MAGNON ENERGY IN THE FERROMAGNETIC PSEUDOBINARY ALLOYS*

By A. Jezierski

Ferromagnetics Laboratory, Institute of Molecular Physics of the Polish Academy of Sciences, Poznań**

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Using the method of effective Hamiltonian and the Coherent Potential Approximation the expression for the magnon energy is derived for the case of the pseudobinary alloys with the SRO. The numerical calculations are made for $Pt_{0.75}(Cr_{1-x}Mn_x)_{0.25}$ alloys.

1. Introduction

In the last few years the problem of magnon energy in the ferromagnetic alloys was investigated intensively. For the long wavelength the magnon energy E_q is given by formula $E_q = Dq^2$, where D is the spin wave stiffness constant and q is the wave vector of magnon.

In this paper we would like to present the new method of calculation of the magnon energy in the pseudobinary ferromagnetic alloys. Recently Morkowski and Jezierski [1] used this method for Ni and Fe based alloys. In this paper we formulate the outline of the method and present the numerical calculations for $Pt_{0.75}(Cr_{1-x}Mn_x)_{0.25}$ alloys.

2. Effective magnon Hamiltonian and equations for coherent potentials

We consider a pseudobinary ferromagnetic alloys $A_{1-c}B_{c(1-x)}Y_{cx}$ where c is the concentration of impurities B and Y, and x is the concentration of one of them. In our case the concentration of Y is cx. The magnetic properties of pseudobinary alloy we shall describe in the term of one band model of ferromagnetism. The system of itinerant electrons may be determined by the Hamiltonian

$$\mathcal{H} = \sum_{l\sigma} \varepsilon_l a_{l\sigma}^+ a_{l\sigma} + \sum_{\substack{lj\sigma \\ l\neq j}}{}' t_{lj} a_{l\sigma}^+ a_{j\sigma} + \sum_l I_l n_{l+} n_{l-}, \tag{1}$$

where ε_l, I_l and t_{lj} denote the atomic potential, Coulomb integral and hopping integral, respectively. Those three parameters take the different values depending on whether sites

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** Address: Zespół Ferromagnetyków, Instytut Fizyki Molekularnej, Polska Akademia Nauk, Smoluchowskiego 17, 60-179 Poznań, Poland.

l and j are occupied by atoms A, B or Y. The operators $n_{l\sigma}$, $a_{l\sigma}^{+}$ are the occupation numbers and the creation operator for electron in the Wannier states at the lattice site R_l with spin σ, respectively. Then we take

$$t_{lj} = \begin{cases} t \text{ if } l \text{ and } j \text{ are the nearest neighbours} \\ 0 \text{ otherwise.} \end{cases} \tag{2}$$

Using the Coherent Potential Approximation we define the coherent Hamiltonian

$$\mathscr{H}_{\mathrm{c}} = \sum_{l\sigma} \varepsilon(\omega) a_{l\sigma}^{+} a_{l\sigma} + \sum_{\substack{lj\sigma \\ l \neq j}}{}' t_{lj} a_{l\sigma}^{+} a_{j\sigma} + \sum_{l} I(\omega) n_{l+} n_{l-}, \tag{3}$$

in which $\varepsilon(\omega)$ and $I(\omega)$ are the coherent potentials. Hamiltonian $\mathscr{H}$ we can rewrite as

$$\mathscr{H} = \mathscr{H}_{\mathrm{c}} + V, \tag{4}$$

where $V = \mathscr{H} - \mathscr{H}_{\mathrm{c}}$ is the perturbation term.

