

## ESR of Nd<sup>3+</sup> and Gd<sup>3+</sup> in YRh<sub>2</sub> and YIr<sub>2</sub> Cubic Intermetallic Compounds\*

J. P. DONOSO, J. F. SUASSUNA, G. E. BARBERIS, D. DAVIDOV and C. RETTORI

*Instituto de Física, UNICAMP, 131W Campinas, SP*

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ESR experiments at liquid helium temperatures has been done on diluted (0.01% - 1%) Nd and Gd in YRh<sub>2</sub> and YIr<sub>2</sub> Laves phases. ~ d shows an isotropic spectra with hyperfine lines corresponding to the various isotopes and a g-value appropied to a  ${}^6A_1$  crystal field ground state. The ~ d resonance shows a single line at  $g = 1.993$ .

Experiências de RPE a baixas temperaturas sob Nd e Gd diluidos em YRh<sub>2</sub> e YIr<sub>2</sub> são apresentadas. ~ d apresenta uma ressonância isotrópica com estruturas hiperfinas correspondente aos vários isótopos e um valor de g apropriado a um estado fundamental,  ${}^6A_1$ . A ressonância de ~ d ~ + apresenta uma única linha isotrópica a  $g = 1.993$ .

Low temperature (1.6 - 15K) X Band Electron Spin Resonance experirnents has been carried out on Nd and Gd dopped YRh<sub>2</sub> and YIr<sub>2</sub> cubic intermetallic compounds.

A series of samples of  $Re_x A_{1-x} B_2$  (RE = Nd, Gd; A = Y; B = Rh, Ir;  $10^{-4} < x < 10^{-2}$ ) were prepared by arc melting the stoichiometric amounts of the corresponding elements in an arc furnace of argon atmosphere. No thermal treatment was necessary in order to get good single phase samples as it was verified by X rays analysis.

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As in others  $AB_2$  compounds ( $A = \text{La, Lu, Ce; B} = \text{Rh, Ir, Ru}$ )<sup>1,2,3</sup>, the  $\text{Nd}^{3+}$  spectra (see figure 1) shows a central line ( $I=0$ ) with a  $g$ -value close to 2.667, appropriated to a  $\Gamma_6$  cubic crystal field ground state<sup>4</sup>. The spectra also shows two sets of eight satellites hyperfine lines corresponding to the  $^{143}\text{Nd}$  ( $I = 7/2$ , 12.3%) and  $^{145}\text{Nd}$  ( $I = 7/2$ , 8.3%) isotopes. The  $\text{Gd}^{3+}$  resonance shows a single line with a  $g$ -value close to 1.993<sup>5</sup>.

Figure 1 shows a typical spectra of 1000 ppm of  $\text{Nd}^{3+}$  in  $\text{YRh}_2$ . Similar spectrum were obtained for  $\text{Nd}^{3+}$  in  $\text{YIr}_2$ . The resonance lines were analysed by the method of Peter *et al*<sup>6</sup>. The linewidth was fitted to the formula  $a + bT$ , and the hyperfine constants were obtained using the second-order hyperfine Breit-Rabi formula<sup>7</sup>. In order to get better determination of the position of the hyperfine lines, the second derivative of the spectra was also recorded.

Table 1 gives the thermal broadening of the linewidth ( $b$ ), residual width ( $a$ ) and  $g$ -value obtained from the spectra. For the low concentrated samples ( $C < 0.5\%$ ) no concentration effects were observed on

