a better quantitative agreement and suggests that the experimentally observed anisotropy is slightly underestimated in the calculation.

The extension of the investigated pressure range up to 39 GPa also gives a qualitative comparison with the elastic anisotropy of iron, as obtained by *ab initio* calculations [4] or derived from XRD measurements [5]. Our results are again in general agreement with the calculations, but appear in disagreement with the results obtained form diffraction.

Our future experiments are aimed to extending this investigation to pressures of ~100 GPa and including the effect of the temperature.

References

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