We assume that the ground state $|\phi_0\rangle$ of $\mathscr{H}_{\mathrm{c}}$ is ferromagnetic and we define, as in paper [1], the magnon creation operator for the effective medium

$$\beta_q^{+} = \sum_{k} b_{k+q,k}(\omega) a_{k+q,+}^{+} a_{k,-}, \tag{5}$$

where the value of $b_{k+q,k}(\omega)$ is determined from the equation of motion in the Random Phase Approximation (RPA)

$$[\mathscr{H}_{\mathrm{c}}, \beta_q^{+}]_{\mathrm{RPA}} = E_q \beta_q^{+}, \tag{6}$$

hence

$$\frac{I(\omega)}{N} \sum_{k} \frac{\langle n_{k,-} \rangle - \langle n_{k+q,+} \rangle}{\varepsilon_{k+q} - \varepsilon_k + I(\omega) m - E_q}, \tag{7}$$

$$b_{k+q,k}(\omega) = d_q(\omega) / \Omega_{k,q}(\omega), \tag{8}$$

$$\Omega_{k,q}(\omega) = \varepsilon_{k+q} - \varepsilon_k + I(\omega) m - E_q \tag{9}$$

$$d_q(\omega) = \{\sum_{k} [\Omega_{k,q}(\omega)]^{-2} (\langle n_{k-} \rangle - \langle n_{k+q,+} \rangle)\}^{-1/2}, \tag{10}$$

here $m = n_- - n_+$ and $n_\sigma = N^{-1} \sum_{k} n_{k\sigma}$.

Then we introduce the effective magnon Hamiltonian $\mathscr{H}_{\mathrm{eff}}$ constructed by β_q^{+} operators

$$\mathscr{H}_{\mathrm{eff}} = \sum_{qq'} A(\boldsymbol{q}, \boldsymbol{q}'; \omega) \beta_q^{+} \beta_{q'}, \tag{11}$$

where

$$A(\boldsymbol{q}, \boldsymbol{q}'; \omega) = \langle \phi_0 | [\beta_q, [\mathscr{H}, \beta_{q'}^{+}]] | \phi_0 \rangle. \tag{12}$$

After some manipulations we get

$$A(\boldsymbol{q}, \boldsymbol{q}'; \omega) = E_q \delta_{qq'} + N^{-1} \sum_{j} e^{i\boldsymbol{R}_j \cdot (\boldsymbol{q} - \boldsymbol{q}')} \{[\varepsilon_j - \varepsilon(\omega)] f_{qq'} + [I_j - I(\omega)] h_{qq'}\}, \tag{13}$$

here

$$f_{qq'} = \sum_k \{b_{k+q,k}(\omega) b^*_{k+q',k}(\omega) (\langle n_{k+q',-}\rangle - \langle n_{k+q+q',+}\rangle)$$

$$- b_{k+q+q',k+q'}(\omega) b^*_{k+q+q',k+q}(\omega) (\langle n_{k+q',-}\rangle - \langle n_{k+q+q',+}\rangle)\}, \tag{13a}$$

$$h_{qq'} = \sum_k \{b_{k+q,k}(\omega) b^*_{k+q',k}(\omega) n_- - b_{k+q,k}(\omega) b^*_{k+q,k+q-q'}(\omega) n_+\} \{\langle n_{k-}\rangle$$

$$- \langle n_{k+q,+}\rangle\} - N[I(\omega)]^{-2} d_q(\omega) d^*_{q'}(\omega). \tag{13b}$$

The perturbation term V determines the scattering of magnons on the local fluctuations of the atomic and Coulomb potentials, therefore we calculate the magnon energy for small wave vector. The magnons of large wave vectors are highly damped by the scattering on local fluctuations. For the small $\boldsymbol{q}$ vectors expressions (13a–b) assume the form

$$f_{qq'} = F(\boldsymbol{q} - \boldsymbol{q}') \cdot \boldsymbol{q}', \tag{14}$$

$$h_{qq'} = B\boldsymbol{q} \cdot \boldsymbol{q}' + C\boldsymbol{q}' \cdot \boldsymbol{q}', \tag{15}$$

where

$$F = 2\beta_1/\Delta, \quad \Delta = I(\omega)m, \quad C = Fn_+,$$

$$\alpha_1 = (3mN)^{-1} \sum_k |\nabla \varepsilon_k|^2 (\langle n_{k-}\rangle - \langle n_{k+}\rangle),$$

$$\beta_1 = (6mN)^{-1} \sum_k \nabla^2 \varepsilon_k (\langle n_{k-}\rangle + \langle n_{k+}\rangle). \tag{16}$$

