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^{89}Y NMR STUDY OF TRANSFERRED HYPERFINE
INTERACTIONS IN YFe_2

by

K.M.B. Alves[§], N. Alves[†], A.P. Guimarães[†],
I.S. Mackenzie* and J.W. Ross*

[†]Centro Brasileiro de Pesquisas Físicas - CNPq/CBPF
Rua Dr. Xavier Sigaud, 150
22290 - Rio de Janeiro, RJ - Brazil

[§]Universidade Federal do Espírito Santo
29000 - Vitória - Brazil

*Schuster Laboratory, University of Manchester, Manchester, UK

ABSTRACT

The NMR data on ^{89}Y in $(\text{R}_x\text{Y}_{1-x})\text{Fe}_2$, where R represents Tb, Dy and Ho, is interpreted in terms of local polarisation of the Fe sublattice by the lanthanide ions.

Key-words: NMR; YFe_2 ; Hyperfine interactions.

The intermetallic compound YFe_2 crystallises in the cubic laves (C15) structure with ferromagnetic order along the $\langle 111 \rangle$ direction below the Curie temperature of 542 K [1]. Other directions of spontaneous magnetisation can be induced by small additions of lanthanide ions of appropriate anisotropy. This study extends existing work [2,3] on the nuclear magnetic resonance of ^{89}Y in YFe_2 to samples substituted on the Y site with Tb, Dy and Ho at concentrations less than 20%. The lanthanide ions have their moments antiparallel to that of the iron sublattice. Experiments in applied fields confirm that the transferred hyperfine field (THFF) set up at the Y nuclei by the iron sublattice is antiparallel to the iron moments.

The compounds were prepared under argon in an arc furnace and annealed for 150 h at 1175 K. X-ray spectra of the pseudo-binary compounds revealed the desired C15 structure with any impurity phase less than 4%. Powdered samples were mixed with silicone oil and the NMR measurements were made at 4.2 K using a Bruker SXP pulsed spectrometer.

In pure YFe_2 the NMR line is narrow and can easily be broadened by the rf excitation power. The line centre, defined as the frequency for which the echo and excitation frequencies coincide, is at $(45.94 \pm 0.02)\text{MHz}$, in excellent agreement with the value extrapolated to 0 K of Riedi and Webber [3]. This frequency corresponds to a hyperfine field of $(22.03 \pm 0.01)\text{T}$ (using the nuclear g factor $g_n = -0.2736$).

Compared to pure YFe_2 , considerably higher rf power is required to excite optimum echoes in the substituted compounds. This suggests the absence of domain wall enhancement in the latter. The

lineshapes for Tb and Ho doped compounds which are presumed to originate in domain resonances, are shown in fig. 1.

In the pseudo-binary compounds containing dysprosium the NMR signals were very weak. The ^{89}Y resonance was not discernible for $x > 0.02$: even then the signals were roughly 100 times smaller than those observed in the alloy $\text{Ho}_{0.05}\text{Y}_{0.95}\text{Fe}_2$. This observation is attributed to a low rf susceptibility arising from the anisotropy of the dysprosium ion. In the sample $\text{Dy}_{0.01}\text{Y}_{0.99}\text{Fe}_2$ the linewidth is approximately the same as in the 5% Ho and Tb samples and the centre is at $(46.1 \pm 0.05)\text{MHz}$.

The structure which appears in the ^{89}Y lineshapes for samples containing Tb and Ho lies to the high frequency side of the peak in pure YFe_2 . The transferred hyperfine field originating from the lanthanide ions is therefore parallel to that from the Fe sublattice. The absence of resolved structure indicates that the THFF is not simply an effect arising directly from the four nearest neighbour lanthanide sites. Analysis shows that the nature of the shifts and broadening is compatible with a THFF contribution brought about by a modification of the Fe THFF by the substituted lanthanide moments. The results of calculations based on this model are shown alongside the experimental points in the figures. Essentially the model assigns a transferred hyperfine field of amount α for each Fe nearest neighbour that an yttrium site shares with a lanthanide substituent. This involves the lanthanide ions in the first three near neighbour shells to each Y: because of the number of shared Fe nearest neighbours the contribution of a lanthanide ion in the first, second or third shells is 6α , 2α or α , respectively. The possible contributions from

the three neighbour shells, of 4, 12 and 12 atoms, range from 0 to 60α . To arrive at a continuous distribution of intensity from these discrete shifts the probability amplitudes are convoluted with a residual Gaussian lineshape of width equal to that observed in $Dy_{0.01}Y_{0.99}Fe_2$. The results shown indicate that $\alpha=0.12$ MHz for Ho and 0.17 MHz for Tb. These values are in approximate proportion to the spins of the ions. Al-Assadi et al. [4] obtained an upper limit of α for fields at Ho nuclei due to Gd neighbours in (Ho)(Gd,Y)Fe₂ of 0.4 T. Taking account of the outer electron hyperfine coupling constants of Campbell [5] this translates to $\alpha_{max}=0.3$ MHz for YFe₂ doped with Gd: this is not inconsistent with our observations above. The ⁸⁹Y resonances in the <111> magnetised (Tb,Y)Fe₂ sample will suffer from asymmetric dipole broadening due to random Tb neighbours. While preserving the centre of gravity this effect will bias the line intensity to lower frequencies and we believe this to be a factor in the poor fit to the data for the 20% Tb sample.

