Proc. 14th Int. Conf. on Muon Spin Rotation, Relaxation and Resonance (μSR2017)
JPS Conf. Proc. **21**, 011029 (2018)
https://doi.org/10.7566/JPSCP.21.011029

Origin of the Multi-Peak Muon Frequency Spectrum in the Heavy Fermion Compound UBe_{13}

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(Received June 22, 2017)

Transverse-field muon spin rotation (TF-μSR) experiments have been carried out on an oriented mosaic of UBe_{13} single crystals as a function of temperature and crystal orientation with respect to an applied magnetic field. The observed frequency splittings are consistent with dipolar fields from the paramagnetic U^{3+} moments and an anisotropic hyperfine interaction with the muons stopping midway on the edges of the cubic uranium sublattice. The disappearance of the splittings above 180 K is attributed to rapid muon diffusion. We find no evidence of a spin polaron bound to the muon in UBe_{13}

KEYWORDS: μSR, UBe_{13}, dipolar field, paramagnetic, orientation

1. Introduction

UBe_{13} is a heavy-fermion superconductor ($T_c = 0.87$ K), where the U^{3+} ions form a simple cubic structure with a large lattice constant of 5.134 Å [1]. This leads to a very narrow conduction band with 5f-electron character, which is believed to be responsible for the heavy-fermion behavior. As expected from the resulting high density of states at the Fermi energy, there is a large muon Knight shift [2, 3]. The TF-μSR lineshapes exhibit two sample peaks with a large frequency splitting, which has been attributed to the dipolar interaction with the paramagnetic U^{3+} ions [4]. The amplitude ratio of the two peaks is close to 2:1 for a magnetic field applied along the [001] direction. This is consistent with the muon stopping site being located midway on the edge of the U^{3+} cubic sublattice, for which there are two magnetically inequivalent sites with θ=90° and θ=0°, where θ is the angle between the local 4-fold axis of symmetry and the applied magnetic field. Recently another interpretation of the TF-μSR frequency splitting in UBe_{13} was proposed [5] based on a model for magnetic polarons [6]. In this model, neighboring U^{3+} moments are strongly coupled to form giant ferromagnetic spin clusters and that the observed frequency splittings below 180 K are attributed to the opening of a spin gap.

In order to determine the correct interpretation of the frequency splitting, we have measured the temperature and orientation dependence of a mosaic of UBe_{13} single crystals at 15 kOe with TF-μSR. We show the angular dependence of the spectra is consistent with an anisotropic interaction originating from the dipolar fields from the neighboring U^{3+} moments including a correction due to the anisotropic part of the Knight shift, which has the same angular dependence. Furthermore, the disappearance of the splitting above 180 K is then almost certainly due to muon diffusion which averages out such dipolar fields. If there is a spin gap opening at this temperature, it is coincidental with the onset of muon diffusion.

2. Experiment

The sample is an oriented mosaic pieced together from 4 single crystals (as shown in Fig. 1), with approximate dimensions of 15 mm ×15 mm ×1 mm along the a, b, and c axes, respectively. The TF-μSR measurements were performeded at $T \geq 3$ K where the sample is in the paramagnetic state. A field of 15 kOe was applied in the [001], [$\sqrt{3}$01], [101], and [111] directions. Assuming the muon

