^{11}B NMR study in the tetragonal CeB_2C_2 compound

Ko-ichi Magishi [a,1], Kuniyuki Koyama [a], Takahito Saito [a], Kiyoshi Mizuno [a], Ryuta Watanuki [b], Kazuya Suzuki [b]

[a] *Faculty of Integrated Arts and Sciences, The University of Tokushima, Tokushima 770-8502, Japan*
[b] *Graduated School of Environment and Information Sciences, Yokohama National University, 79-5 Tokiwadai, Hodogaya-ku, Yokohama 240-8501, Japan*

Abstract

We carried out the ^{11}B NMR experiments of CeB_2C_2 and determined the parameters of the electric field gradient and the components of the hyperfine coupling constants at ^{11}B nucleus site in order to elucidate the magnetic properties. The nuclear quadrupole frequency and the asymmetry parameter are estimated to be $\nu_Q = 0.78$ MHz and $\eta = 0.22$. The hyperfine coupling constants are highly anisotropic and are deduced to be $A_X = +0.39$ kOe/μ_B and $A_Y = -0.51$ kOe/μ_B. From the analysis, the anisotropic hyperfine coupling can be explained by the atomic dipolar field from the 4f electrons.

Key words: CeB_2C_2; ^{11}B NMR; antiferromagnetic transition

1. Introduction

RB_2C_2 (R = rare earth) has been attracting a great deal of interest, because the multipolar ordering and interaction play key roles in the magnetic properties. One of the isostructural compounds, CeB_2C_2, undergoes magnetic transitions to the antiferromagnetic (AFM) phases at $T_{N1} = 7.3$ K and $T_{N2} = 6.5$ K[1]. From the measurements of the magnetic susceptibility and the magnetization, it is shown that the Ce moments align in the *c*-plane in the AFM state[1]. Also, from the neutron scattering experiment at zero field[2], it is indicated that the magnetic structure has a long periodicity and can be described by the propagation vector k = [0.161 0.161 0.10], which is suggested to be a screw structure. But, it has not been made clear about the reason why the magnetic structure is so complicated, although there are no evidence for magnetic properties related to quadrupolar ordering and even for properties affected by quadrupolar interaction in CeB_2C_2. Thus, further studies are indispensable to clarify the magnetic properties, where an experiment by a microscopic probe is important. The nuclear magnetic resonance (NMR) technique has provided useful information on the magnetic state of the compound.

In this paper, we determined the parameters of the electric field gradient and the components of the hyperfine coupling constants at ^{11}B nucleus site of CeB_2C_2 from the ^{11}B NMR experiments in order to clarify the magnetic properties from the microscopic viewpoint.

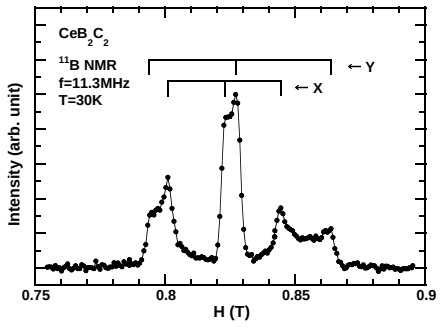

Fig. 1. ^{11}B NMR spectrum of the powder sample of CeB_2C_2 at 11.3 MHz and 30 K.

[1] E-mail:magishi@ias.tokushima-u.ac.jp

2. Results and Discussion

Figure 1 shows the ^{11}B NMR spectrum of the powder sample of CeB_2C_2 at 11.3 MHz and 20 K. In the external magnetic field, the grains are easily aligned in c-plane because of the highly anisotropic susceptibilities. As the field direction is random in c-plane, the spectrum shows the two-dimensional powder pattern in c-plane with satellite lines due to the electric quadrupole interaction, because I=3/2 for ^{11}B nucleus. If we take the principal axes of the electric field gradient (EFG) tensors to be $|V_{XX}| \leq |V_{YY}| \leq |V_{ZZ}|$, the values of each component are determined as $|\nu_X| = 0.30$ MHz and $|\nu_Y| = 0.47$ MHz from the difference between the resonance fields for each pair of satellite lines, because the maximum principal axis ($= Z$) of the EFG tensors is along the c-axis. Here, $\nu_\alpha = eQV_{\alpha\alpha}/2h$, $V_{\alpha\alpha}$ is the α component of EFG, and Q is the nuclear quadrupole moment. Also, ν_Z is estimated to be 0.77 MHz from the formula as $\nu_X + \nu_Y + \nu_Z = 0$, and the asymmetric parameter is obtained to be $\eta = (V_{XX} - V_{YY})/V_{ZZ} = 0.22$. The remarkable feature is that the EFG at the ^{11}B site is rather asymmetric. Also, the nuclear quadrupole frequency is deduced to be $\nu_Q = \nu_Z(1 + \eta^2/3)^{1/2} = 0.78$ MHz. These values are almost the same as those of other RB_2C_2 compounds, such as NdB_2C_2[3].

