The localized-itinerant magnetic system \( \text{Gd}_{1-x} \text{Y}_x \text{Co}_3 \) described by a statistical distribution mean-field model

A.L. Lima\textsuperscript{a,*}, P.J. von Ranke\textsuperscript{b}, M.S. Reis\textsuperscript{a}, A.Y. Takeuchi\textsuperscript{a}, A.P. Guimar\textsuperscript{aes}a, I.S. Oliveira\textsuperscript{a}

\textsuperscript{a}Centro Brasileiro de Pesquisas Fisicas, Departamento de Mat\textsuperscript{e}ria Condensada e F\textsuperscript{is}ica Estat\textsuperscript{istica} , Rua Dr. Xavier Sigaud, 150 - Urca - Rio de Janeiro, 22290-180, Brazil

\textsuperscript{b}Univ. do Est. do Rio de Janeiro, R. S\textsuperscript{ao} Francisco Xavier, 524, Rio de Janeiro 20550-013, Brazil

Abstract

Magnetization curves of the localized-itinerant intermetallic system \( \text{Gd}_{1-x} \text{Y}_x \text{Co}_3 \) are calculated from a statistical distribution of Gd-ions in a mean-field approximation. The Gd subsystem is considered magnetically localized, whereas the magnetic properties of Co are described through a density of states model, built from the experimental \( M \) vs. \( H \) curve of \( \text{YCo}_3 \). We measured magnetization curves for \( x = 0.0, 0.2, 0.4, 0.78 \), and compared to theoretical results. Excellent agreement between the theory and experimental data was obtained. © 2002 Elsevier Science B.V. All rights reserved.

Keywords: RE compounds; 3d metals; Mean-field approximation

1. Introduction

Among the rare earth–transition metal intermetallic compounds, those with formula \( \text{RCO}_3 \) present interesting features [1]. The magnetic state of Co ions in these compounds is very sensitive to the magnetic field acting on the 3d electrons and a sharp transition on the \( M \) vs. \( H \) curve is observed in \( \text{YCo}_3 \) at a field around 82 T, for which the magnetic moment of Co ions jumps from \( 0.98 \mu_B \) to \( 1.22 \mu_B \) [2]. This instability of the 3d magnetism in \( \text{YCo}_3 \) is related to the existence of sharp peaks in the density of states (DOS) near the Fermi level [3,4].

The replacement of Yttrium by Gadolinium in \( \text{YCo}_3 \) introduces a magnetic species into the rare earth sublattice, which increases the molecular field acting on cobalt [4], leading to the above referred transition at Gd concentration around \( x = 0.225 \) [5]. In this work we consider the following approach to the series of intermetallic compounds \( \text{Gd}_{1-x} \text{Y}_x \text{Co}_3 \): the Gd sub-

system is assumed to be magnetically localized and well described in the framework of the Heisenberg hamiltonian taken in a molecular field approximation. We consider that Gd ions are randomly distributed in the RE sites, and introduce a statistical distribution of R-ions. For the Co subsystem, we used a rigid band model within a molecular field approach, which reproduces the magnetization curve of \( \text{YCo}_3 \) reported by Goto et al. [6]. The equations are solved self-consistently in respect to the magnetic moments of each sublattice and the model reproduces the behavior of the experimental data.

2. Model

The total magnetic moment of the Co-subsystem is given by the difference between spin-up and spin-down electrons in the split band:

\[
M_{\text{Co}} = \mu_B \left\{ \int_{\epsilon_F}^{\epsilon_{\uparrow}} \frac{D_{\uparrow}(\epsilon) \, d\epsilon}{1 + \exp \left( \beta(\epsilon + \mu_B B_{\text{Co}} - \epsilon_F) \right)} \right\} - \left\{ \int_{\epsilon_F}^{\epsilon_{\downarrow}} \frac{D_{\downarrow}(\epsilon) \, d\epsilon}{1 + \exp \left( \beta(\epsilon + \mu_B B_{\text{Co}} + \epsilon_F) \right)} \right\}, \tag{1}
\]
where \( D_1(\varepsilon) \) and \( D_1(\varepsilon) \) are the density of states (DOS) for the itinerant up and down electrons respectively. Here, \( \alpha_1 = \mu_B B_{\text{Co}} \) and \( \alpha_1 = -\mu_B B_{\text{Co}} \) give the bottom energy for the up and down DOS, respectively, and \( \varepsilon_F \) is the Fermi energy, determined from the conservation of the number of itinerant electrons \( n_e \):

\[
\begin{align*}
  n_e = & \int_{\alpha_1}^{\varepsilon_F} \frac{D_1(\varepsilon) \, d\varepsilon}{1 + \exp \left[ \beta (\varepsilon + \mu_B B_{\text{Co}} - \varepsilon_F) \right]} \\
  & + \int_{\alpha_1}^{\varepsilon_F} \frac{D_1(\varepsilon) \, d\varepsilon}{1 + \exp \left[ \beta (\varepsilon - \mu_B B_{\text{Co}} - \varepsilon_F) \right]}
\end{align*}
\]  

(2)

\( B_{\text{Co}} \) is the molecular field acting on the Co lattice:

\[
B_{\text{Co}} = B_{\text{ext}} + \lambda_{\text{Co-Co}} M_{\text{Co}}.
\]  

(3)

For the localized subsystem one starts from the Zeeman–Heisenberg Hamiltonian relative to the \( i \)th magnetic site:

\[
H = 2J_b \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j - g \mu_B B_{\text{ext}} \vec{S}_i \cdot \vec{S},
\]  

(4)

where the symbols have their usual meaning.

