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MAGNETIC AND LATTICE PROPERTIES OF CeBi

by

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ABSTRACT

The magnetic structures of CeBi have been examined as a function of field with neutron diffraction. At low fields unusual domain reorientation effects are observed. For H >18 kOe a 3+, 1- spin configuration is found. A first-order transition to induced ferromagnetic behavior occurs at 47.5 kOe. X-ray experiments at low temperature show that no lattice distortion occurs at either the Néel temperature or the I - IA transition at 12.5 K. A volume discontinuity is observed at the low temperature transition.

INTRODUCTION

The compound CeBi (NaCl structure) is of interest because of its anomalous magnetization[1,2] and unusual magnetic structures in zero field.[3] At T_N (25 K) the magnetic structure is type I in which ferromagnetic (001) sheets are stacked in an alternating +,- sequence. The spin direction is parallel to [001]. However, at 12.5 K CeBi undergoes a first-order transition to the type IA magnetic structure, in which the spin direction remains unaltered but the ferromagnetic sheets are stacked in the ++-- sequence. The IA structure is unusual in that it is not predicted by molecular field theory, but has been observed in a number of uranium compounds.[4] Recently Cooper et al.[5] and Bartholin[6] have reported magnetization experiments on single crystals. These measurements have shown that the moments are parallel to the cube axis in all fields and that for 15 <H <45 kOe an intermediate phase exists in which the magnetization is 1/2 the value in the fully ordered state (= 2.1 μ_B/Ce atom).

Neutron experiments

The experiments were performed at the CP-5 Research Reactor with a 60 kOe superconducting magnet assembly. The field was applied parallel to [001] throughout. The following reflections (together with their interpretation) were examined as a function of field: (110) - type I modulation with the propagation direction $\tau \parallel H$, (210) - type I modulation $\tau \perp H$, (11 1/2) - type IA modulation $\tau \parallel H$, (2 1/2 0) - type IA modulation $\tau \perp H$, and the (111) and (200) nuclear reflections which are sensitive to a net ferromagnetic contribution and are equivalent to the magnetization. For the (111) reflection the nuclear contribution is $N(111)=b_{Ce} - b_{Bi}= -0.377 \times 10^{-12}$ cm, and the magnetic contribution $M(111) = 0.27 \times f \times \mu$, where f is the form factor (=0.91) from Blume et al.[7] and the dipole approximation.[8] Thus $M(111)=0.245 \times \mu$, where μ is the moment per Ce in Bohr magnetons. The polarized-neutron technique measures the ratio M/N so the (111) reflection is very sensitive to a ferromagnetic component.

a)Type IA phase, T = 5 K.

Figure 1 (left hand side) shows the field dependence of the (110) and (11 1/2) reflections together with the ferromagnetic component. Initially with H=0 only the type IA reflections are present. As H increases the (11 1/2) increases and the (2 1/2 0) decreases (not shown). This behavior corresponds to a domain reorientation such that preferred domains have $\tau \parallel H$, i.e. the longitudinal susceptibility is greater than the transverse, and was observed by Cable and Koehler.[3] For H $\sim$15 kOe we believe fluctuations in the arrangement of the ferromagnetic (001) sheets leads to a lack of long-range coherence and the resulting loss of antiferromagnetic intensity. A sharp rise in the ferromagnetic component occurs at this field. For 18 <H <47.5 kOe both the (110) and (11 1/2) reflections are present, as well as a ferromagnetic component of 1.05 μ_B/Ce atom. No intensity was observed at the (210) or (2 1/2 0) positions. A combination of these modulations leads to the conclusion that the spin configuration is a 3+, 1- sequence of the ferromagnetic (001) sheets. For H=47.5 kOe the 3+, 1- structure collapses, leading to a totally induced ferromagnetic state with 2.1 μ_B/Ce atom.

b)Type I phase, 12.5 <T <25 K.

