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SEMI-EMPIRICAL STUDY OF IMPLICIT EXCHANGE INTERACTION IN RARE TARTH METAL-WEAKLY MAGNETIC METAL SYSTEM

Abstract*: For the first time the exchange interaction of Ruderm-Kittel-Kasuya-Yosida (RKKY) type is studied semi-empiricallyin compounds of binary systems of rare –earthmetal (REM)-weakly magnetic metal (WMM) (REM=Gd,Tb,Dy,Ho,Er,Tm; WMM=Al,In) using experimental values of paramagnetic Curie temperature $(\theta_P)$of these compounds. The prediction of theory of RKKY about existence of direct proportional dependence of experimental values of $\theta_P$on de Gennes factor for equiatomic compounds of heavy REM with WMM similar pure REM.As a whole, it is found that for REM compounds with WMM as well as for pure REM the exchange interaction of RKKY type is characteristic.*

Key words*: exachange interaction, magnetic susceptibility, paramagnetic temperature, magnetic moment, de Gennes factor.*

Language*: English*

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Introduction

In rare-earth metals (REM) and compounds based on them, the question of the origin of the atomic magnetic order becomes especially important. In isolated REM atoms, the previously missed 4f-layer of the electron shell is sequentially built up. This layer lies deep and is shielded from external influences by a layer of $5s^2$ $5p^6$ even in the crystalline state of rare-earth metals. For heavy REMs, it is characteristic that the average radius of the 4f shell is 1/10 of the interionic distance. Therefore, direct exchange interaction (overlapping) between the electrons of the 4f-layers of neighboring ions is almost impossible. However, studies show that rare-earth metals and their compounds with other metals have magnetic ordering, due to the exchange interaction of 4f-electrons localized in the nodes of the crystal lattice through conduction electrons, called the indirect exchange interaction of the Ruderman-Kittel-Kasuya-Yosida (RKKY) [1-5]. Such an interaction is carried out as follows: the electrons of the 4f-layer located in the n-node (determined by the radius vector $\vec{R}_n$) of the crystal lattice affect the conduction electrons and magnetically polarize them. Polarized conduction electrons, in turn, affect the electrons of the 4f layer located in the m - site (determined by the radius vector $\vec{R}_m$) of the lattice. Thus, the arising ordered state of the magnetic moments of the electrons of the 4f-layers is destroyed when they are heated to a certain temperature $T = \theta_p$ (called the paramagnetic Curie temperature), which is characteristic of each rare-earth metal. At temperature $T = \theta_p$ a magnetic phase transition occurs, magnetic ordering - magnetic disorder (paramagnetism). Thus, θ_p it is the energy characteristic (measure) $(k_Б T)$ of the exchange interaction of the RKKY type in REMs and compounds based on them.

The temperature dependence of the magnetic susceptibility of REMs and compounds based on them directly reflects the paramagnetic Curie temperature [according to the Curie – Weiss law $\chi = C/(T - \theta_p)$, where is the C- Curie – Weiss constant]. The experimental dependence $\chi^{-1}(T)$ determines the value θ_p. Information on the paramagnetic temperature of the Curie of rare-earth metals depending on their atomic number, and in compounds based on them, on the concentration of alloyed components, is necessary for the development of theoretical ideas about the nature of exchange interactions in these objects.

The purpose of this work is to study the effect of weakly magnetic metals (WMM) - paramagnetic aluminum metal and indium diamagnetic metal on the indirect exchange interaction in heavy rare-earth metals and to verify the applicability of the RKKY theory for intermetallic compounds in binary systems REM-WMM $REM\text{–}WMM\ (REM = Gd, Tb, Dy, Ho, Er, \mathrm{Tm}; WMM = Al, In)$ using their experimental values θ_p.

II. Results and its discussion.

In a number of works, for example in [6, 7], it was previously established that the dependences $\chi(T)$ of heavy REMs (REMs = Gd, Tb, Dy, Ho, Er, Tm) and their compounds with aluminum and indium in a wide temperature range (300–2000 K), covering their solid state, the melting process and the liquid state, is described by the Curie - Weiss law. From the experimental dependence $\chi^{-1}(T)$, the values θ_p were determined.