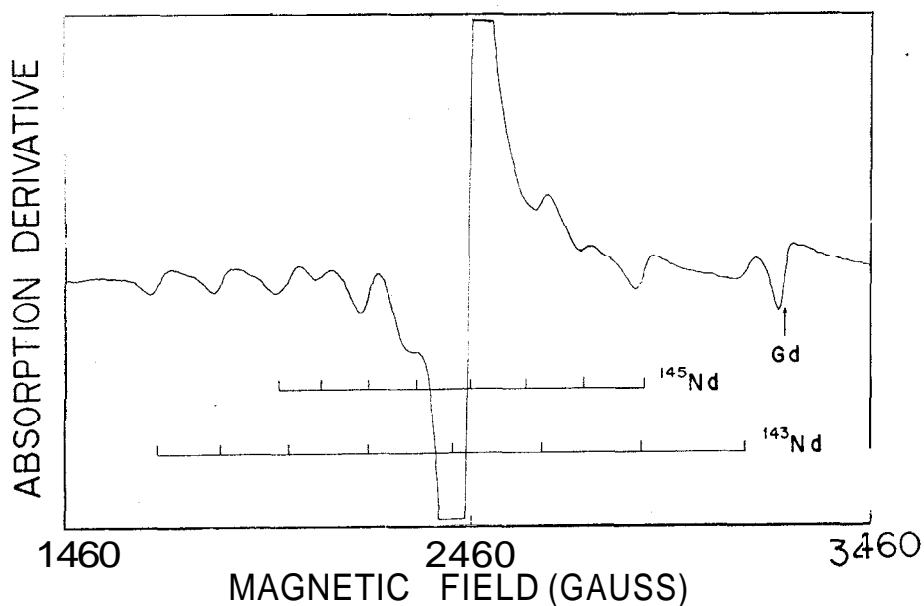


Fig.1 - ESR spectra of 1000 ppm of Nd in  $\text{YRh}_2$  at  $T=1.5$  K. The resonance of natural impurities of Gd is also indicated.

Table I - Experimental ESR data of Nd<sup>3+</sup> and Gd<sup>3+</sup> in YRh<sub>2</sub> and YIr<sub>2</sub>.

Alloy	C %	$a(G)$		$b(G/K)$		$g$ -value	
		$T = 0$	$1.5 < T < 15K$	$T = 1.5 K$	$T = 1.5 K$		
Nd : YRh <sub>2</sub>	1	277 ± 20	5.2 ± 1	2.655 ± 0.010			
"	0.1	35 ± 4	6.1 ± 0.7	2.640 ± 0.005			
"	0.05	30 ± 3	6.4 ± 0.8	2.640 ± 0.005			
"	0.02	35 ± 4	6.1 ± 0.7	2.640 ± 0.005			
Gd : YRh <sub>2</sub>	0.2	110 ± 10	2 ± 0.2	1.993 ± 0.007			
"	0.05	46 ± 5	1.9 ± 0.2	1.999 ± 0.005			
"	0.01	40 ± 4	2.1 ± 0.2	1.999 ± 0.005			
Nd : YIr <sub>2</sub>	1	270 ± 20	16 ± 6	2.646 ± 0.010			
"	0.3	68 ± 7	14 ± 4	2.640 ± 0.006			
"	0.1	60 ± 5	17 ± 7	2.645 ± 0.008			
"	0.05	46 ± 4	13 ± 3	2.630 ± 0.010			
"	0.01	50 ± 5	15 ± 5	2.630 ± 0.010			
Gd : YIr <sub>2</sub>	0.35	127 ± 15	2.2 ± 0.5	1.994 ± 0.010			
"	0.08	155 ± 15	1.8 ± 0.5	1.990 ± 0.010			
"	0.05	153 ± 15	2.0 ± 0.5	1.995 ± 0.010			
"	0.04	130 ± 20	2.5 ± 0.5	1.998 ± 0.010			
"	0.02	120 ± 20	2.6 ± 0.5	1.993 ± 0.010			

these parameters, indicative of the absence of bottleneck effects in the relaxation mechanisms. However, for the high concentrated samples (C > 0.5%) and low temperatures ( $T < 5K$ ) some interaction effects has been observed on the linewidth and g-value.

