ISSN 0029-3865

CBPF-NF-054/91

ELECTRIC FIELD GRADIENT AT THE ^{59}Co NUCLEUS OF FERROMAGNETIC YCo_3*

by

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*Presented at I.C.M. Edinburgh, September 1991. To be published in J. Magn. Magn. Mat.

ABSTRACT

The structure of YCo_3 is of the $PuNi_3$ type with three inequivalent cobalt sites in the lattice. The spin echo decay of the ^{59}Co NMR at 43 MHz (18 h site) was found to have an oscillatory component, indicating an electric field gradient at the nucleus equivalent to a quadrupole splitting frequency of 210 kHz. No clear oscillations could be detected at the NMR frequencies of the 3b and 6c sites but a signal, attributed to nuclei in domain walls, was observed near 48 MHz.

1. Introduction

The intermetallic compound YCo_3 belongs to the R3m space group and has the $PuNi_3$ structure. There are three inequivalent cobalt sites (3b, 6c, 18h) which have spin (orbital) moments of 0.57 (0.16), 0.71 (0.23), 0.45 (0.02) μ_B, respectively [1-3].

The observation of the ^{59}Co NMR of YCo_3 is complicated by the high magnetocrystalline anisotropy of the material which leads to narrow domain walls of limited mobility in polycrystalline material. (At 4.2 K a field ~ 10 T is required for technical saturation [4].) Also, the Y-Co phase diagram is complicated and a sample of nominal composition YCo_3 usually contains other phases such as YCo_5 or Y_2Co_{17}.

Yoshie et al [1,2] discussed earlier NMR work on YCo_3 and, from measurements in fields up to 5.5 T, deduced that the effective field at the ^{59}Co nucleus in zero external field was +3.5, +6.1 and -4.2 T for the 3b, 6c and 18h sites respectively. They suggested that the NMR lines reported at other frequencies were not due to domain signals from YCo_3. The positive effective field (parallel to the magnetisation) at the 3b and 6c sites arises from the large contribution (65 T/μ_B) of the orbital moment relative to the spin contribution of -13T/μ_B.

Since energy band calculations suggest [5] that YCo_3, unlike YFe_3 [6], is close to a magnetic instability we are at present performing high pressure experiments on YCo_3. During preliminary experiments at atmospheric pressure we have made the first observation of an electric field gradient (EFG) at the 18h cobalt site. There was no detectable EFG at the 3b and 6c sites but an EFG was observed at ~ 48 MHz (-4.8 T).

2. Experimental

The ^{59}Co NMR spectrum of a powder sample of YCo_3 was measured at 4.2 K in zero external field using an automatic spin echo spectrometer [7] and a commercial Bruker spectrometer. The lines at 61 and 43 Mz reported earlier [1,2] were observed using RF power up to the maximum available (~ 200 W) but the lines were ~ 10 MHz wide and no definite peak was observed at 35 MHz. At low power a peak appeared in the spectrum at 48 MHz.

The transverse relaxation of the ^{59}Co NMR was measured using the usual two pulse spin echo sequence. The echo height as a function of pulse spacing at 43 and 48 MHz is shown in fig 1. The echo decay is not a simple exponential and contains an oscillatory component which is indicative of an EFG at the nucleus. In the presence of an EFG the magnitude of the spin echo following two RF pulses separated by a time τ is, ignoring relaxation, given by,

$$E(2\tau) = \sum_{r=0}^{2I-1} C(r)\cos(2\pi r\nu_m\tau + \delta_r) \qquad (1)$$

where I is the nuclear spin, C(r) and δ_r are constants and ν_m the frequency splitting due to the EFG [8]. In principle up to five harmonics could be observed due to a single EFG at the ^{59}Co nucleus but in practice only two have been observed.

