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Itinerant metamagnetism in rare earth-transition metal compounds

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Intermetallic compounds of rare-earth and transition metals present the possibility of using the large magnetic moment of the first with the high Curie temperature of the second. We first discuss the nature of the coupling between the spin of the rare-earth and transition metal. We assume that it happens within the d band coming from the 5d and 3d levels and describe it using the Van Vleck model for ferromagnetism. We then consider the particular case of Cobalt compounds where Cobalt can be magnetic or not depending of the rare-earth metal. We describe the appearance of magnetism as a collective metamagnetism due to the position of the Fermi level in these compounds in a steep decrease of the density of states. Calculation of the density of states confirms this hypothesis.

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INTRODUCTION

Intermetallic compounds between rare-earth and transition metals present interesting magnetic properties [1]. Among them we first point out that a large magnetization would be obtained if one would be able to align the large magnetic moment of a rare earth of the second part of the series with the moment of the transition metal. Only Nickel, Cobalt and Iron can be magnetic in these compounds and, in all cases, the spin of the rare earth couples antiferromagnetically to the spin of the transition metal making the interesting compounds ferrimagnetic. In the first part, we will discuss the physical origin of this general rule. In the second part, we will address ourself the question of the occurrence of magnetism of the transition metal and particularly why Cobalt in the series TCo_2 (where T is a rare-earth) is magnetic only for some rare-earth. Moreover the transition is generally second order except for the three cases Er, Ho and Dy where it is of first order. We will explain this behaviour by a kind of collective metamagnetism as described by Wohlfarth and Rhodes [2].

I - THE RARE-EARTH TRANSITION METAL COUPLING

When the 3d moment exists, a general rule is observed in all known intermetallic compounds. The spin of the rare-earth couples antiferromagnetically to the spin of the 3d moments. The exceptions, which have been thought to exist in compounds with Mn, turn out to have no real ferromagnetic interactions. In these intermetallic compounds, one can consider three main types of interactions: between rare earth metals, between transition metals and between rare earth and transition metals. The first one is of the RKKY type and is, by far, the smallest. The second one is usually large and the third has been shown to be fairly large [3]. The antiparallel coupling between 4f and 3d spin moments has been first explained by Wallace [4] with a model in which the interaction takes place via the polarization of the s conduction electrons and is of the RKKY type. Wallace argues that the distances in intermetallic compounds are such that antiferromagnetic coupling arises. This is difficult to reconcile with the experimental fact that this coupling occurs irrespective of composition, electron concentration, or crystal structure. Furthermore, in amorphous alloys, antiparallel coupling is observed. Gomes [5] also assumes a coupling via s electrons but he takes them uniformly polarised as in a Zener model. Such coupling occurring within the s band contradicts the fact that critical

temperatures are much like transition metal ones where coupling is known to be within the d band. Campbell [6] was the first to suggest such a coupling. He proposed that the f electron spin creates a positive local d moment through the ordinary f-d exchange and that there is a direct interaction within the d band with any other d moment as in normal transition metal alloys. The coupling between moments in transition metals has been explained qualitatively by Friedel [7] with the concept of the virtual bound state. Campbell assumes that the rare earth metal behaves like a transition metal at the beginning of the series which is reasonable. However we point out that Friedel's theory is valid for an impurity in a matrix and that Campbell's explanation holds mainly for an impurity of rare earth in a transition metal. We think that the physical background of this theory holds for the intermetallic compounds. Thus we proposed another point of view for the interaction within the d band i.e. we also assume that the f electron spin creates a positive local d moment and we show that the coupling between the d moments is antiferromagnetic. Our explanation relies on the Van Vleck model [8] for ferromagnetism in Nickel. He argued that correlation in transition metal make the states of high ionization unlikely. For Ni, atoms can be in d^9 or d^{10} configurations. The states of higher polarisation give rise to a coupling between pairs of neighbouring atoms. For instance there is a ferromagnetic coupling between two Ni atoms in the d^9 configuration because of the possibility for this pair to go in the $d^{10} + d^8$ or $d^8 + d^{10}$ states. As a rough estimate, second order perturbation with respect to the transfer integral t associated with the transition from a d state of an atom to the d state of its neighbour gives the excess of the energy of singlet ground state 1t over the triplet 3t

$$^1t - ^3t = 2t^2 \left| \frac{2}{T} - \frac{3}{S} \right|$$

where T is the mean excess energy of the 2 triplet states of $d^8 + d^{10}$ over the energy of the $2d^9$ and S the mean excess energy of the 3 singlet states. Here we assume that the rare earth atom is in the d^1 state. The same kind of argument for $d^1 + d^8$ states shows that the coupling in that case is antiferromagnetic. This stems from the fact that this is the only possibility for the single electron to visit the d^8 atom. Thus the coupling between Nickel and a rare-earth metal is always antiferromagnetic. Similar results are likely to be obtained for Cobalt and Iron.

Iron is always magnetic in intermetallic compounds, contrary to Ni, which in general is not. In about half of the compounds with Cobalt, Co is magnetic. TCO_2 compounds are on the borderline: higher concentrations of Cobalt atoms make it magnetic, less non magnetic. For this particular series, if T is Y, La and Lu, Cobalt is non magnetic but becomes magnetic for a magnetic rare-earth. The transition, which is, in general, second order in all these compounds, is first order with Dy Ho and Er. Bloch and Lemaire [3] proposed a model to explain the susceptibility of TCO_2 and Bloch et al [9] used a phenomenological Landau theory for the order of the transition in Dy Ho and Er. These last authors fitted their results to a Stoner theory using the various derivatives of the density of states at the Fermi level.