Neglecting the influence of low lying crystal field excited states of Nd<sup>3+</sup>, and in the single band approximation, the ratio between the thermal broadening of the linewidth for Nd<sup>3+</sup> and Gd<sup>3+</sup> gives an exchange ratio<sup>2</sup>

$$\frac{\langle J^2(q) \rangle_{Nd}}{\langle J^2(q) \rangle_{Gd}} = 1.36 \frac{b_{Nd}}{b_{Gd}} \quad (1)$$

Using the data of Table I, we found this ratio to be about 4 and 8 for  $\text{YRh}_2$  and  $\text{YIr}$ , respectively. Larger exchange parameter for  $\text{Nd}^{3+}$  than for  $\text{Gd}^{3+}$  was also observed in other  $\text{AB}_2$  compounds<sup>1,2,3</sup>. This tendency toward smaller exchange parameter in the first half of the rare-earth series with the increasing of the 4f occupation number seems to be a general behavior which has already been observed in the superconductor  $\text{LaAl}_2$ <sup>8</sup> and predicted theoretically<sup>9</sup>.

For a single band metal the g-shifts of  $\text{Nd}^{3+}$  and  $\text{Gd}^{3+}$  will give an exchange ratio for  $q = 0$ <sup>2</sup>

$$\frac{J(0)_{\text{Nd}}}{J(0)_{\text{Gd}}} = - \frac{\Delta g_{\text{Nd}}}{\Delta g_{\text{Gd}}} \quad (2)$$

Since the g-shift of  $\text{Gd}^{3+}$  is too small to be measured, we can not compare the results given by (2) and (1) in order to detect any wavevector dependence of the exchange parameters in these compounds.

From Table I we can see that there is some tendency toward positive g-shift for  $\text{Gd}^{3+}$  in both compounds (in insulator  $g = 1.993$ ) which will give a positive  $q = 0$  component of the effective exchange parameter. On the other side if we take the g-value of  $\text{Nd}^{3+}$  in insulator to be 2.667,<sup>10</sup> it is clear from Table I that the g-shift of  $\text{Nd}^{3+}$  is negative, indicating that the  $q = 0$  component of the effective exchange parameter will be also positive ( $g_J - 1 < 0$ ). Therefore our experimental data seems to indicate no change in the sign of the exchange parameter upon going from  $\text{Nd}^{3+}$  to  $\text{Gd}^{3+}$ . On the other hand, if we take the maximum possible g-shift for  $\text{Gd}^{3+}$  ( $\sim 0.01$ ) and the minimum possible g-shift for  $\text{Nd}^{3+}$  ( $\sim -0.02$ ), formula (2) will give a ratio of two approximately; showing again the tendency toward smaller exchange parameter as the 4f occupation number increases, as mentioned before. This reduction could be understood in terms of a recent calculation by Troper *et al.*<sup>11</sup> where a larger radius for  $\text{Nd}^{3+}$  4f shell compared with that of  $\text{Gd}^{3+}$  might reduce or eventually induce a change in the sign of the f-d effective parameter for  $q = 0$  because the inter site to intra site exchange interaction ratio of the 4f localized magnetic moment and the d-conduction electrons will be bigger for  $\text{Gd}^{3+}$  than that of  $\text{Nd}^{3+}$ .

The hyperfine constants  $^{143}\text{A} = 209 \pm 2 \text{ G}$ ,  $^{145}\text{A} = 132 \pm 2 \text{ G}$  and  $^{143}\text{A} = 208 \pm 4 \text{ G}$ ,  $^{145}\text{A} = 131 \pm 4 \text{ G}$  measured for  $^{143}\text{Nd}^{3+}$  and  $^{145}\text{Nd}^{3+}$  isotopes in  $\text{YRh}_2$  and  $\text{YIr}_2$  respectively are smaller than those reported for insulators ( $^{143}\text{A} = 215\text{G}$ ,  $^{145}\text{A} = 135\text{G}$ )<sup>12</sup>. This negative conduction electrons contribution to the hyperfine constants, might be attributed mainly to the contact hyperfine interaction<sup>7</sup>, (note that  $g_J - 1 > 0$  will give  $\Delta A < 0$ ).

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