In order to analyse the data shown in fig 1 in the frequency domain the technique of linear prediction by singular value decomposition (LPSVD) was employed [9,10]. The spin echo data shown in figure 1 was analysed using the LPSVD program to fit 200 points, sampled at 0.1 μs intervals, to a sum of terms of the form $A_k\cos(2\pi\nu_k + \phi_k)\exp(-t/\lambda_k)$. The value of λ_o (zero frequency) corresponds to the normal transverse relaxation time, apart from a factor of two ($T_2 = 2\lambda_o$) and the other values of λ_k represent the damping of the oscillatory components of the spin echo of frequency ν_k. The results are shown in table 1.

3. Discussion

At the highest RF power available the ^{59}Co spin echo signal of YCo_3 at 43 MHz decays with a transverse relaxation time of 71 μs and exhibits an oscillatory decay with frequencies of 206 and 410 kHz, table 1. We interpret the upper frequency, which is heavily damped, as the second harmonic produced by the quadrupole splitting of 206 kHz in agreement with equation (1). As the RF power is decreased a zero frequency component with a $T_2 \sim 10$ μs increases in importance but the value of the oscillatory component only changes slightly. The highest power signals therefore arise from the domain but a domain wall edge contribution arises as the power decreases.

In contrast to the results at 43 MHz, the frequencies and damping factors associated with the 48 MHz line are strongly dependent on RF power. There is a significant zero frequency component with short, ~ 5-8 μs, transverse relaxation and the frequency of the main oscillatory component increases from 198 kHz to 323 kHz as the power is decreased. There is also a higher frequency signal at ~ 500 kHz which is not a harmonic of the lower frequency. This complicated response suggests that at the lowest RF power the 48 MHz line arises from Co atoms near the centre of a domain wall and contributions from across the wall increase with increasing RF power.

4. Conclusion

The transverse ^{59}Co NMR spin echo decay of YCo_3 supports the view [1,2] that the NMR frequency of the 18h site is 43 MHz. The electric field gradient at this site is equivalent to a frequency of 210 kHz. A line observed at 48 MHz is also due to the 18h site but arises from atoms within a domain wall.

Caption

Figure 1 The ^{59}Co NMR spin echo decay of YCo_3 at 4.2 K as a function of the RF pulse separation. At each frequency the RF power decreases from (a) to (c).

