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**Names and affiliations of applicants** (* indicates experimentalists):

- *D. Antonangeli, *D. L. Farber, Energy & Environment Directorate, Lawrence Livermore National Laboratory, USA.

## Report:

We have determined selected elements of the elastic tensor of hcp cobalt at simultaneous high pressure and temperature, namely the elastic moduli $C_{11}$, $C_{33,}$ $C_{66}$ and $C_{44}$, using an analogues approach to that used in previously high pressure and ambient temperature velocity and density measurements [1]. High quality single crystals [2] (30 to 40 μm diameter and 20 μm thickness, with surface normal parallel to the [110] direction) were loaded in a rhenium gasket and pressurized in a resistively heated diamond anvil cell (HTDAC) using neon as pressure transmitting medium. An innovative design of the cell, specifically optimized for Inelastic X-Ray Scattering (IXS) experiments on single crystals, allowed us to collect high quality data on phonons at high pressure in the 300-1000 K temperature range. Critical to our ability to achieve the required high-temperature stability (Co samples stayed above 300 C for more than a week, and, over that period, at 500 C for two days and at 700 C for almost one) were the controlled vacuum and careful insulation of portions of the cell. Higher temperatures, although likely achievable, were not investigated because of the proximity of the Co hcp-to-fcc phase transition [3]. The pressure was determined *in situ* by the shift of the fluorescence line of a $SrB_4O_7:Sm^{2+}$ chip placed in the sample chamber [4], while the temperature was determined from two thermocouples placed in contact with the two diamonds and crosschecked with the ruby fluorescence (at lower temperatures) and the Stokes/anti-Stokes ratio of the collected phonons. The experiment was performed with an overall energy resolution of 3 meV and a momentum resolution of 0.3 $nm^{-1}$. We obtained the sound velocities from the initial slope of selected acoustic modes and then the elastic moduli solving the Christoffel equations. Typical errors are about 2% for the sound velocities and 3-4% for the elastic moduli.

The evolution of the measured $C_{ij}$ with temperature at constant density (directly derived from the diffraction patterns collected in parallel to the IXS spectra) is illustrated in Figure 1. At the density value of 9.40±0.02 g/cm$^3$, corresponding to a pressure of about 13.5 GPa at ambient temperature, no significant temperature effects are observed. This evidence suggests that the elasticity of hcp cobalt under compression at high temperature is favourably described within the frame of a quasi-harmonic approximation, within which the elastic properties and sound velocities are functions of the density only, irrespectively of the pressure-temperature conditions. Consequently, the shape of the elastic anisotropy previously determined at high pressure and ambient temperature [1] remains likely the same over a wide P-T range, indicating anharmonic high-temperature effects to be minimal at constant density.

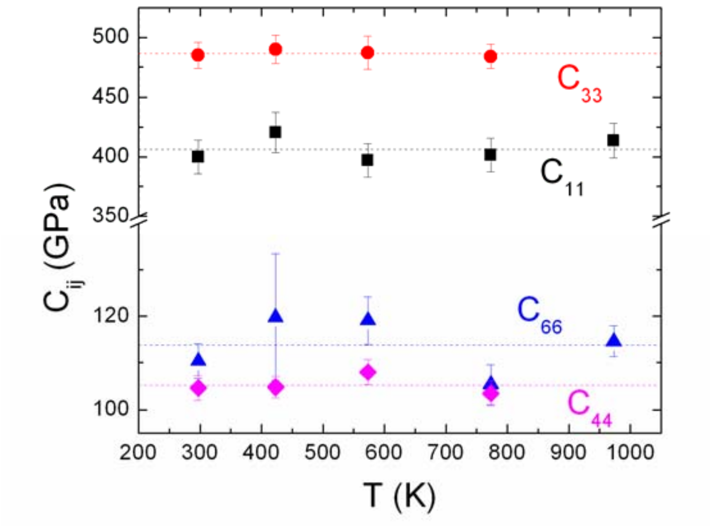


***Figure 1****: Temperature evolution at constant density (ρ=9.40 g/cm$^3$) of four of the five elastic moduli of hcp cobalt.*
*The lines through the experimental points are guides to the eyes fixed to the mean values of the various moduli in the investigated temperature range.*

These conclusions on hcp cobalt are in disagreement with recent and controversial *ab initio* calculations performed for hcp iron [5]. Despite the fact that a very similar pressure evolution of the elastic moduli and of the elastic anisotropy is predicted for Co and Fe at high pressure [6], in Fe, high-temperature effects at constant density have been suggested. These lead to the crossing between $C_{11}$ and $C_{33}$ and hence, to a reversed elastic anisotropy [5]. The reasons for this difference are still under investigation. Possibly, the approximation used in the calculations (as pointed out in [7]) limit the reliability of the theoretical findings, or the lower temperature of the present experiments with respect to calculations did not allow us to probe these effects. Alternatively, there may be significant differences in the behaviours of hcp cobalt and hcp iron at high temperature, with a more harmonic behaviour for Co.

## References

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