MAGNETIC *P–T* PHASE DIAGRAMS OF CeSb AND CeBi*

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Neutron diffraction experiments on CeSb and CeBi under high pressure up to 4.6 GPa revealed the new features of the magnetic P–T phase diagrams. The development of each magnetic phase corresponds to the unusual enhancement of the electrical resistivity or the shrinking of the crystal lattice. The phase diagram of CeSb above about 2 GPa is very similar to that of CeBi above ambient pressure.

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1. Introduction

The heavier Ce-monopnictides, CeSb and CeBi exhibit highly unusual and anisotropic magnetic properties as well as Kondo-effect like transport properties in spite of their simple NaCl-type crystal structures and low-carrier-density [1]. The magnetic properties of these compounds were mainly explained by a fundamental microscopic analysis based on the anisotropic p–f mixing effect between the Ce $4f$ electrons and the neighboring pnictogen $5p$ valence-holes with Γ_8 symmetry [2]. CeSb is well known with its complicated magnetic phase diagrams below 2 GPa or 10 T revealed by the extensive neutron diffraction studies [3]. Magnetic structures consist of a

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stacking of ferromagnetic (001) planes with a given sequence. The magnetic moments, which are perpendicular to the ferromagnetic planes, are originated from Γ_8-like state of Ce-ions with the moment of 2 μ_B. Non-magnetic (001) planes with the Γ_7 Ce-ions appear in the so-called AFP phases below 1 GPa. The developments of high pressure techniques on the measurement of transport properties revealed new features of the phase diagram of CeSb up to 8 GPa [4]. A huge enhancement and a sharp drop of the resistivity appear at T_H and T_L above about 2 GPa. This brought forward new problems to be solved, that is, the apparent discrepancy of the phase diagram at around 2 GPa, or whether the magnetic orders exist or not above 2 GPa. On the other hand, in contrast to CeSb case, there have been few reports on the P–T phase diagram of CeBi so far. Nevertheless, the resistivity data show an unusual hump and an inflection point at T_H and T_L, and give the similar phase diagram to that of CeSb above about 2 GPa. Thus, systematic neutron diffraction studies beyond 2 GPa are inevitable to confirm the P–T phase diagrams of these compounds. In this paper, we briefly present our neutron diffraction studies up to 4.6 GPa.

2. Neutron diffraction studies of the magnetic phase diagrams

The neutron diffraction experiments were carried out on the triple-axis spectrometer TAS-1 installed at 2G beam port in JRR-3M reactor in JAERI, Tokai. The high pressure was produced by the conventional piston-cylinder clamp-type cell(McWhan cell) below about 3 GPa and by the newly developed anvil-type cell, in which sapphire or moissanite(single crystal SiC) were used as opposite anvils, above about 3 GPa.

Fig. 1 shows the P–T phase diagram of CeSb obtained in this work together with the data of the previous neutron diffraction [3], the resistivity measurements [4] and X-ray diffraction [5]. Below 1 GPa, the lowest temperature phase AF-IA with the stack ($\uparrow\uparrow\downarrow\downarrow$), all the AFP phases and the highest temperature phase AF-I with the ($\uparrow\downarrow$) are confirmed in our measurements. The transition temperatures are identical with that in ref. [3]. However, above 1 GPa, AF1 and AF2 phases exist in very narrow temperature ranges and disappear at about 2 GPa. Furthermore, $T_{\mathrm{AF-IA}}$ and $T_{\mathrm{AF-I}}$ shift to considerably higher temperatures of 31 K and 38 K. Above 2 GPa, AF-I and AF-IA phases were clearly observed as higher and lower temperature phases. The new phase boundaries of $T_{\mathrm{AF-IA}}$ and $T_{\mathrm{AF-I}}$ are smoothly connected through the all P–T area investigated in this work. These results solve the problems mentioned above. Fig. 2 shows the P–T phase diagram of CeBi together with the resistivity data. In marked contrast to CeSb case, the phase diagram consists of only two magnetic phases AF-I and AF-IA. The lower temperature phase AF-IA disappears at around 2 GPa.

