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High-pressure x-ray studies of the UCo_3B_2 compound and ambient magnetic properties

E Sterer, I Halevy, H Ettedgui and E N Caspi

Physics Department, Nuclear Research Centre—Negev, PO Box 9001, Beer-Sheva, Israel

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Abstract

Substituting B for Co in the strong permanent magnet materials ACo_5 (A = Ln or U) substantially modifies the magnetic properties as a function of the B/Co ratio. Preliminary neutron diffraction studies on $TbCo_3B_2$ show site-dependent magnetic moments for both the Tb and the Co atoms. The changing interatomic distances and magnetic properties with changing B/Co ratio lead to a rich magnetic phase diagram as a function of pressure. It is our intention to study some of these materials using high-pressure Mössbauer spectroscopy in the future. As a preliminary step it is essential to study the high-pressure crystallographic phase diagram of these materials. This work shows preliminary high-pressure crystallographic results on UCo_3B_2 to 42 GPa, indicating a phase transition around 6 GPa.

1. Introduction

Materials of the $A_{n+1}Co_{3n+5}B_{2n}$ family (A = Ln or U, $n = 1$, 2, 3, and ∞) are derived from the ($n = 0$) ACo_5 structure by substituting B for Co. The ACo_5 structure ($P6/mmm$ space group) is a layered hexagonal structure that was considered potentially a strong permanent magnet. The substitution of B for Co is preferential and takes place only at the planes that are shared by cobalts and lanthanides and not at the planes that contain only cobalt [1] (figure 1). A complete substitution is achieved for ACo_3B_2 ($n = \infty$), shown in figure 2. This structure exists for most of the lanthanides, and partly for U ($n = 0$, 1, ∞).

The above materials were studied in the past using bulk magnetization methods and assumptions such as antiparallel (parallel) alignments between heavy-Ln (light-Ln) and Co moments [2–7]. Calculating the magnetic moments of Ln = Y, Gd [2–4], all the Co atoms, regardless of different crystallographic sites, were assumed to have the same magnetic moment. In other cases [7, 8] the Co moments were calculated assuming that the Ln ions always carry the full free-ion moment. These assumptions lead to inconsistencies [2–9].

Recent band structure calculation attempts to determine the magnetic moments per crystallographic site for Ln = Y, Nd [10, 11] gave similar results to the bulk measurements.

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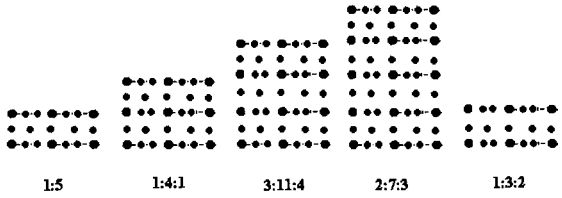

Figure 1. The $A_{n+1}Co_{3n+5}B_{2n}$ family with $n = 1, 2, 3$, and ∞.

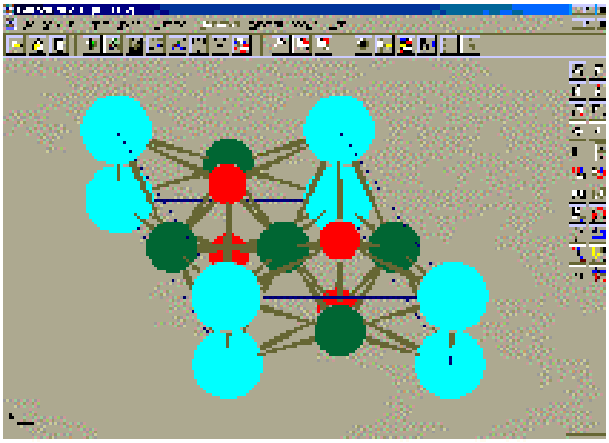

Figure 2. The UCo_3B_2 unit cell.
(This figure is in colour only in the electronic version)

NMR measurements [12–15] could not determine the magnetic moments per crystallographic site either. Thus, the need for a systematic neutron diffraction study is evident.

Preliminary neutron diffraction studies [16, 17] have shown that the Ln = Tb and Co moments are site dependent, and a more substantial study is now under way at the SINQ neutron source (PSI, Switzerland).

To complete the picture, a high-pressure Mössbauer study could elucidate the kinds of exchange interaction between the different neighbouring magnetic moments, provided that their spatial distribution is known. In order to achieve that, a high-pressure crystallographic study such as that presented here is needed.

2. Experimental details

UCo_3B_2 with nominal composition was prepared by arc-melting stoichiometric amounts of the constituents under an argon atmosphere. Since natural B is a neutron absorber, isotopic $^{11}B(99\%)$ has been used. The microstructures were examined by SEM, and the phases were analysed by means of EDS to determine their chemical compositions.

