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**Low temperature magnetism in YbPtBi
by ^{170}Yb Mössbauer spectroscopy**

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We report on ^{170}Yb Mössbauer spectroscopy data in the cubic *fcc* alloy YbPtBi, in the temperature range 0.06 - 30 K. The zero field spectra show a two component structure above 1.5 K, which can be analysed as due to 85% of Yb^{3+} ions at a site with cubic symmetry and 15% at a site with non-cubic symmetry. Below 0.3 K, the spectra are resolved and can also be interpreted in terms of two sites, but with a dominant non-cubic site ($\sim 60\%$) with Yb ions bearing small magnetic moments. The spectra with a large applied magnetic field give information on the Yb^{3+} C.E.F. level scheme and on the exchange interaction. The relation of the Mössbauer data with the results of μSR measurements is discussed.

Keywords: Yb intermetallics, magnetic ordering, Mössbauer spectroscopy.

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The intermetallic compound YbPtBi, crystallising into a cubic *fcc* structure (MgAgAs type), has recently attracted much interest due to its intriguing low temperature properties. The specific heat shows a small peak at 0.45 K, attributed to a magnetic transition, and the ratio C/T reaches very high values ($8 \text{ JK}^{-2}\text{mol}^{-1}$ at the lowest temperature) [1]. Subsequent work tried to unravel the problem of the Yb^{3+} ground state [2-4]. Zero field μSR experiments [3] give evidence for the coexistence of spin-glass like and paramagnetic domains in the sample below 0.5 K, in roughly equal proportions; the inferred magnitude of the Yb^{3+} magnetic moment in the spin-glass domains is $0.1 \mu_B$. In the present work, we report on a Mössbauer spectroscopy study, on the isotope ^{170}Yb ($E_0=84 \text{ keV}$, $I_g = 0$, $I_e=2$), of a polycrystalline YbPtBi sample, grown by a Bi flux method, in the temperature range 0.06 - 30 K, in magnetic fields from 0 to 7 T.

The spectrum at 4.2 K in zero field, represented in figure 1a, shows the presence of two components: a rather broad single line and a split symmetrical spectrum. The single line corresponds to a Yb^{3+} ion at a cubic site, whereas we interpret the split spectrum as a three line hyperfine quadrupolar spectrum due to a Yb^{3+} ion at a low symmetry site, with a relative weight of 15(2)%. The quadrupolar moment tensor of the Yb^{3+} ion at this latter site is such that: $Q_{ZZ} = -Q_{XX}$, $Q_{YY} = 0$, with the rather large value: $Q_{ZZ} \simeq 14$. It is striking to observe that the unique Yb site in the isostructural compound YbPdBi has very similar characteristics (figure 1b).

Figure 1: Zero field ^{170}Yb Mössbauer absorption spectra at 4.2 K in YbPtBi (a) and YbPdBi (b).

In YbPtBi this low symmetry quadrupolar component is resolved between 1.5 and 30 K, with a slowly decreasing weight (7% at 30 K). It is rather surprising to find such a low symmetry site in cubic compounds. The regular Yb site in YbPtBi and YbPdBi

is the cubic tetrahedral ($1/4 \ 1/4 \ 1/4$) site; the occurrence of a non-axial quadrupolar spectrum means that the Yb ion lies at a strongly distorted site. It is worth noticing that the weight of the low symmetry site above 1.5 K ($\sim 15\%$) is the same as that of the “fast” component observed in the μ SR spectra of YbPtBi above 1 K [3].

The spectrum at 0.06 K in zero field is shown in figure 2a. A possible interpretation is to assign this spectrum to a magnetic hyperfine interaction, with a hyperfine field of 125 T, corresponding to a spontaneous Yb^{3+} moment of $1.25 \mu_B$. An alternative interpretation, more coherent with that of the 4.2 K spectrum, assigns this spectrum to a superposition of a very broad single line, corresponding to paramagnetic Yb^{3+} ions at a cubic site, and of a low symmetry quadrupolar spectrum, similar to that at 4.2 K, but with a higher relative weight of $\sim 60(5)\%$ and a much broader right-side line. The broadening of this line is compatible with the presence of a distribution of small hyperfine fields of a few 10 T, corresponding to Yb^{3+} magnetic moments of a few $0.1 \mu_B$. At 0.4 K, the weight of this low symmetry component has decreased to $\sim 20\%$.

Figure 2: ^{170}Yb Mössbauer absorption spectra in YbPtBi at 0.06 K in zero field (a) and in a field of 7 T (b).