The fitting procedures imply a centre frequency for the ⁸⁹Y resonance at the limit of zero lanthanide concentration, thus giving a measure of the anisotropy of the Fe sublattice THFF. The values of (46.0 ± 0.05) and (46.1 ± 0.05) MHz for Tb <111> and Ho<100> substitution indicate that if such anisotropy exists it is no more than about 0.2%.

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FIGURE CAPTION

Fig. 1 - NMR spectra of ^{89}Y in $\text{Ho}_x\text{Y}_{1-x}\text{Fe}_2$ and $\text{Tb}_x\text{Y}_{1-x}\text{Fe}_2$.

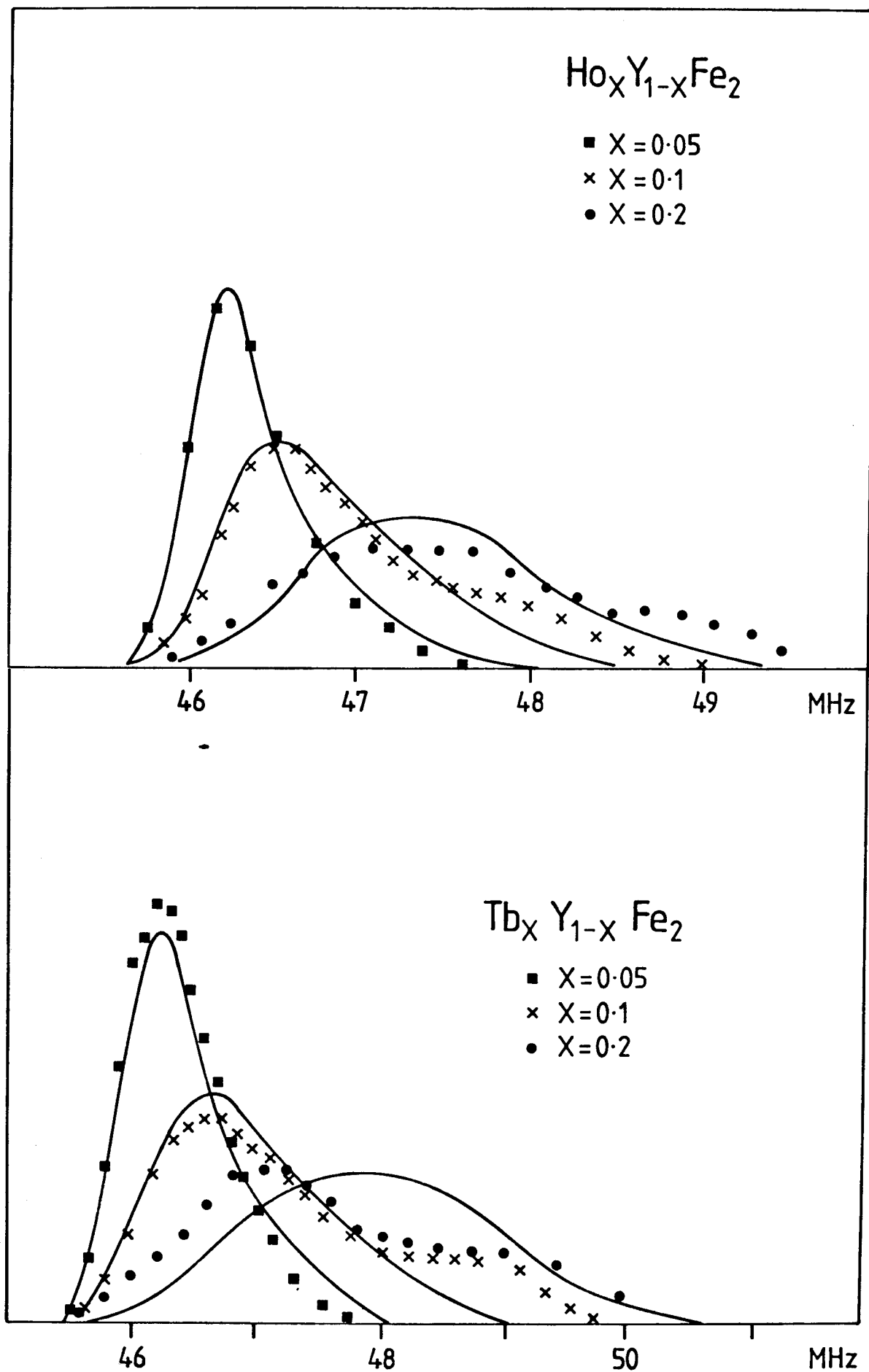


Fig. 1

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