Our ambient pressure XRD data are shown in figure 3. Low-statistics and low-resolution neutron powder diffraction measurements were taken at the IRR-2 reactor; the results indicated no magnetic ordering down to 10 K.

High-pressure x-ray powder diffraction measurements (figure 4) up to 42 GPa were taken using an imaging plate and a Mo tube.

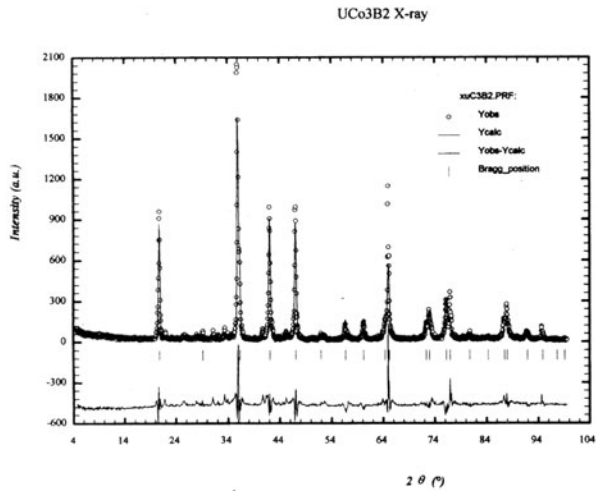

Figure 3. X-ray powder diffraction of UCo_3B_2 with Cu Kα radiation at ambient pressure.

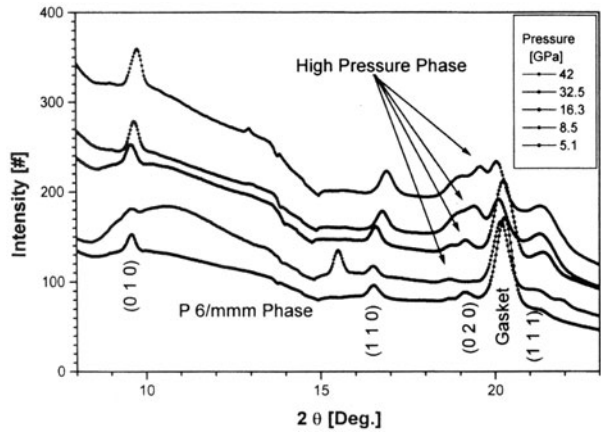

Figure 4. High-pressure XRD data taken at 5.1, 8.5, 16.3, 32.5, and 42 GPa. Above 8.5 GPa an extra peak is emerging at about $2\theta = 19°$.

The pressure was achieved using a miniature opposing-plate diamond anvil cell [18] with 500 μm culets. The pressure was calibrated using the ruby fluorescence method. To increase the angular diffraction range a Be backing plate was used. SQUID measurements for UCo_3B_2 in the temperature range 4–300 K are shown in figure 5.

3. Results and discussion

The x-ray ambient pressure measurement (figure 3) indicates a main phase of UCo_3B_2 in agreement with [1] and morphology. Rietveld analysis indicates that the UCo_3B_2 sample has the $P6/mmm$ ACo_5 structure with $a = 4.9560(1)$ Å and $c = 3.0720(7)$ Å at ambient pressure.

The high-pressure x-ray powder diffraction measurements are shown in figure 4. Above 8.5 GPa we find an extra diffraction line that we currently attribute to an as yet undetermined high-pressure phase, persisting up to 42 GPa. Current attempts to determine this crystallographic phase using an Ag tube are under way.

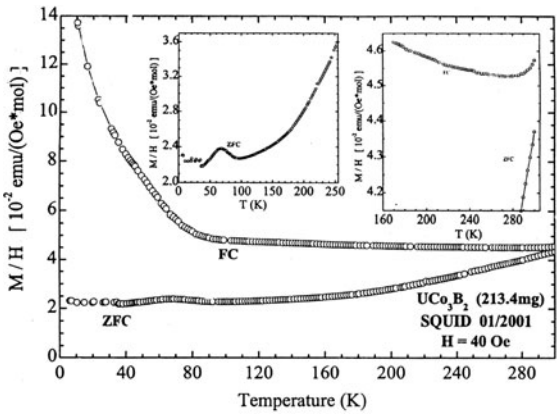

Figure 5. SQUID measurements for UCo_3B_2 in the temperature range 4–300 K.

SQUID magnetization measurements (figure 5) show some interesting magnetic features:

(1) A magnetic transition-like peak at 60 K.
(2) A separation between the ZFC and FC curves at $T < 300$ K.

These results are in disagreement with our neutron diffraction data. We propose a small ordered Co magnetic moment at UCo_3B_2 at $T < 60$ K, similar to the $TbCo_3B_2$ results (SINQ; to be published), where a small ($<1\ \mu_B$) Co magnetic moment is observed above the Tb magnetic transition temperature ($T = 35$ K).

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