In the framework of the RKKY theory, using the molecular field representation to explain the experimental θ_p REM values, the following expression is obtained [1, 5, 8, 9]:

$$\theta_p = \frac{3\pi n^2}{k_Б \Omega^2 E_F} A_{sf}^2(0) G \sum_{n \neq m} F\left(2\vec{k}_F \left|\vec{R}_n - \vec{R}_m\right|\right) \quad (1)$$

where: n - is the number of conduction electrons per atom; Ω - atomic volume; $A_{sf}(0)$ – Integral of the s – f - exchange interaction, independent of $\vec{k}_F$; E_F and $\vec{k}_F$ – energy and wave vector on the Fermi surface; $\left|\vec{R}_n - \vec{R}_m\right|$ - the distance between the rare-earth magnetic ions, located in the nodes of the crystal lattice n and m; $F\left(2\vec{k}_F\left|\vec{R}_n - \vec{R}_m\right|\right) = F(y)$ - Ruderman-Kittel function defined by the expression:

$$F(y) = (y\cos y - \sin y)/y^4 \, ; \quad (2)$$

$$G = (g_J - 1)^2 J(J+1) \quad (3)$$

de Gennes factor [9] for REM. In (3), g_J - the Lande factor is determined by the following expression:

$$g_J = 1 + [J(J=1) + S(S+1) - L(L+1)]/2J(J+1), \quad (4)$$

where: S, LuJ - respectively, the total quantum numbers of the spin, orbital, and total mechanical moments of the electrons of the 4f-layer.

In the framework of the RKKY theory, to calculate the integral of the indirect exchange interaction, the following expression was obtained [1,5]:

$$A = \frac{9\pi n^2}{E_F \Omega^2} A^2{}_{sf}(0) \sum_{n \neq m} F\left(2\vec{k}_F\left|\vec{R}_n - \vec{R}_M\right|\right) \quad (5)$$

Given (5) and (3), from expression (1) we obtain a proportional dependence of the values θ_p for pure rare-earth metals on their de Gennes factor:

$$\theta_p = \frac{A}{3k_Б} G \quad (6)$$

The de Gennes factor for the studied compounds can be calculated by the additivity rule:

$$G = (1 - x)G_{REM} + xG_{WMM} \quad (7)$$

where: is the content of WMM (Al, In) in atomic fractions; $G_{\text{РЗМ}}$ and G_{WMM} – respectively, de Gennes factors for REM and WMM. Since the term of the ground state of the trivalent ion WMM – ${}^1S_0$, therefore $G_{WMM} = 0$. When this fact and (7) are taken into account, for the value θ_P of the studied compounds we find:

$$\theta_P = \frac{A}{k_Б}(1 - x)(g_J - 1)^2 J(J+1) \quad (8)$$

The outer electron shell of trivalent rare-earth ions is almost identical ($5s^2 5p^6$), they are located in the nodes of the crystal hexagonal lattice, which remains almost unchanged when passing from one metal to another. The integral of indirect exchange by (5) depends on n, $A_{sf}(0)$, Ω, E_F and lattice sums (function $F(y)$). To a first approximation, all these quantities can be considered constant [10]. From expression (8) it follows that the values θ_p for the compounds under study should be proportional to the de Gennes factor, similar to pure REMs. Thus, expression (8) makes it possible to semi-empirically verify this prediction of the RKKY theory.

In [6, 7], it was found that the experimental values of the effective numbers of magnetic moments per heavy P3M^{3+} ion, in all studied heavy REMs and compounds with aluminum and indium satisfactorily correspond to the theoretical values of free ions of heavy P3M^{3+}. This indicates that the 4f electrons responsible for the magnetic properties of the objects under study are localized at the sites of their crystal lattice in the same way as in pure heavy rare-earth metals. A weakly magnetic medium (Al, In) and high temperature ($T \approx 2000$ K) do not affect the energy state of 4f electrons in the studied objects.