As shown in Fig. 1 and Fig. 2, AF-I phase clearly relates to the unusual enhancement of the resistivity at T_{H} and the development of AF-IA phase leads to the rapid decrease of the resistivity at T_{L}. These results indicate that the mechanism of the carrier scattering or the carrier number itself is highly different between the two magnetically ordered phases. The sudden shrinking of the crystal lattice is observed at T_{S}, which agrees well with T_{H}. The origin of this shrinking is clearly evidenced by the direct observation of the modulation of 4f electron orbital on CeSb [6]; the planes with the Γ_8-like state of Ce-ions, which have small effective ionic size due to the p–f mixing effect, appear in the lattice of Ce ions with Γ_7 CEF ground state.

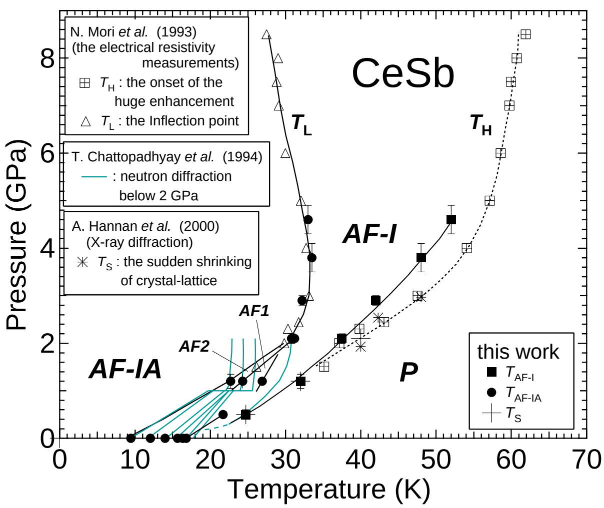

Fig. 1. The magnetic P–T phase diagram of CeSb.

It should be pointed out that in CeSb non-magnetic Γ_7 planes disappear at about 1 GPa and the phase diagram above 2 GPa bears a close resemblance to the phase diagram of CeBi above ambient pressure, which has no non-magnetic plane. As pointed out for lighter monopnictides CeP and CeAs in Ref. [7, 8], this behavior is probably understood in terms of the common physical basis for the whole Ce-monopnictides system. In this idea, although the difference of the CEF splittings or pnictgen atoms between the compounds should be considered, the carrier density can be a common physical parameter. That is, the application of pressure increases the carrier density. As a result of this, the p–f mixing effect is highly enhanced. Indeed, the carrier number are estimated to be about 0.04 and 0.06 per Ce for CeSb and CeBi, respectively [9] and the calculated energy gain of the p–f mixing effect in CeBi is much larger than that in CeSb [2]. However, the future development of theoretical works is highly desired to elucidate the

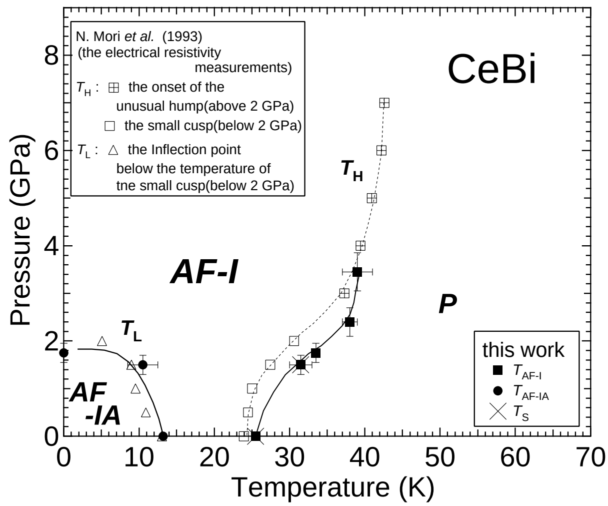

Fig. 2. The magnetic P–T phase diagram of CeBi.

problems such as the correspondence between the unusual enhancement of the resistivity and the magnetic orders, or the strong stabilization of the AF-I phase by applied pressure in spite of the small difference of the energy between the AF-I and the AF-IA phases at ambient pressure [2].

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