Figure 2 shows the T dependences of the shift, $\delta = (H_0 - H_{res})/H_{res}$. This shift is composed by the Knight shift and the quadrupolar shift. As the principal values of the EFG tensors are found to be almost T independent, the quadrupolar shift is T independent. Thus, the T dependence of this shift is originated from the spin Knight shift, which is related to the magnetic susceptibility χ[4], as shown in the inset of Fig. 2.

Figure 3 shows the plot of the shift against the susceptibility χ above 30 K with temperature as an implicit parameter. The linearity indicates that the shifts are found to be proportional to χ. The hyperfine coupling constants at ^{11}B site are obtained from the $\delta - \chi$ plots. On the assumption that the hyperfine coupling constants at the B sites, defined by $A_\alpha = N_A \mu_B d\delta_\alpha/d\chi_\alpha$, are due to the Ce 4f electrons, A_α's are deduced from the slopes $d\delta_\alpha/d\chi_\alpha$, where N_A and μ_B are the Avogadro's number and the Bohr magneton, respectively. From the analysis, we obtained as $A_X = +0.39$ kOe/μ_B and $A_Y = -0.51$ kOe/μ_B. As A_Z is obtained as -1.00 kOe/μ_B[5], the isotropic and anisotropic hyperfine coupling constants are deduced as $A_{iso} = -0.37$ kOe/μ_B and $A_{ani} = +0.38$ kOe/μ_B, from the formula as $A_{iso} = (A_X + A_Y + A_Z)/3$ and $A_{ani} = (A_X - (A_Y + A_Z)/2)/3$. A_{ani} agrees in order of magnitude with that calculated by the dipole field due to surrounding Ce ions (+0.40 kOe/μ_B). Therefore, it may be concluded that the dominant contribution for the hyperfine coupling is the atomic dipolar field.

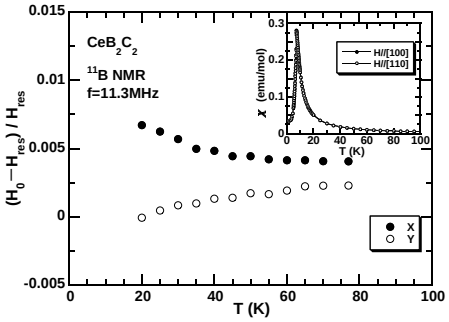

Fig. 2. T dependences of the shift, $\delta = (H_0 - H_{res})/H_{res}$. Inset shows the T dependence of the magnetic susceptibility, χ.

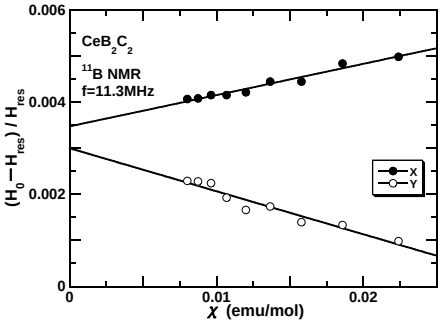

Fig. 3. The plot of the shift, $\delta = (H_0 - H_{res})/H_{res}$, against the susceptibility, χ, with temperature as an implicit parameter.

3. Summary

The ^{11}B NMR experiments on CeB_2C_2 are carried out, and the parameters of the EFG and the components of the hyperfine coupling constants at ^{11}B nucleus site are determined in order to get the microscopic information for the magnetic properties. The values of the EFG tensors are determined as $|\nu_X| = 0.30$ MHz and $|\nu_Y| = 0.47$ MHz. The hyperfine coupling constants are obtained to be $A_X = +0.39$ kOe/μ_B and $A_Y = -0.51$ kOe/μ_B. Also, the isotropic and anisotropic hyperfine coupling constants are deduced as $A_{iso} = -0.37$ kOe/μ_B and $A_{ani} = +0.38$ kOe/μ_B. A_{ani} agrees in order of magnitude with that expected from the dipole field due to surrounding Ce ions, suggesting that the hyperfine coupling can be explained by the atomic dipolar field from the Ce 4f electrons.

References

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