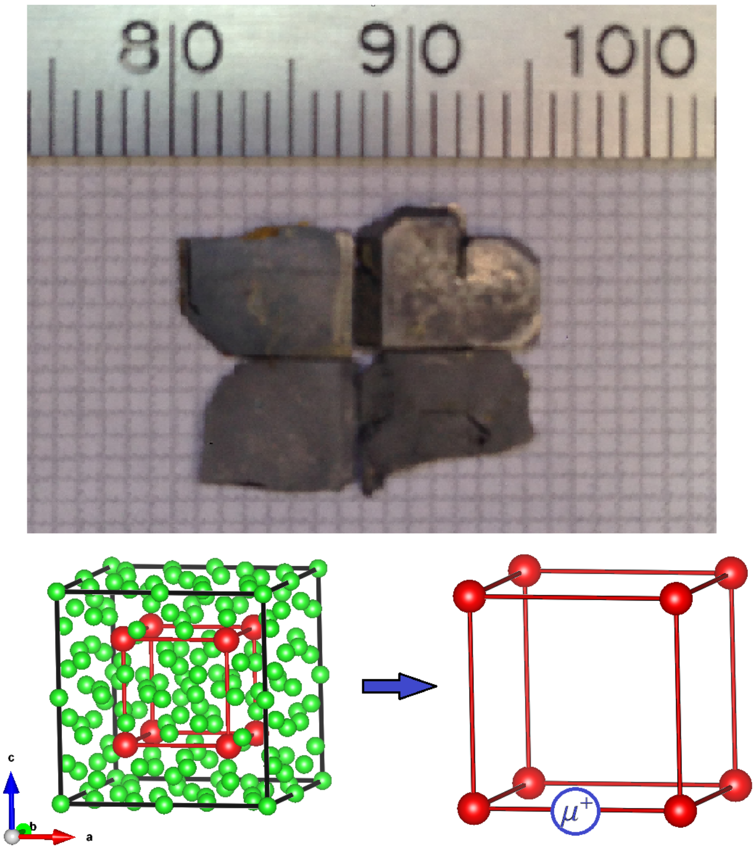

Fig. 1. Top: Mosaic of UBe_{13} single crystals on a millimeter grid. Bottom: UBe_{13} unit cell and the U^{3+} sublattice with the proposed μ^+ site, which is midway between the U^{3+} on the cube edge.

site proposed in [4] (see Fig. 1), magnetic dipolar field calculations were carried out for the cubic U^{3+} sublattice to reconstruct the TF-μSR frequency spectra. The Hamiltonian considered is

$$\mathscr{H} = -\gamma_n \mathbf{I} \cdot \mathbf{H}_0 - \gamma_n [\mathbf{I} \cdot \overleftrightarrow{\mathrm{K}} \cdot \mathbf{H}_0] - \gamma_n \mathbf{I} \cdot \mathbf{H}_{\mathrm{dip}} \tag{1}$$

where $\gamma_n = \mu_B g/\hbar$, μ_B is the Bohr magneton, and g is the g-factor. The first term is due to the Zeeman interaction between the muon spin $\mathbf{I}$ and the applied magnetic field $\mathbf{H}_0$. The second term is due to the hyperfine interaction described by the second-rank Knight shift tensor $\overleftrightarrow{\mathrm{K}}$, which includes both isotropic and anisotropic terms, $\overleftrightarrow{\mathrm{K}} = \overleftrightarrow{\mathrm{K}}_{\mathrm{iso}} + \overleftrightarrow{\mathrm{K}}_{\mathrm{ani}}$. The last term is due to the classical magnetic dipole interaction between the muon and the U^{3+} moments, which is calculated as follows

$$\mathbf{H}_{\mathrm{dip}} = \sum_i \left(\frac{3(\boldsymbol{\mu}_i \cdot \mathbf{r}_i)\mathbf{r}_i}{r_i^5} - \frac{\boldsymbol{\mu}_i}{r_i^3} \right) \tag{2}$$

where r_i is the distance between the muon site and the U^{3+}moment at site i with a magnetic moment of $\boldsymbol{\mu}_i$. In this paper, a finite-size lattice calculation is implemented, which doesn't employ a Lorentz sphere. Therefore, the dipolar field calculated here includes both the dipolar field and Lorentz field due to U^{3+} moments inside and outside of the Lorentz sphere, respectively, and the demagnetization field that is typically distinguished in the literature.

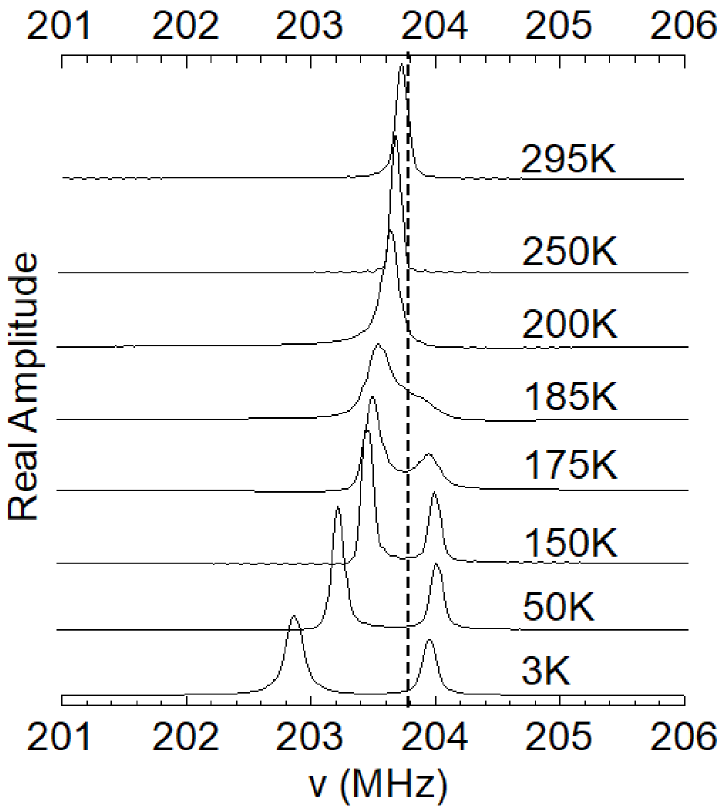

Fig. 2. Temperature dependence of the fast Fourier transform of the TF-μSR spectra for UBe_{13} in a field of 15 kOe applied parallel to the [001] direction. The dotted line indicates the precession frequency ν of the muon in pure silver.

