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MAGNETIC PROPERTIES OF $R_{1-x}^{(1)}R_x^{(2)}Al_2$ ALLOYS*

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Using the multiband s - f model we derive the formulae determining the Curie temperature and magnetic moment as functions of concentration x for $R_{1-x}^{(1)}R_x^{(2)}Al_2$ intermetallic alloys, where $R^{(1,2)}$ denote magnetic rare earth metals. These formulae, applied to $R_{1-x}^{(1)}R_x^{(2)}Al_2$ alloys ($R^{(1)} = La, Lu, Y, Zr$ and $R^{(2)} = Gd$) give the linear dependence of the Curie temperature and magnetic moment versus x in full agreement with experimental data.

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1. Introduction

The Curie temperature and magnetic moment in the paramagnetic state of $R_{1-x}^{(1)}Gd_x^{(2)}Al_2$ samples ($R = La, Lu, Y$) as functions of the concentration x ($x \in [0, 1]$) have been measured in [1, 2] and more recently ($R = Zr$) in [3]. A linear dependence of the Curie temperature T_C and of the magnetic moment M versus x has been found with T_C changing from zero ($x = 0$) to $T_C = 170$ K ($x = 1$) and M changing from zero ($x = 0$) to $M = 7.94 \mu_B$ ($x = 1$), in such a way that $M(x)/x = 7.94 \mu_B$ ($x \in [0, 1]$).

The explanation of the observed T_C behaviour of the mentioned samples (but not of the magnetic moment) has been given in the papers [4] and [2], using the formalism invented in [5, 6].

In Ref. [7] the multiband s - f model has been successfully applied to explain the magnetic properties of the $Gd(Al_{1-x}Me_x)_2$ alloys ($Me = Cu, Ag, Pd, In, Sb, Pb, Bi, Sb, Si$). The method presented in [7], after some modifications, can be also successfully applied to the present case ($R_{1-x}^{(1)}R_x^{(2)}Al_2$ alloys), where we can additionally explain the behaviour of the magnetic moment of the samples as a function of the concentration x .

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2. Curie temperature and magnetic moment

In Ref. [7] the Curie temperature T_C and the magnetic moment M of $GdAl_2$ have been calculated. The corresponding formulae can be directly applied to the more general case of RAI_2 , where R is a magnetic rare earth element. We recall here these formulae. The Curie temperature can be calculated from the following implicit equation:

$$T_C = \frac{S(S+1)}{3k} A, \quad (1)$$

where

$$A = \frac{5(I^{(5d)})^2 F^{(5d)}}{2W^{(5d)}} + \frac{(I^{(6s)})^2 F^{(6s)}}{2W^{(6s)}} + \frac{(I^{(3s)})^2 F^{(3s)}}{W^{(3s)}} + \frac{3(I^{(3p)})^2 F^{(3p)}}{W^{(3p)}} \quad (2)$$

$$F^{(a)} = f\left(t^{(a)} - \mu - \frac{W^{(a)}}{2}\right) - f\left(t^{(a)} - \mu + \frac{W^{(a)}}{2}\right), \quad (3)$$

$$(a = 5d, 6s, 3s, 3p)$$

$$f(z) = (\exp(\beta z) + 1)^{-1}. \quad (4)$$

In (2) the s - f coupling constant has been denoted by $I^{(a)}$ and the bandwidth of the corresponding band by $W^{(a)}$ with the gravity centre $t^{(a)}$. The upper index a corresponds to $5d$, $6s$ bands of R and to $3s$, $3p$ bands of Al and μ is the chemical potential.

The magnetic moment at T_C is given by:

$$M = 2B\sqrt{S(S+1)} \mu_B, \quad (5)$$

where

$$B = 1 + \frac{5I^{(5d)}F^{(5d)}}{2W^{(5d)}} + \frac{I^{(6s)}F^{(6s)}}{2W^{(6s)}} + \frac{I^{(3s)}F^{(3s)}}{W^{(3s)}} + \frac{3I^{(3p)}F^{(3p)}}{W^{(3p)}}. \quad (6)$$

Having in mind an alloy such as $R_{1-x}R_x^{(2)}Al_2$ we have to perform the averaging procedure in (1) and (5) over the alloy configurations in order to get the equation for T_C and M . Similarly to [7] we get:

$$T_C = \frac{(1-x)S^{(1)}(S^{(1)}+1)}{3k} A^{(1)} + \frac{xS^{(2)}(S^{(2)}+1)}{3k} A^{(2)}, \quad (7)$$

$$M = 2 \left[(1-x)B^{(1)}\sqrt{S^{(1)}(S^{(1)}+1)} + xB^{(2)}\sqrt{S^{(2)}(S^{(2)}+1)} \right] \mu_B. \quad (8)$$