This interpretation strengthens the identification of the sample domains giving rise to the “fast” μ SR component with the regions where the Yb ion lies at a non-cubic site: the thermal variation of the size of these domains is very similar in both types of measurements, except around 0.5 K where the μ SR derived weight is $\sim 50\%$ vs 20% with Mössbauer spectroscopy. As to the cubic spectral component, its large width indicates the presence of Yb^{3+} paramagnetic fluctuations down to the lowest temperature. The measured Yb^{3+} fluctuation frequency $1/T_1$ is constant and equal to 2 GHz below 1 K. In terms of single ion Kondo fluctuations, this gives the small Kondo temperature:

$$k_B T_0 \sim h/T_1 \simeq 0.1 \text{ K}.$$

The spectra at 0.06 and 4.2 K in high magnetic field ($H \geq 1.5 \text{ T}$) are characteristic of a Yb^{3+} ion having a low lying Γ_8 quartet, with line broadenings showing the presence of sizeable axial distortions of the Yb cubic site. They consist of two lines (figure 2b), expected when the magnetic moment, hence the hyperfine field, is parallel to the applied field. In these high field spectra, there is no hint of the presence of Yb ions at a non-cubic site whereas at low fields (0.5 and 1 T) at 4.2 K the low symmetry spectral component is present. At 0.06 K the spectra for 0.4 and 1 T show five lines, which is characteristic of a cubic Yb^{3+} ion in the presence of an antiferromagnetic (AF) exchange interaction, when the applied field is too small to align the magnetic moments along its direction. As alignment occurs for $H_a = 1.5 \text{ T}$, the exchange field magnitude is $H_{\text{ex}} \sim H_a/2 = 0.75 \text{ T}$.

The magnetisation curve at 0.35 K, taken from ref.2, together with the Mössbauer derived magnetic moment values at 0.06 and 4.2 K, are represented in figure 3.

Figure3: Magnetisation (from ref.2) and Mössbauer derived moment values as a function of magnetic field in YbPtBi.

When the magnetic moments are not aligned along the external field direction, the Mössbauer technique yields the magnitude of the moment, whereas the magnetisation data yields its projection onto the field direction. The Mössbauer derived moment values at 0.06 K interpolate smoothly with the magnetisation data at 0.35 K for a field of 1.5 T, confirming that the alignment of the AF structure along the field direction occurs for this field value. The moment value extrapolated to zero field at 0.06 K is $m_0 \simeq 1.4 \mu_B$ which is the expected value for the spontaneous moment of a Γ_6 C.E.F. ground state. Then the exchange energy scale is: $E_{\text{ex}} = m_0 H_{\text{ex}} \sim 0.7 \text{ K}$, which is close to

$T_N = 0.45$ K, and the (assumed isotropic) molecular field constant: $\lambda \simeq -0.4$ T/ μ_B . Using the above information, we tried to derive the cubic C.E.F. level scheme of the Yb^{3+} ion from the magnetisation curves. The solid and dashed lines in fig.3, as well as the theoretical spectrum in fig.2b, are calculated using $\lambda = -0.3$ T/ μ_B and the following level scheme: Γ_6 ground state, Γ_8 at 16 K and Γ_7 at 75 K. The agreement is satisfactory and the derived C.E.F. scheme agrees qualitatively with the inelastic neutron scattering data [5].

To summarise, the ^{170}Yb Mössbauer spectroscopy data in YbPtBi show the presence of two kinds of Yb sites: a cubic site and a low symmetry site, probably distributed in domains. The occurrence of the low symmetry Yb environment could be due to a Jahn-Teller distortion, linked to the presence of a low lying Γ_8 state; in the isostructural compound YbPdBi , the ^{170}Yb Mössbauer data have shown that all the Yb sites are of the low symmetry type. In YbPtBi , the importance of the distorted site domains is strongly diminished by increasing temperature or magnetic field, suggesting that this compound is at the verge of a Jahn-Teller instability. Below 0.3 K, the Mössbauer data can be interpreted in a way that confirms and extends the μSR results: 60% of the Yb ions are at the low symmetry site and bear small magnetic moments ($<0.5 \mu_B$), whereas the Yb ions at the cubic sites remain paramagnetic down to 0.06 K and fluctuate with a frequency 2 GHz. The Mössbauer data with a magnetic field could give an estimation for the exchange energy scale (0.7 K) and for the AF molecular field constant (-0.3 T/ μ_B).

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