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Report:

Based on the measured dispersions of longitudinal and transverse acoustic phonon branches in single crystalline hcp-Cobalt, the five independent elastic moduli C_{11}, C_{33}, C_{44}, C_{12} and C_{13} were determined with high accuracy to 39 GPa at room temperature, completing and refining, especially in the case of transverse modes, the previous results (see experimental reports HS-1970 and HS-2046) [1].

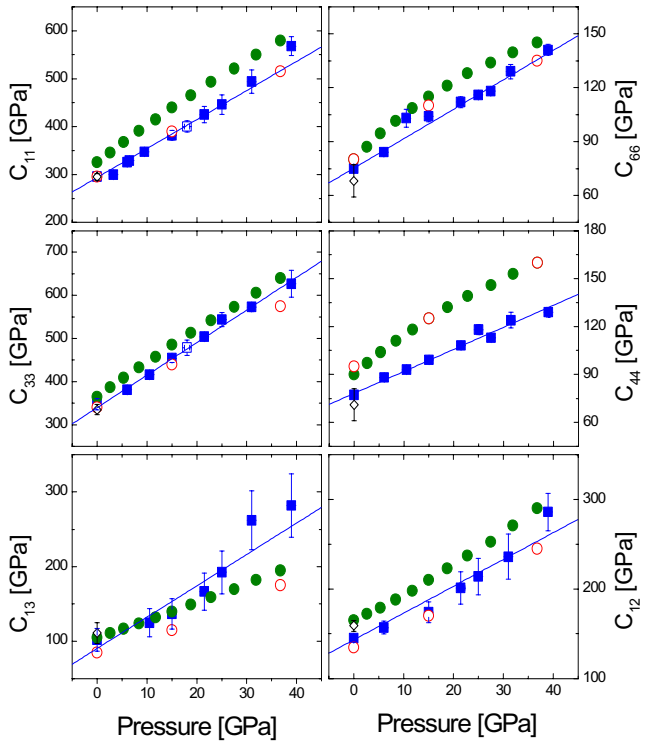

***Figure 1**: Pressure evolution of the hcp-Co elastic moduli. IXS results, obtained using helium (full squares) and neon (open squares) as pressure transmitting medium; room pressure ultrasonic measurements (open diamonds) [2]; ab initio calculations within the GGA approximation (full circles) and LDA approximation (open circles) [3]. The pressure values for the calculations were obtained using our measured equation of state. The solid line is a linear fit to our data.*
C_{66}=½(C_{11}-C_{12}) is reported as well for comparison .

High quality single crystals (45 to 80 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 in order to ensure hydrostatic pressure conditions. For one run neon was used rather than helium, recording values for the elastic moduli in excellent agreement with the ones previously obtained (see Figure 1), clearly demonstrating that gas absorption by the sample, as well as other pressure medium effects are negligible. 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 [4,5]. The experiment was performed with an overall energy resolution of 3 meV and a momentum resolution of 0.2 nm^{-1}. Three to five points were recorded in the linear part of the dispersion curve 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.

The pressure evolution of the elastic moduli is reported in Figure 1 and compared with *ab initio* calculations [3] and ultrasonic measurements [2]. The pressure derivatives of the various C_{ij} are well described by a linear law (see solid lines). We note that $C_{11}(P=0) < C_{33}(P=0)$ and $\partial C_{11}/\partial P < \partial C_{33}/\partial P$, so that the elastic anisotropy between the basal (a-b) plane and the c-axis, already present at room condition, is increasing with pressure. Furthermore, $C_{44}(P=0) < C_{66}(P=0)$, while for other hcp metals such as beryllium, rhenium, zinc and zirconium [2] $C_{66}(P=0) < C_{44}(P=0)$. This anomaly disappears with increasing pressure, since $\partial C_{44}/\partial P < \partial C_{66}/\partial P$ leading to a crossing of the two moduli at about 12 GPa. Our results are in good agreement with room pressure ultrasonic measurements [2], except for C_{12}, where the IXS value is lower by about 11%. Results from *ab initio* calculations [3] yield in most of the cases higher values, with the exception of C_{13}. The calculated pressure evolution is close to the experimentally determined one for $C_{11,}$ C_{33}, C_{66} and C_{12}, but $\partial C_{44}/\partial P$ and $\partial C_{13}/\partial P$ are, respectively, too high and too low. A more critical comparison suggests that the calculations tend to underestimate the increasing anisotropy between C_{33} and C_{11}, and, above all, do not predict the observed crossing between C_{44} and C_{66}, because of the high value for the C_{44} pressure derivative. In general we observe a better quantitative agreement (in particular for C_{11} and C_{66}) with calculations performed within the Local Density Approximation (LDA) rather than within the Generalized Gradient Approximation (GGA), while the IXS values for C_{33} and C_{12} lay in-between the two approximations. In summary, although there are small discrepancies between our IXS results and calculation, there is a good overall agreement. The present experimental results are therefore of great value for further refinement of the *ab initio* methods, and might be used to directly address the choice of the pseudo-potential, the treatment of electron correlation and exchange interactions, as well as the applied strains used for the determination of the elastic moduli.

Moreover, a new kind of high temperature DAC, dedicated to IXS measurements, was tested for simultaneous high pressure-high temperature experiments. Neon proved to be a good pressure transmitting medium for such kind of measurements, while further work, improving the long term stability at high temperatures, is required to obtain an accurate determination of phonon energies at elevated temperatures and pressures.

References

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