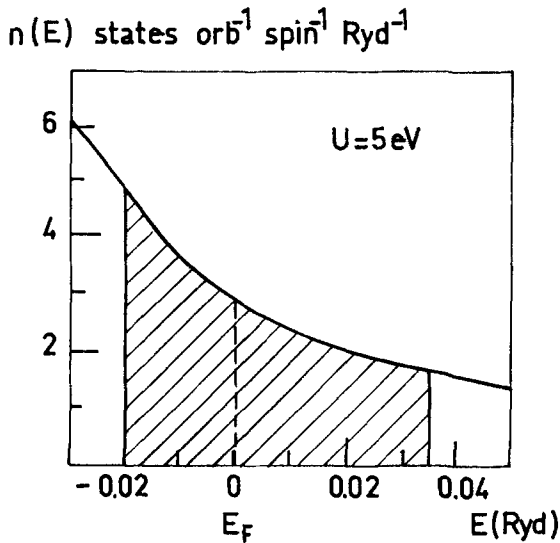


Fig. 1 : Density of states of YCo_2 near the Fermi level

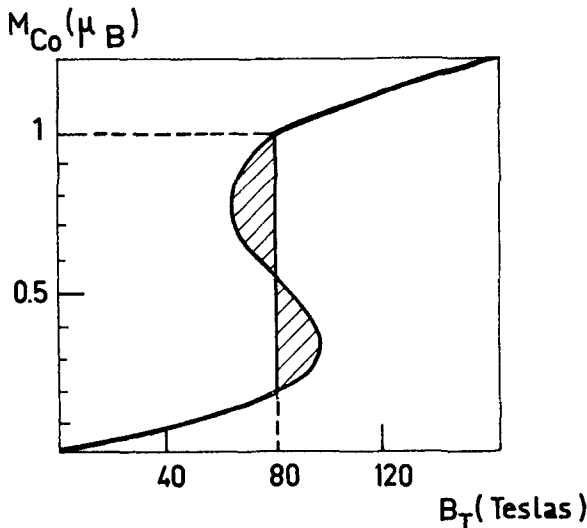


Fig. 2 : Magnetization curve of YCo_2 deduced from figure 1.

We have developed this model [10] and first calculated the density of states of TNi_2 , TFe_2 and TCO_2 . The results show that the Stoner criterion is fulfilled for Iron, but not for Ni, in accordance with the experimental result. Cobalt is borderline. The Stoner criterion is nearly fulfilled and the Fermi energy lies in a steep decrease in the density of states. This explains why YCo_2 is a Pauli paramagnet and that paramagnons effects are important. Moreover the position of the Fermi level is favorable for collective metamagnetism as described by Wohlfarth et al [2]. Figure 1 shows the density of states near the Fermi level and Figure 2 the

magnetization on the Cobalt atom as a function of an applied field which results from the behaviour of the density of states. Such a large magnetic field needed to magnetize Cobalt can be obtained easily using the exchange field due to the magnetic rare earth atoms: i.e. If we replace Yttrium atoms by Ho, Er or Dy atoms, the field created by the rare earth atoms can magnetize the Cobalt. Thus the following picture would apply to this compounds (see figure 3).

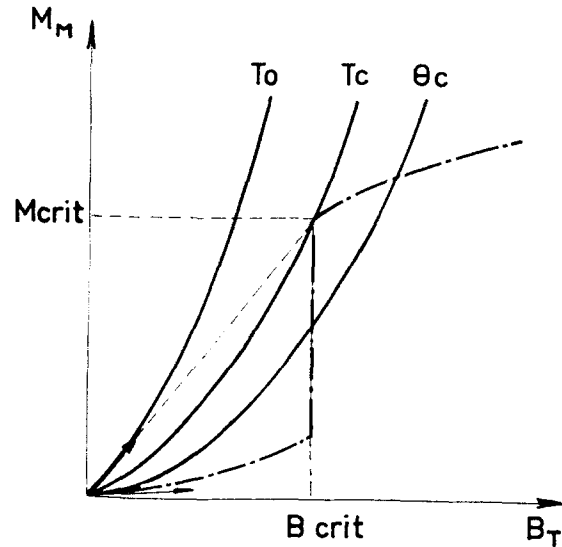


Fig. 3 : Variation of the Cobalt magnetization with the total field B_T in RCo_2 compounds.

The internal field which magnetizes the Cobalt atom is λm_f where λ is a molecular field constant and m_f is the magnetization of the rare earth atoms. The effective field on the rare earth is λm_d where m_d is the magnetization of the Cobalt atom. Thus we have to solve self consistently the set of equations

$$m_d = f(\lambda m_f, T)$$

$$m_f = g \mu_B J B_J \left(\frac{\lambda m_d}{kT} \right)$$

where f is the function of fig. 2 and B_J a Brillouin function. Figure 3 shows the graphical discussion. For temperature greater than T_c , the magnetization is zero. It appears discontinuously at temperature T_c where there is a first order transition. Table I gives the calculated values for T_c . Second order transitions occur when the susceptibility of the d electrons is large enough so the Brillouin curve intersects the curve first at $m_f = m_d = 0$. This is the case for the other compounds which have higher T_c because, in this temperature range, the susceptibility of the d electrons increases with temperature.

RCo_2	T_c calculated in K	T_c exp. in K
DyCo_2	138	135
HoCo_2	84	77
ErCo_2	43	33

Transition temperatures of the RCo_2 compounds with heavy rare earths.

One can also predict and it is observed that in DyCo_2 and ErCo_2 above T_c , an applied magnetic field can induce the transition on the Cobalt atom [11]. This itinerant metamagnetism is not limited to the TCO_2 series and seems to be a rather general phenomenon. It

has been found in YCo_3 and $ThCo_5$ [12]. It must happen every time, in a compound, the Fermi level lies between the region of high density of states due to the transition atom and that of low density of states due to the rare-earth atom.

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