The energy interval between the ground and first excited levels is large compared to c $k_Б T$, and the population of the excited level is very small. Therefore, when calculating G for heavy rare earth metals and the studied compounds, one can use the values of J and g_J for the basic levels of free ions of heavy rare earth metals:

$$REM^{3+}[Gd^{3+}(J = 7/2,\ g_J = 2);$$

$$Tb^{3+}(J = 6,\ g_J = 3/2);$$

$$Dy^{3+}(J = 15/2,\ g_J = 4/3);$$

$$Ho^{3+}(J = 8,\ g_J = 5/4);$$

$$Er^{3+}(J = 15/2,\ g_J = 6/5);$$

$$Tm^{3+}(J = 6,\ g_J = 7/6)].$$

The results of calculations according to (6) and (8) are presented, respectively, in Fig. 1 and 2. The analysis of Fig. 1 shows that the dependences $\theta_p(G)$ for the studied equiatomic compounds of heavy rare earth metals with aluminum (p. 2-6) are almost linear and satisfactorily correspond to the linear nature of the dependence $\theta_p(G)$ for heavy rare earth metals (p. 1). From Fig. 2 it can be seen that the dependences for the studied equiatomic compounds of heavy rare-earth metals with indium (p. 2-5) also have an almost linear character and satisfactorily correspond to the linear nature of the dependence $\theta_p(G)$ for heavy rare-earth metals (p. 1). Consequently, the change θ_p in the compounds studied is quite close to what the theories of the RKKY. This indicates that the exchange interaction in the studied compounds is an interaction of the RKKY type, as in pure heavy rare-earth metals.

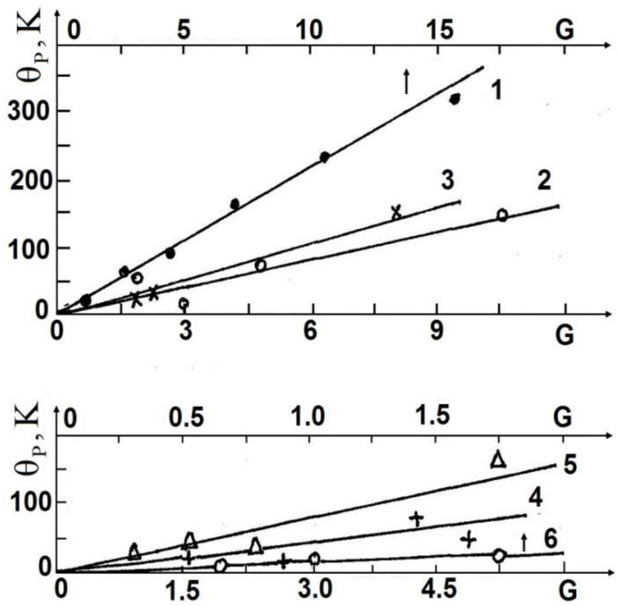

Fig. 1. Dependencies $\theta_p(G)$ for REM compounds with aluminum.

p. 1 - REM (REM = Gd, Tb, Dy, Ho, Er, Tm); p. 2 - REM$_2$ Al; p. 3 – REM Al; p. 4- REM$_3$ Al$_2$; p. 5 - REM Al$_2$; p. 6 - REM Al$_3$.

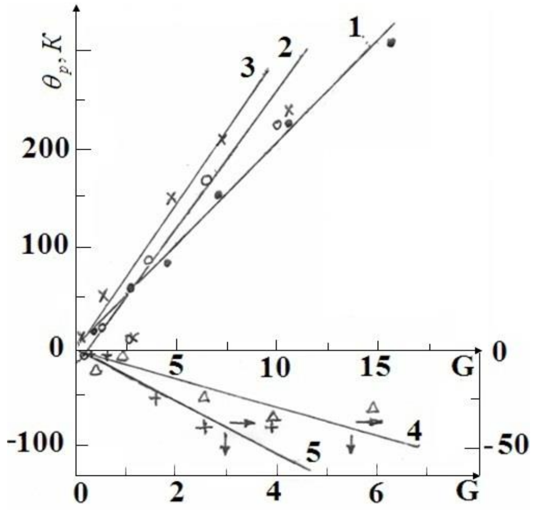

Fig. 2. Dependencies θ_p (*G*) for REM compounds with indium.

p. 1 - REM (REM = Gd, Tb, Dy, Ho, Er, Tm); p. 2- REM_5 In_3; p. 3- REM_2 In;
p. 4 - REM_3 In_5; p. 5 - REM In_3.

III. Conclusions.

1. For the first time, a semi-empirical study confirms the prediction of the theory of the RKKY, i.e. the same proportional relationship between the experimental value of the paramagnetic Curie temperatures and the de Gennes factor for equiatomic compounds of rare-earth metals with aluminum and indium was established, similarly to pure heavy REMs.

2. In general, it was found that for all compounds of the studied REMs (Al, In) systems, as well as for pure heavy REMs, an exchange interaction of the RKKY type is characteristic.

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