Magneto-elastic effects in compressed cobalt

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Characterizing elasticity of 3d transition metals under compression has been at the center of experimental development in high-pressure physics and geophysics over the past decade as cores of terrestrial planets are primarily composed of iron. As the study of elasticity on the high-pressure hcp phase of iron has proven challenging, a lot of effort has focused on cobalt which crystallizes in the hcp phase at ambient pressure (P). The discovery of the high P phase transition from the hcp to the fcc phase near 100 GPa raises a number of interesting question, e.g. the role of magnetism and elasticity in phase stability. Here we perform density functional theory based computations on the magneto-elastic properties of both phases, paying particular attention to the effect of magnetism on the elastic constants with the goal to elucidate the experimental findings.

In agreement with experiments we find hcp Co stable over the fcc phase for a large volume range. For both phases we find a magnetic phase with initial moments near 1.65 μ_B that decrease slowly with P due to delocalization effects. At higher P magnetism is lost almost instantaneously from the fcc phase; for the hcp phase it more slowly vanishes.

The elastic constants for hcp Co at ambient P are in good agreement with ultrasonic experiments. For the magnetic hcp phase the elastic moduli start deviating from a monotonic increase above 65 GPa. The shear constants (c_{44} and c_{66}) show significant softening: the anomaly coincides with the loss of magnetism. The longitudinal constants (c_{11} and c_{33}) also show softening in that volume range. Aggregate sound velocities reflect these anomalies. For magnetic and non-magnetic hcp Co the compressional wave velocity (v_P) and the shear wave velocity (v_S) are similar at low compression and depend linearly on density, following Birch's law. v_S for the magnetic phase shows a strong softening, decreasing over some compression range, before recovering the non-magnetic value at highest P. The compression dependence of sound velocities agrees well with experiments to above 100 GPa. The agreement between experiments and computations for magnetic hcp cobalt indicate that in the experiments cobalt remained in the hcp structure to highest P. The strong magneto-elastic coupling in the shear elastic constants for hcp Co at high P computed here as well as the anomaly in v_P and v_S measured shows that Co can be used as an analogue to hcp iron only with great caution.

Hyperaccumulation of U in organic-rich alpine soils, Dischma Valley, Davos, Switzerland

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Mountain wetlands have been shown to be efficient uranium filters resulting in uranium concentrations of up to 3'000 ppm based on dry weight [1]. We recently found uranium concentrations up to 7'000 ppm in organic-rich soils of the Dischma Valley (Eastern Swiss Alps). This formerly glaciated valley close to Davos is cut into crystalline rocks of the Upper Austroalpine Silvretta Nappe. The major lithologies are orthogneisses, paragneisses, and amphibolites.

Uranium-rich histosols are widespread in the Dischma Valley with hot-spots corresponding to areas with the highest organic and moisture content. The uranium in the soils has a natural isotopic composition and long-lived daughter isotopes of ^{234}U (e.g. ^{226}Ra) and ^{235}U (e.g. ^{231}Pa) are missing. This clearly points to a process where U is solubilized from a source rock, then migrates with the solution and finally becomes immobilized in organic-rich and water-logged soils. Interestingly, there are no particularly U-rich rocks or U-ores described in the Dischma area.

The distribution of artificial radionuclides such as plutonium, ^{241}Am and ^{137}Cs within the soil profiles shows that soils at the study site have not been significantly disturbed by anthropogenic activities.

Soil profiles show a good correlation between the distribution of uranium and that of other redox sensitive elements such as Mo and Se with a maximum concentration at a depth of 30 cm. The porewater profiles show that the highest U content in the soil coincides with the zone of sulfate reduction. These two findings suggest that reduction may play a role in the immobilization of U. However, determination of the U valence state in these soils does not indicate predominance of U(IV) over U(VI) [2].

To evaluate the potential health impact of U in Dischma soils, we measured U content in locally captured drinking water and found concentrations below 25 ppb U.

[1] Owen & Otton (1995) *Ecological Engineering* **5**, 77-93.
[2] Roquier *et al*. (2009) *GCA*, this volume.