Figure 1 (right hand side) shows the field dependence of the (110) and (11 1/2) reflections, together with the ferromagnetic component at 14 K. In contrast to the low temperature behavior, the transverse susceptibility in the type I phase is greater than the longitudinal (as one expects for an antiferromagnet) and the (110) decreases as H increases. For H between 10 and 17 kOe the behavior is complex, and, we believe, represents both the domain reorientation effects and the inherent instability of the I and IA structures in the presence of an applied field. This behavior extends over a wider field range as the temperature is increased towards T_N (25 K). The lack of any magnetic intensity at the (210) or (2 1/2 0) positions eliminates the possibility of a canted spin arrangement. For

17.5 <H <47.5 kOe the 3+, 1- configuration is again present. The critical field for induced ferromagnetism shows little temperature dependence for T <20K, in agreement with magnetization results.

X-ray experiments

We have examined the behavior of the lattice parameter of CeBi at low temperature with X-ray diffraction from the (800) planes of a single crystal. The results are shown in Fig.2. A careful search for a lattice distortion in the ordered state gave an upper limit of $|(c-a)/a| < 1 \times 10^{-4}$ for any tetragonal distortion. As the figure shows, on warming through the IA-I transition (12.5K) the relative volume discontinuity associated with the first-order transition is $(8 \pm 1) \times 10^{-5}$. The thermal expansion in the type I magnetic phase is first positive (T <20 K) then negative for T >20 K. The lattice parameter at 5K is 6.4873 (1) Å. The change in the lattice parameter between 25 and 30K represents a linear expansion coefficient of 7×10^{-6}/°K.

DISCUSSION

The experiments reported here confirm the 3+, 1- configuration for the intermediate field state in CeBi as first suggested by Tsuchida and Nakamura.[9] In fact their phase diagram is in excellent agreement with our results and we present a modified phase diagram with all the magnetic structures defined in Fig. 3. The dashed lines represent boundaries that have not been experimentally verified. The variations in the intensities of the (110) and (11 1/2) at low fields (see Fig.1) arise from domain reorientation effects and/or the instability of the I and IA phases to the application of a magnetic field and, as such, are not represented in the phase diagram. For H> 47.5 kOe and T< 25 K the correct description of the phase is paramagnetic rather than the "induced ferromagnetism" used in the literature.[9] However, the anisotropy in this state is considerable, and the spins cannot be rotated significantly away from the cube axis.[5,6] As discussed by Cooper et al.[5] the easy direction for the mements in CeBi should be <111> if the crystal field is the dominant interaction. Direct measurements of the crystal-field splittings in CeBi have found them to be small[10] so that it is more likely that the exchange interactions define the easy axis of magnetization.

The mechanism that stabilizes the IA magnetic structure remains a mystery. Particularly since <u>no</u> distortion, which would allow the introduction of an additional term in the free energy, is observed at the I - IA transition at 12.5 K. The close analogy between the uranium compounds with the I and IA structures[4] (and their unusual behavior in a magnetic field) and CeBi is even more striking when one recalls that these uranium compounds, like CeBi, maintain cubic symmetry below their respective ordering temperatures.[11]

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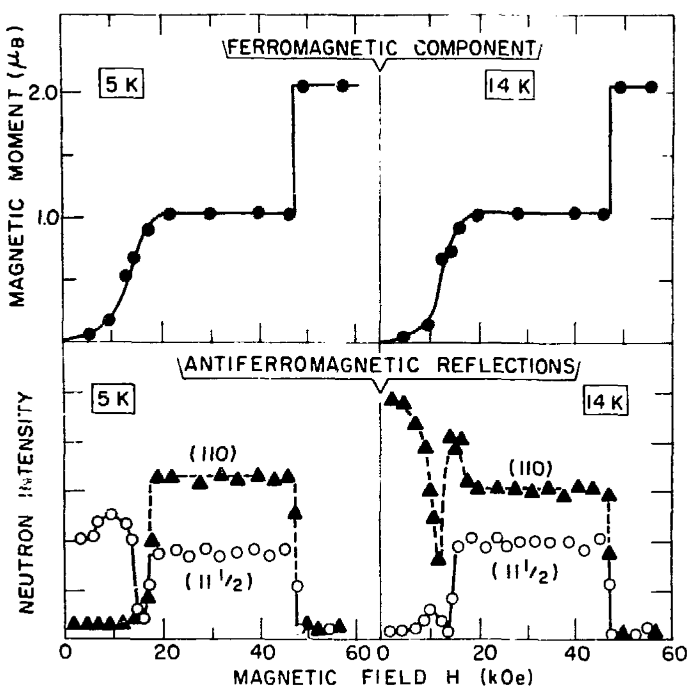

