



Experiment title:

Investigation of the acoustic anisotropy of hcp metals at high pressure by inelastic x-ray scattering

Experiment number:

HS-1970

Beamline:

ID28

Date of experiment:

from: 13.11.2002 to: 24.11.2002

Date of report:

19 February 2003

Shifts:

24

Local contact(s): M. Krisch

Received at ESRF:

Names and affiliations of applicants (* indicates experimentalists):

- *G. Fiquet, *J. Badro, F. Guyot, Laboratoire de Minéralogie Cristallographie, Universités Paris VI, IPGP, F-75252 Paris Cedex 05, France.
- *D. Antonangeli, *M. Krisch, *H. Requardt, ESRF, France.
- *F. Occelli, *C. Aracne, *D. Farber, Energy & Environment, Lawrence Livermore National Laboratory, USA.

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} as a function of pressure up to 25 GPa at room temperature.

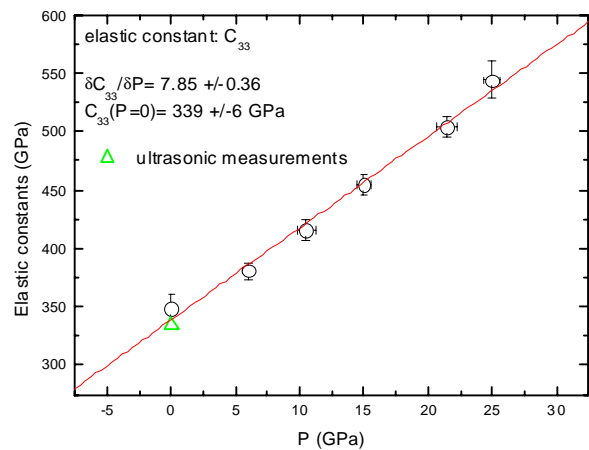
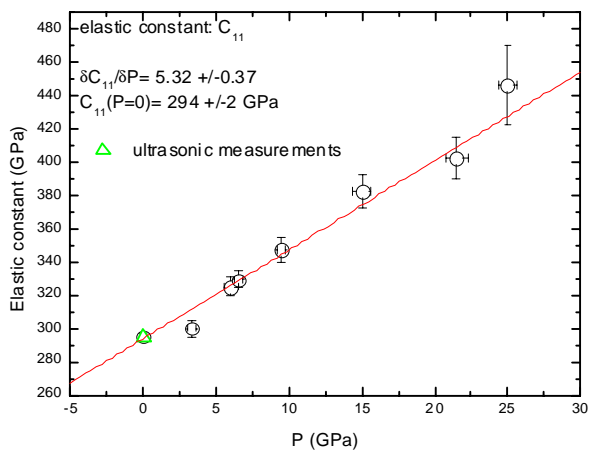


Figure 1: Evolution of the elastic moduli C_{11} and C_{33} with pressure. Lines are linear fits to the data. The determined pressure derivative and the extrapolation to room pressure are reported as well. Ultrasound measurements at room pressure are indicated as triangles.

High quality single crystals (90 μm diameter and 15-20 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. To cover the entire pressure range, four cells with slightly different characteristics were used. 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} , recording either the complete dispersion (8-10 q points) or a few points at low q. The sound velocities were derived from a linear fit to the lower part of the phonon dispersion curves. The elastic moduli are 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 C_{ij} '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 $C_{ij}(P)$ 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 sound velocity in the meridian (a-c) plane for each pressure and thus comparisons with the anisotropy estimated from first principle calculations [4].

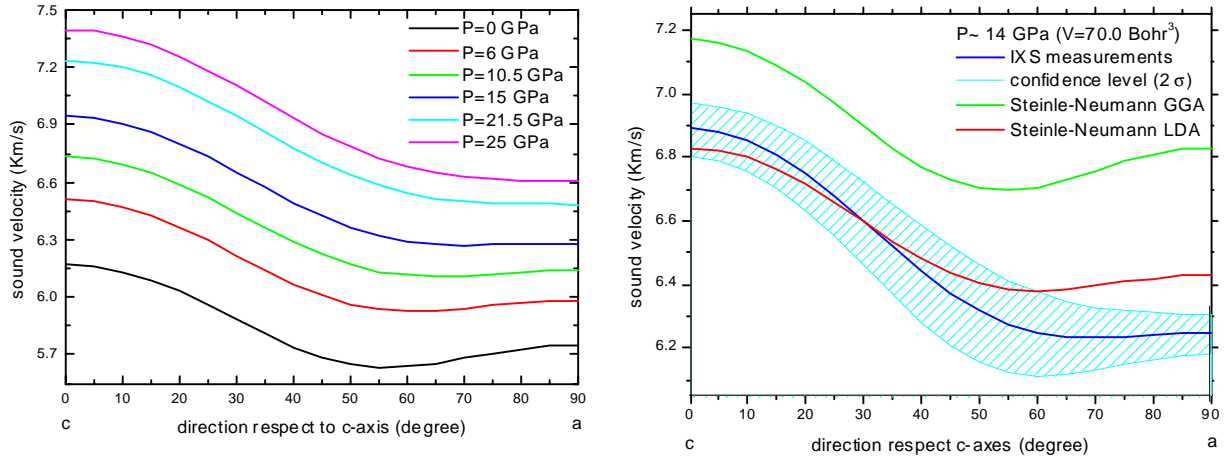


Figure 2: (left panel) Anisotropy of the longitudinal sound velocity in the meridian a-c plane as a function of pressure; (right panel) Comparison between IXS results and first principle calculations performed in the general gradient approximation (GGA) and in the local density approximation (LDA) at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

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

References

- [1] H. Fujihisa and K. Takemura, *Phys. Rev. B*, **54**, 5 (1996)
- [2] C.S. Yoo *et al.*, *Phys. Rev. Lett*, **84**, 4132 (2000)
- [3] R. F. S. Hearmon, *The Elastic Constant of Crystals and Other Anisotropic Materials* in Landolt Börnstein, New Series III, Vol. 11 (Springer, Berlin, 1979)
- [4] Steinle-Neumann *et al.*, *Phys. Rev. B*, **60**, 791, (1999)