The equations for the coherent potentials $\varepsilon(\omega)$ and $I(\omega)$ we find using the Green function method. The magnon Green function $G_{qq'}(\omega)$ satisfies the following equation

$$G_{qq'}(\omega) = g_q \delta_{qq'} + g_q \sum_k A_{qk} G_{kq'}(\omega), \tag{17}$$

here

$$g_q = (\omega - E_q)^{-1}, \tag{18}$$

$$A_{qk} = A(\boldsymbol{q}, \boldsymbol{k}; \omega) - E_q \delta_{qk}. \tag{19}$$

Equation (17) can be written in the term of magnon T-matrix

$$G_{qq'}(\omega) = g_q \delta_{qq'} + g_q T_{qq'} g_{q'}, \tag{20}$$

where T-matrix is given by

$$T_{qq'} = A_{qq'} + \sum_k A_{qk} g_k T_{kq'}. \tag{21}$$

Taking the configurational average of Eq. (20) we get

$$\langle G_{qq'}(\omega)\rangle = g_q \delta_{qq'} + g_q \langle T_{qq'}\rangle g_{q'}. \tag{22}$$

In the CPA we put $\langle T_{qq'}\rangle = 0$ and we get the conditions for the coherent potentials $\varepsilon(\omega)$ and $I(\omega)$. The magnon energy is determined by the pole of average Green function $\langle G_{qq'}(\omega)\rangle$.

In the Wannier representation equation (21) may be written as

$$T_{lj} = A_{lj} + \sum_{mn} A_{lm} g_{mn} T_{nj}, \tag{23}$$

where

$$T_{lj} = N^{-1} \sum_{qq'} e^{-i(ql - q'j)} T_{qq'}, \tag{24}$$

$$A_{lj} = N^{-1} \sum_{qq'} e^{-i(ql - q'j)} A_{qq'}, \tag{25}$$

$$g_{mn} = N^{-1} \sum_{q} e^{-i(m-n)q} g_q. \tag{26}$$

In order to solve equation (23) we assume the cluster model in which we consider the interaction between central atom and its nearest neighbours. In the cluster model the T-matrix elements have the form

$$T_{lj} = T^1_{\beta\gamma} = \frac{\tau_{lj}[1 + t_j(g_0 + R_{lj} g_1)]}{1 - \tau_{lj} t_j (g_0 + R_{lj} g_1)\,(g_0 R_{jl}^{-1} + g_1)}, \tag{27}$$

where β and γ denote the type of atom in l or j site, and

$$T_{ll} = T^0_{\beta\beta} = t_l[1 + g_1 \sum_{j \neq l}' T_{jl} + g_0 \sum_{j \neq l}' A_{lj} T_{jl}]. \tag{28}$$

The summation includes only nearest neighbours.

$$\tau_{lj} = A_{lj}/(1 - (A_{ll} g_0 + A_{lj} g_1)), \tag{29a}$$

$$t_j = A_{jj}/(1 - A_{jj} g_0), \tag{29b}$$

$$R_{lj} = A_{ll}/A_{lj}, \tag{29c}$$

$$g_0 = g_{ll} = N^{-1} \sum_{q} (\omega - E_q)^{-1}, \tag{29d}$$

$$g_1 = g_{lj} = N^{-1} \sum_{q} e^{iq \cdot (R_l - R_j)} (\omega - E_q)^{-1}. \tag{29e}$$

