

# Pressure effect on the crystal lattice of unconventional superconductor UCoGe.

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Several unconventional superconductors, i.e. those where non-phonon mediated superconductivity is considered, can be found among U-based compounds. Such materials occur at the onset of magnetic order, and magnetic fluctuations have to be considered as a key ingredient of a pairing mechanism. A recently investigated example of such an unconventional compound is UCoGe, reported to be a weak ferromagnet ( $T_C = 2.8$  K) and superconductor ( $T_c = 0.8$  K) [1]. High-pressure experiments are a useful tool to provide information about the relationship of magnetism and superconductivity (SC). UCoGe was found to be easily tunable by hydrostatic pressure whereby ferromagnetism is suppressed and vanishes near  $p_c = 1.4$  GPa but superconductivity is enhanced and survives in the paramagnetic phase up to at least 2.2 GPa [2,3]. In other superconducting ferromagnets such as UGe<sub>2</sub> or URhGe, SC exist only in a ferromagnetic phase under pressure, close to the critical point, and then both ferromagnetism and SC disappear continuously at the critical pressure  $p_c$  [4,5].

The sensitivity of magnetic properties to interatomic spacing is also demonstrated in the case of lattice expansion stimulated by hydrogen absorption. This expansion, partly controlled by the hydrogen pressure, can simulate to some extent a negative pressure. The studies performed on UCoGe indicated a stabilization of ferromagnetism with  $T_C$  shifted up to the vicinity of 50 K for the dihydride UCoGeH<sub>2</sub>. In this context it was surprising to detect the fully reproducible loss of the weak ferromagnetism in UCoGe for the  $\alpha$ -hydride (roughly UCoGeH<sub>0.1</sub>) with a small but non-negligible volume expansion of 0.25% [6]. As volume contraction has to be generally expected for high-pressure experiments, we face the peculiar situation with magnetism disappearing with both volume contraction and expansion. Such a paradox brings about the necessity to determine the real lattice reaction to applied hydrostatic pressure.

The structural behaviour of UCoGe with pressure was studied using a diamond anvil cell (DAC) and a modified Bruker D8 diffractometer (Mo-K $\alpha$  radiation). Experimental data were collected at room temperature and pressure increasing gradually up to  $p = 30$  GPa. UCoGe crystallizes in the orthorhombic structure of the TiNiSi type (space group  $Pnma$ ). High-pressure XRD data showed that the TiNiSi type of structure was preserved up to the highest applied pressure. A Le Bail analysis of the high pressure diffraction patterns yielded data about the pressure variation of the lattice parameters. The quality of the diffraction data was insufficient for full Rietveld analysis however, the attempted refinement gave information about interatomic uranium distances ( $d_{U-U}$ ), which decrease under applied pressure. The most apparent fact deduced is that the pressure variations of  $b$  and  $c$  are much weaker than for  $a$ .

The observed anisotropy of compressibility with the  $a$ -axis as the soft direction obeys the same rule as in the compounds with the ZrNiAl structure type [7], pointing to a profound unifying underlying mechanism for the anisotropy of compressibility. This work also illustrates the fact that the hydrogenation-induced volume expansion cannot be mechanically taken as the equivalent of “negative” pressure, because the geometry of the expansion can be dramatically different than the geometry of compression under hydrostatic pressure. The equilibrium bulk modulus was estimated both from the fit of the Birch and Murnaghan equation of state to the relative volume changes  $V/V_0$  calculated at each pressure  $-B_0 = 1/k_V$ , where  $k_V$  is the volume compressibility (Figure 1) and the sum of individual compressibilities along given lattice directions  $-B_0 = 1/(k_a + k_b + k_c)$  (Figure 2). Individual compressibilities were obtained from a linear fit of the pressure variations of each individual lattice. The equilibrium bulk modulus is relatively high ( $B_0 \cong 340$  GPa) when compared to the UTX compounds with the ZrNiAl structure type [7], but it is in line with results obtained on UTSi-H compounds which form in a structure similar to TiNiSi type ( $B_0 = 257$  GPa for UPdSiH<sub>1.0</sub> [8]).

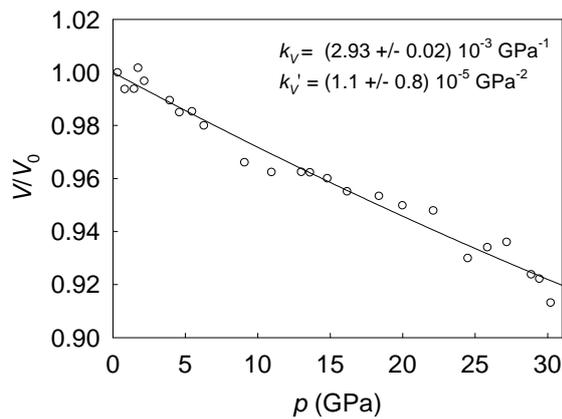


Fig. 1. Relative volume as a function of pressure for UCoGe. The line represents the fit of the Birch and Murnaghan equation.

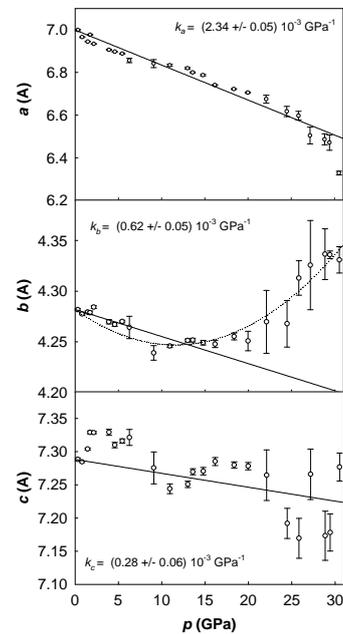


Fig. 2. Pressure dependence of lattice parameters  $a$ ,  $b$  and  $c$  for UCoGe. The lines represent the fits mentioned in the text.

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