Fig. 1. Variation of ferromagnetic component (upper portion) and (110) and (11½) antiferromagnetic reflections (lower portion) in type IA (5 K) and type I (14 K) phases as a function of magnetic field.

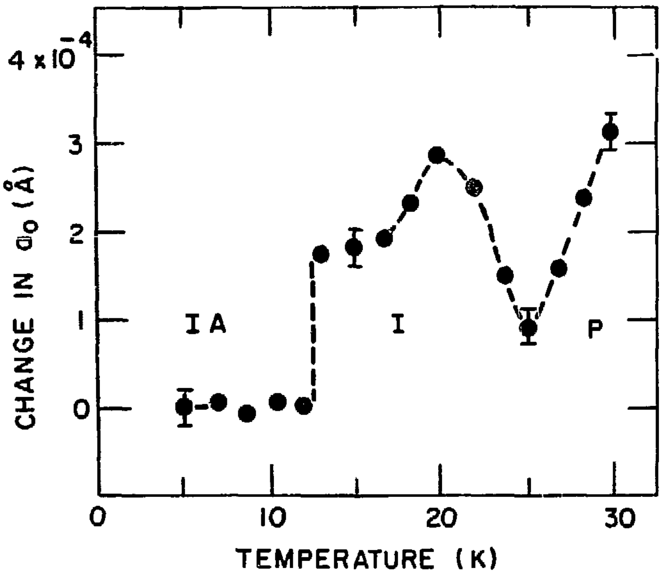

Fig. 2. Change of lattice parameter (relative to value of 6.4873 Å at 5 K) of CeBi as a function of temperature.

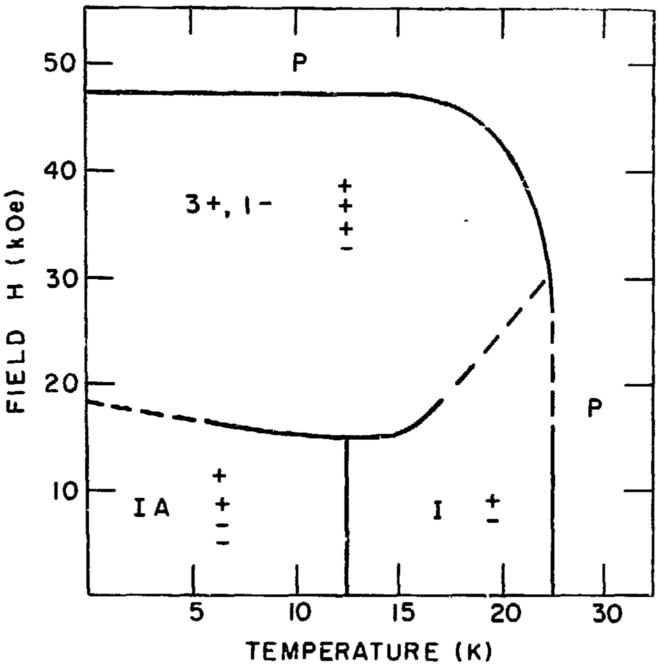

Fig. 3. Phase diagram for CeBi.