The configurational average of T-matrix elements we can calculate if we introduce c_l^β quantities as follows:

$$c_l^\beta = \begin{cases} 1 \text{ if site } l \text{ is occupied by } \beta \text{ atom} \\ 0 \text{ otherwise.} \end{cases} \tag{30}$$

The using the definitions

$$\langle c_l^\beta c_j^\gamma \rangle = c^\beta \delta_{\beta\gamma} + c^\beta c^\gamma (1 - \alpha), \quad l \neq j, \tag{31}$$

here α is the SRO parameter, we can write

$$\langle T_{lj} \rangle = \sum_{\beta\gamma} \langle c_l^\beta c_j^\gamma \rangle T^1_{\beta\gamma}, \tag{32}$$

and

$$\langle T_{lc} \rangle = T^0_{AA} + c[T^0_{BB} - T^0_{AA} + x(T^0_{YY} - T^0_{BB})]. \tag{33}$$

From conditions (32)–(33) we get the selfconsistent equations for coherent potentials $\varepsilon(\omega)$ and $I(\omega)$.

3. *Numerical results for the pseudobinary ferromagnetic $Pt_3Cr_{1-x}Mn_x$ systems*

We tested our model for $Pt_{0.75}(Cr_{1-x}Mn_x)_{0.25}$ system. To start with we present, in a short form, the magnetic and structural properties of $Pt_3Cr_{1-x}Mn_x$ alloys for $0 \leqslant x \leqslant 1$. For all x the alloys crystallize in the Cu_3Au type structure. Pt-Cr systems have f.c.c. structure up to 60 at % Cr, but Pt–Mn alloys crystallize up to 40 at % Mn. The maximum of magnetization is about 25 at % Cr or Mn. First measurements for Pt-Cr system were made by Kussmann et al. [2]. The neutron diffraction measurements (Pickart and Nathans [3]) showed that Pt_3Cr alloys are ferrimagnetics with two sublattices. The magnetic properties of ordered and disordered Pt-Cr systems were investigated by Bessnus and Meyer [4] and the dependence on the effects of the atomic environment was studied by Goto [5].

However, the atomic structure and ferromagnetic properties of PtMn alloys were investigated by Sidorov and Dubinin [6]. Menzinger et al. [7] reported the local antiferromagnetic ordering in ferromagnetic Pt_3Mn alloys near the stoichiometric composition. The experimental investigations of Pt_3Cr and Pt_3Mn alloys indicate the existence of the phase transition from the ferrimagnetic to ferromagnetic state.

Recently, Williams and Lewis [8] studied the magnetic properties of pseudobinary $Pt_3Mn_xCr_{1-x}$ systems, and they found the region of concentration x ($0.2 \leqslant x \leqslant 0.5$) in which the phase transition takes place. From the magnetization measurements Williams and Lewis estimated the values of spin wave stiffness constant D for $Pt_3Cr_xMn_{1-x}$ alloys. The dependence of D vs x is very interesting, because for $0.1 \leqslant x \leqslant 0.9$ the values of D are almost constant and equal to $\frac{1}{3}D$ for $x = 0$ or $x = 1$.

In this section we present the numerical calculations of the spin wave stiffness constant for the $Pt_{0.75}(Cr_{1-x}Mn_x)_{0.25}$ system in which the short range order exists. Such system is not quite equivalent to $Pt_3Cr_{1-x}Mn_x$ alloys but we think that the theoretical results for $Pt_{0.75}(Cr_{1-x}Mn_x)_{0.25}$ system may be compared with experimental results for $Pt_3Cr_{1-x}Mn$ alloys. In the numerical calculations we consider the one band model of ferromagnetism. The energy of electron ε_k was taken in the tight binding approximation for the f.c.c. structure. We assume the bandwidth of alloy as for Pt [9]. The spin wave stiffness constant we got from the solution of equations (32)–(33) for the following values of parameters.

$$\varepsilon_{Pt} = \varepsilon_{Mn} = \varepsilon_{Cr} = 0, \quad u = I_{Mn} - I_{Pt}, \quad w = I_{Cr} - I_{Pt}.$$