The quantities $A^{(i)} = A^{(i)}(I^{(i-5d)}, I^{(i-6s)}, t^{(i-5d)}, t^{(i-6s)}, W^{(i-5d)}, W^{(i-6s)})$ and $B^{(i)} = B^{(i)}(I^{(i-5d)}, I^{(i-6s)}, t^{(i-5d)}, t^{(i-6s)}, W^{(i-5d)}, W^{(i-6s)})$ ($i = 1, 2$) are given

by (2) and (6), respectively. The parameters for Al ($3s, 3p$) in $A^{(i)}$ and $B^{(i)}$ remain unaffected.

The equation for the chemical potential μ of the alloy can be determined from the equation:

$$2 \left[(1-x) \left(\langle n_{\uparrow}^{(1-5d)} \rangle + \langle n_{\uparrow}^{(1-6s)} \rangle \right) + x \left(\langle n_{\uparrow}^{(2-5d)} \rangle + \langle n_{\uparrow}^{(2-6s)} \rangle \right) + \langle n_{\uparrow}^{(Al-3s)} \rangle + \langle n_{\uparrow}^{(Al-3p)} \rangle \right] = (1-x)n^{(1)} + xn^{(2)} + 6 = 6 + n^{(1)} + x(n^{(2)} - n^{(1)}), \quad (9)$$

where

$$\langle n_{\uparrow}^{(i-5d,6s)} \rangle \quad (i=1,2) \quad \text{and} \quad \langle n^{(Al-3s,3p)} \rangle$$

are the averaged occupation numbers of electrons including the band degeneracies (cf. [7]). Each of the $R^{(i)}$ atoms ($i=1, 2$) contributes $n^{(i)}$ electrons and two Al atoms contribute $2 \times 3 = 6$ electrons into the system, as visualized in the relation (9).

3. Numerical results

In order to get $T_C = T_C(x)$ and $M = M(x)$ we have to solve the system of implicate Eqs. (7) and (9) selfconsistently, and to calculate M from (8). We consider here the alloy $R_{1-x}Gd_xAl_2$, where $R = La, Lu, Y, Zr$. Two of them (La, Lu) are nonmagnetic rare earth elements. Therefore for them $S^{(1)} = 0, S^{(2)} = 7/2$ (Gd) and the formulae (7) and (8) become simpler.

In Figs. 1 and 2 we show the dependence of the Curie temperature calculated from (7) and (9). We have assumed the same parameters for Al as in [7]. The parameters for Gd and La or Lu are completely irrelevant because Eq. (9) determines such a position of the chemical potential μ , which is below the lower $5d$ and $6s$ band edges of Gd and La or Lu. In such a situation the mentioned bands are empty and therefore their contribution is zero. The magnetic moment M at T_C as a function of x , determined by (8) for $R_{1-x}Gd_xAl_2$, ($R = La, Lu$), is a linear function of x in such a way that the ratio $M(x)/x = 7.94 \mu_B$, what agrees with experiments very well [1, 2]).

In the case of $R_{1-x}Gd_xAl_2$, where R stands for such elements as Y and Zr, the formulae (7), (8) and (9) are applicable, too. These elements are nonmagnetic ($S^{(1)} = 0, S^{(2)} = 7/2$ (Gd)) and their valence bands (Y: $4d^15s^2$, Zr: $4d^25s^2$) possess the same orbital degeneracies as $5d, 6s$ bands of Gd, La or Lu. Also in this case the lower band edges of the $4d$ and $5s$ bands of Y and Zr lie higher than the chemical potential determined by (9). Therefore, also here, the only relevant parameters are the ones for Al. It is clear then, that the T_C dependence on x calculated from (7) and (9) gives the same results as in Figs. 1 and 2. The $T_C = T_C(x)$ dependence seems to be universal then, for all $R_{1-x}Gd_xAl_2$ alloys ($R = La, Lu, Y, Zr$) and also the ratio $M(x)/x = 7.94 \mu_B$, what is the conclusion from (8). For $R = Y$ (see