3. Results

Figure 2 shows the temperature dependence of the TF-μSR lineshape at 15 kOe. The observed frequency splitting is similar to that previously reported [2–4]. By removing the isotropic part of the Knight shift and the demagnetization field, which is given by the difference between the precession frequency of the muon in the applied magnetic field (estimated from the precession frequency of the muon in an Ag reference sample) and the average precession frequency of the UBe_{13} TF-μSR spectra, the TF-μSR spectra for various field orientations can be reproduced by a magnetic dipolar calculation using Eq. (2) [see Fig. 3]. Note that each peak frequency in Fig. 3 is indexed by the angle θ between the 4-fold symmetry axis the muon sits on and the applied field. The observed splittings are about 38.5 % smaller than expected, assuming each U^{3+} ion carries a moment equal to 0.0426 μ_B from bulk magnetization [4, 7–9]. This can be explained by an anistropic component of the Knight shift, which has the same orientation dependence as the magnetic dipolar field from the localized U^{3+} ions. The frequency shift from the anisotropic Knight shift is assumed to have an opposite sign to the frequency shift produced by the magnetic dipolar field and is estimated to be $K_{\rm ani} = 0.113\left(1 - 3\cos^2\theta\right)$.

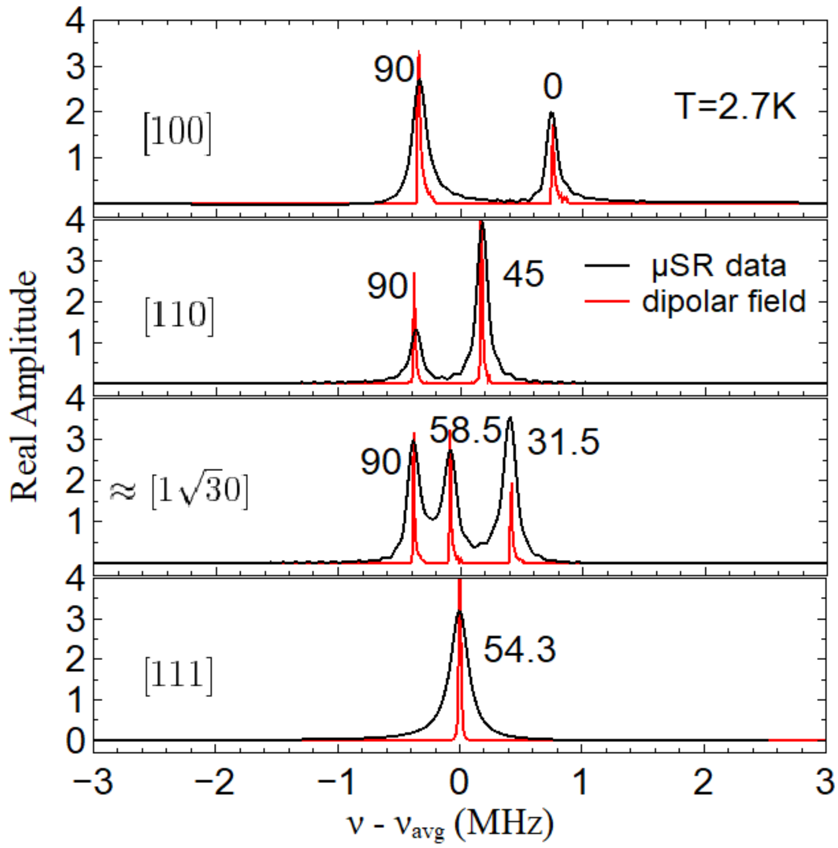

Fig. 3. TF-μSR frequency spectra (black) compared to the magnetic dipolar field calculated spectra (red) for various crystal orientations with respect to the applied field. Note that $\nu_{\rm avg}$ corresponds to the average precession frequency.

4. Conclusion

We have demonstrated that the observed frequency splittings arise from the magnetic dipolar field at the muon stopping site generated by the field-induced spin polarized U^{3+} moments. The splittings disappear above 180 K which is most likely due to the onset of muon diffusion. There is no evidence of a giant moment from a spin polaron bound to the muon or a spin gap opening at 180 K in

UBe_{13} given the average precession frequency (and thus the isotropic part of the Knight shift and the demagnetization field together) varies smoothly through this temperature region for each orientation of the applied magnetic field.

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