In order to apply the relation (4) to the case of Gd\(_{1-x}\)Y\(_x\)Co\(_3\) compounds, the first thing to be noticed is the fact that the number of terms in that series obviously depends on the Gd concentration, \((1-x)\). The Gd ions are assumed to be distributed at random through the rare earth sites. Considering only first neighbor interaction, the probability that a Gd ion will have ‘\( n \)’ other Gd ions as first neighbors is given by [7]:

\[
P(\xi, n, x) = \frac{\xi! (1-x)^n (\xi-n)!}{n! (\xi-n)!},
\]  

(5)

where \( \xi \) is the number of rare earth first neighbors, that is, \( n = 0, 1, \ldots, \xi \). On the molecular field approximation, upon the above assumptions, the Hamiltonian (4), per magnetic ion, will be:

\[
H(n, x) = 2J_b P(\xi, n, x)n \langle \vec{S} \rangle_T \cdot \vec{S} - g \mu_B B_{\text{ext}} \vec{S},
\]  

(6)

where \( \langle \vec{S} \rangle_T = M_{\text{Gd}} / 7 \mu_B N_{\text{Gd}} \), with \( M_{\text{Gd}} \) the magnetic moment of Gd sub lattice, and \( N_{\text{Gd}} = (1-x)N_R \) \( (N_R = \text{number of } R \text{ sites}) \) is the number of Gd ions. The molecular field acting on the \( i \)th site will be given by

\[
B_{\text{Gd}}(n, x) = B_{\text{ext}} + \lambda_{\text{Gd-Gd}}^{(0)} (1-x) \sum_{0}^{\xi} P(N, n, x)M_{\text{Gd}},
\]  

(7)

where \( \lambda_{\text{Gd-Gd}}^{(0)} = 2J_0 n / 7 \mu_B N_R \). In the present paper, the experimental results are expressed as magnetic moment per formula unit and the total magnetic moment is calculated self-consistently from

\[
M_{\text{total}} = M_{\text{Gd}}^{\text{total}} - 3M_{\text{Co}}.
\]  

(9)

3. Experimental

Polycrystalline samples were prepared by arc-melting the constituent metals in argon atmosphere, followed by annealing at 1000°C, under dynamic vacuum for 48 hours, in order to minimize lattice defects. X-ray diffraction was performed in order to check the quality of the samples. The \( M \) vs. \( T \) curves were measured under an applied field of 1T, between 4.2 K and room temperature.

4. Results and conclusions

In order to calculate the magnetic field dependence of the Co–magnetization, \( M_{\text{Co}} \), we adopted a simple profile for the DOS, which was constructed by a set of connected linear equations. Fig. 1(a) shows the DOS model curve built from the experimental results of Goto et al. [8], and Fig. 1(b) shows the theoretical curve superimposing the experimental data performed in ultrahigh magnetic fields up to 110 T at 10 K. The magnetic-field region (I), in Fig. 1(b), presents a high increase in magnetization as well as in the region (III), where the metamagnetic transition is observed. These two magnetization enhancements occurs when the down peak, number 5 in Fig. (1a), crosses over the up peaks 2 and 4 considered in our model DOS. The magnetization increases observed in region (II) is due to small spin changes that occurs when the down peak 5 is moves along the region 3, where the DOS presents a very low increases. Finally, above 90 T, the magnetization is completely saturated achieving the value \( M_{\text{Co}}(\text{Co}/\mu_B) = 1.2 \), which is equal to the area sum under the three peaks in Fig. (1g). Since the DOS is constructed from the experimental data, it includes the information about the three possible values of the magnetic moment that the cobalt can have inside a cell unit of RCo\(_3\) [1], as long as the concentration of the cobalt remain the same in the

Fig. 1. (a) Full lines: theoretical results. Open dots: experimental results after Goto et al. [2], (b) the DOS model and the DOS x Fermi function for different values of the applied field, (c) 0 T, (d) 10 T, (e) 82 T (f) 85 T and (g) 120 T.
whole series of Gd\textsubscript{1−x}Y\textsubscript{x}Co\textsubscript{3}, the DOS is supposed to be the same also. It is worth noting that we must consider at least three peaks in our model DOS in order to reproduce the experimental $M$ vs. $B_{\text{ext}}$ data. Fig. 2 shows $M$ vs. $T$ curves measured from 4.2 K up to RT for various compounds, namely, $x = 0.0, 0.2, 0.4, 0.78$. All curves were taken at $B_{\text{ext}} = 1$ T, in order to avoid domains walls that are not included in the model. Continuous lines are results from model calculation. As it can be seen, there is very good agreement between theoretical results and experimental data.

The Co itinerant subsystem in Gd\textsubscript{1−x}Y\textsubscript{x}Co\textsubscript{3} was described using a rigid band model with DOS build from the experimental results of Goto et al. [8]. The localized magnetic Gd-subsystem was treated in molecular field approximation, and the random distribution of localized magnetic ions was described introducing a statistical function. The total magnetization was calculated self-consistently from Eq. (5) and very good agreement is found between the model and experimental curves.

Acknowledgements

The authors would like to thank Prof. P. Panissod for helpful discussions. This work is supported by CNPq, CAPES and FAPERJ.

References