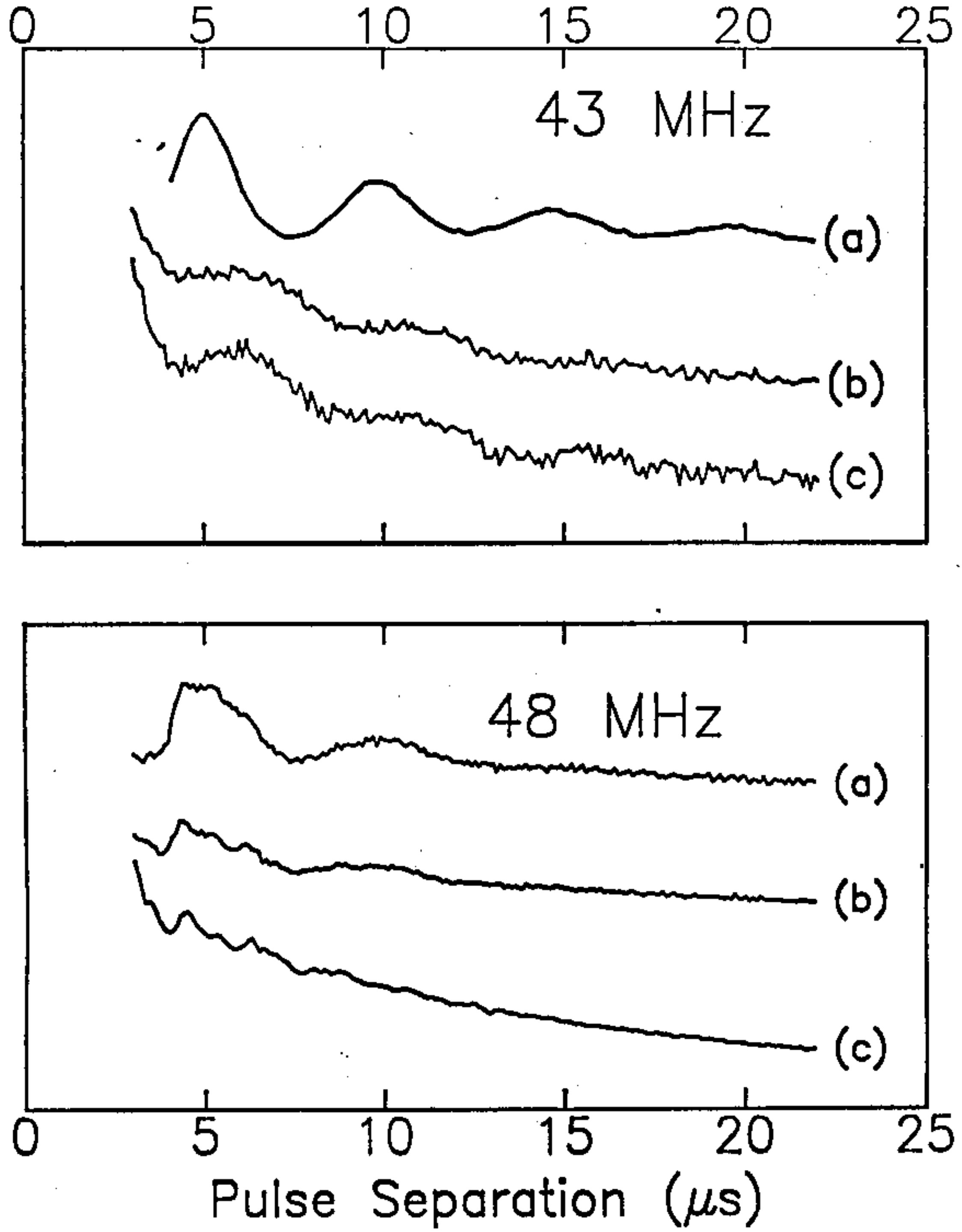
0
5
10
15
20
25
43 MHz
(a)
(b)
(c)
48 MHz
(a)
(b)
(c)
0
5
10
15
20
25
Pulse Separation (μs)

FIG. 1

Table 1

The relative amplitude (A), frequency of oscillation (ν) and damping factor (λ) derived from the LSPD analysis of the ^{59}Co NMR spin echo decays of YCo_3 shown in figure 1.

Frequency (MHz)		A	ν (kHz)	λ (μs)
43	a	100	0	35.3
		67	206	5.4
		14	410	3.6
43	b	100	0	26.2
		70	0	5.2
		22	209	5.6
43	c	100	0	6.2
		39	0	37.3
		37	233	3.8
48	a	100	0	27.5
		43	198	4.0
		15	585	1.9
48	b	100	0	29.5
		28	0	4.0
		12	223	7.0
		15	535	2.8
48	c	100	0	19.6
		22	0	2.3
		10	323	2.1
		13	500	2.4

References

1. H Yoshie, T Fuji, H Nagai, A Tsujimura and Y Nakamura, J Phys Soc Japan 54 (1985) 2725.

2. H Yoshie and Y Nakamura, J Phys Soc Japan 57 (1988) 3157.

3. F Tasset: Thesis, University of Grenoble (1975).

4. T Goto, M Yamaguchi, T Kobayashi and I Yamamoto, Solid State Commun 77 (1991) 867.

5. V L Moruzzi, A R Williams, A P Malozemoff and R J Gambino, Phys Rev B28 (1983) 5511.

6. J G M Armitage, T Dumelow, P C Riedi and J S Abell, J Phys: Condens Matter 1 (1989) 3987).

7. T Dumelow and P C Riedi, Hyp Int 35 (1987), 1061.

8. H Abe, H Yasuoka and A Hirai, J Phys Soc Japan 21 (1966) 77.

9. H Barkhuijsen, R de Beer, W M J Bovée and D van Ormondt, J Magn Res 61 (1985) 465.

10. T Dumelow, P C Riedi, J S Abell and O Prakash, J Phys F: Met Phys 18 (1988) 307.