The short range order parameter α we take as $-\frac{1}{3}$. The sums like $N^{-1}\sum_k |\nabla\varepsilon_k|^2$ and $N^{-1}\sum_k \nabla^2\varepsilon_k$ were calculated by integration over $\frac{1}{8}$ at the first Brillouin Zone for the f.c.c. lattice [10]. For the simplification of the numerical calculations we take the Debye type

of density of magnon states to calculate sums like equation

$$N^{-1}\sum_{k} k^2 e^{ik\cdot R} = -\frac{d^2 f(R)}{dR^2} - \frac{2}{R}\left(\frac{df(R)}{dR}\right), \tag{34}$$

where

$$f(R) = 3(\sin x - x\cos x)/x^3, \quad x = \kappa_D R \tag{35}$$

and κ_D is the Debye wave vector determined by the condition

$$\frac{4\pi}{3}\kappa_D^3 = \frac{(2\pi)^3}{v} N, \tag{36}$$

where v is the volume of the sample and N is the number of electrons. The magnon Green function g_0 was calculated using the lattice Green function [11].

For $I_{Pt} = 1.5$ eV the dependence of D vs concentration x changes insignificantly for different values of u and w (figure 1*a* and *b*). The completely different dependence of D

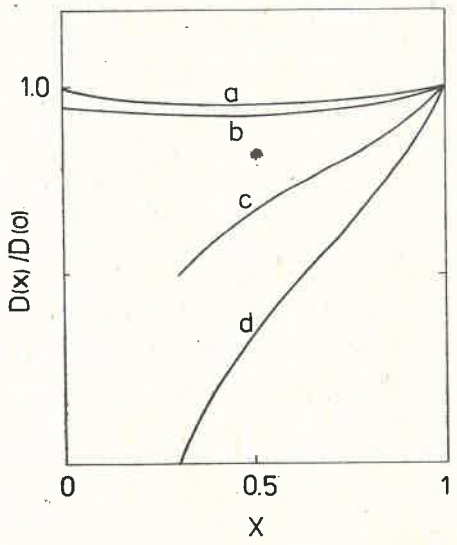

Fig. 1. The dependence of the spin wave stiffness constant D vs concentration x for $Pt_{0.75}(Cr_{1-x}Mn_x)_{0.25}$ alloy for different values of parameters: a — $u = -0.2$, $w = -0.2$; b — $u = -0.2$, $w = -1.0$; c — $u = 0.1$, $w = -0.1$; d — $u = -0.1$, $w = 0.1$

vs x we got for $I_{Pt} = 0.5$ eV (figure 1*c* and *d*). The change of u and w gives different inclination of $D(c)$. The values of I_{Pt} were fitted so to have the subband with spin down completely filling. Our theoretical modelcorre sponds incompletely to the physical situation in $Pt_3Cr_{1-x}Mn_x$ alloys. In the theoretical consideration we assumed that the system has the short range order and we took the cluster consisting of $Z+1$ atom (Z is a number of nearest neighbours). The theoretical results may be compared with experimental data only in the ferromagnetic region. For $I_{Pt} = 1.5$ eV the theoretical results D vs x have similar dependence as experimental data [8].

4. Conclusions

The problem of magnon energy in the pseudobinary $Pt_3Cr_{1-x}Mn_x$ systems is very interesting but it is complicated. In this paper we used the simple theoretical model and calculated the average exchange contribution to the stiffness constant. The previous papers (Edwards and Fung [12], Morkowski and Jezierski [1]) showed the role of magnon scattering contribution to the stiffness constant. For Pt-Mn-Cr systems the magnon scattering contribution may be significant. The present calculations give the first information about dependence D vs concentration in pseudobinary $Pt_{0.75}(Cr_{1-x}Mn_x)_{0.25}$ system with the short range order.

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