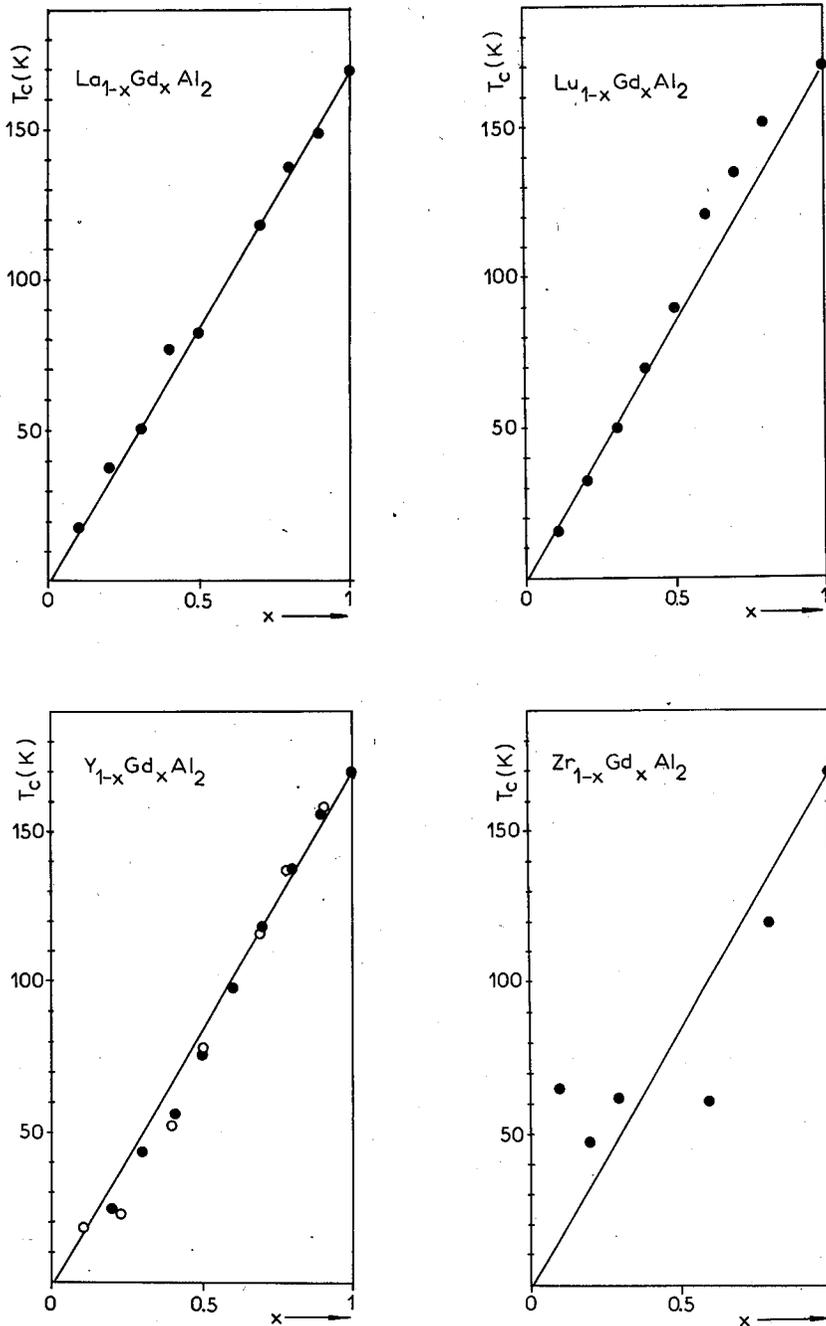


Fig. 1-4. Plot of the Curie temperature vs. concentration x , calculated from Eqs. (7) and (9). The relevant parameters in eV (only for Al) are:

$$I^{(3s)} = -0.093; \quad t^{(3s)} = 0; \quad W^{(3s)} = 4; \quad I^{(3p)} = 0.077; \quad t^{(3p)} = 2;$$

$$W^{(3p)} = 3.5; \quad n^{(1)} = 3(\text{La, Lu, Y}), \quad 4(\text{Zr}); \quad n^{(2)} = 3(\text{Gd}).$$

Fig. 3) the experimental points very closely lie to the mentioned universal linear dependence of $T_C = T_C(x)$, for $R = Zr$ (Fig. 4) the agreement is, however, not so good. In the latter case the deviation from the straight line may be caused by the clusterization process in the $Zr_{1-x}Gd_xAl_2$ samples. In our paper we have used the unperturbed density of states in a form of a rectangle for all the bands considered here ($5d, 6s, 3p, 3d, \dots$). In this case the density of states is a constant in the wide energy range. When the chemical potential lies in this range for $x \in [0, 1]$ we can obtain linear dependence of $T_C = T_C(x)$ and $M(x)/x = \text{const}$ only. May be, in the case of $Zr_{1-x}Gd_xAl_2$ the unperturbed density of states in a form of rectangle is a poor approximation.

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