

Contribution of magnons to the properties of [Co/Ag] super lattice

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Abstract: In this work we study the elementary excitations and the magnetic properties of super lattice [Co/Ag]. The study is obtained in framework of the Heisenberg model for a ferromagnetic system made of N atomic planes. The exchange and the dipolar interactions, the magneto-crystalline anisotropy and surface anisotropy are all taking in account. In the presence of the exchange alone, the analytical expressions of the excitation spectrum $E(k)$ and the magnetization per spin $m(T) = \langle S_z \rangle / S$ are obtained using the Green function formalism. The values of the exchange integrals deduced from the comparison of $m(T)$ with experimental measurements are in good agreement with results of previous studies for analogous magnetic super lattices. A numerical study of the combined effect of dipolar interactions and surface anisotropy is also reported.

I- Introduction

Recently, more interest was given to the study of the magnetic multi-layers. Their new properties gave rise to several applications in various technological fields such as the micro-electronics and the magneto-optical recording. Thus several experimental and theoretical studies were carried out to try a comprehension of the various interactions intervening in this type of systems [1-8]. In this work, we study the contribution of magnons to the magnetic properties of the super lattices [Co/Ag]. The excitation spectrum and magnetization per spin were calculated within the framework of the spin waves theory. For this type of systems, symmetry is broken along the axis perpendicular to the film plan; what implies a discrete treatment along this axis. The combined effect of the dipolar interactions and the surface anisotropy, much more important in rough surfaces and interfaces [9-11], plays an important role in a long range magnetic stability of the quasi-two-dimensional systems. We introduced them into the corresponding Heisenberg Hamiltonian of exchange. The calculated excitation spectra and magnetization per site are in coherence with what we had obtained before for similar magnetic super lattices [M/Cu] containing 3d transition metals M= Ni, Fe, Co and (Ni-Fe) alloys [12-14]. The comparison between calculated and measured magnetization per spin is very satisfactory leading to the exchange integral values coherent with the values usually found for super lattices containing these transition metals.

II - General formulation

We consider a super lattice [Co/Ag] made up of a cobalt layer with N atomic plans ferromagnetically coupled and deposited on another layer of silver. In a configuration where the easy magnetization axis (OZ) is perpendicular to the plan of magnetic film (OXY). The corresponding Heisenberg hamiltonian including, in addition to the exchange and dipolar interactions the surface and magneto-crystalline anisotropies, can be written [12-14]

$$\mathcal{H} = - \sum_{\langle ij \rangle} J_{ij}^{\parallel} (S_i^x S_j^x + S_i^y S_j^y + \Delta S_i^z S_j^z) - \sum_{\langle ii' \rangle} J_{ij}^{\perp} (\vec{S}_i \vec{S}_{i'}) + \frac{g^2 \mu_B^2}{2} \sum_{\langle ij \rangle} \frac{1}{r_{ij}^3} \left\{ \vec{S}_i \vec{S}_j - 3 \frac{(\vec{S}_i \vec{r}_{ij})(\vec{S}_j \vec{r}_{ij})}{r_{ij}^2} \right\} + \alpha \sum_i (S_i^y)^2 \quad (1)$$

J_{ij}^{\parallel} indicates the exchange integral between the first neighbors in the same plan. J_{ij}^{\perp} is the exchange integral between the first neighbors belonging to different plans. α and Δ are respectively the surface anisotropy and the magneto-crystalline anisotropy. By carrying out the Fourier and Holstein-Primakoff transformations [15], the hamiltonian (1) is written:

$$\mathcal{H} = \sum_{l,m} \sum_k \left\{ A_{lm}(k) a_{k,l}^+ a_{k,m} + \frac{1}{2} B_{lm} (a_{k,l}^+ a_{-k,m}^+ + a_{k,l} a_{-k,m}) \right\} \quad (2)$$

A_{lm} and B_{lm} are obtained for the plans l and m

($1 \leq l \leq N$ et $1 \leq m \leq N$) such that:

$$A_{lm}(k) = S \left\{ \sum_{\gamma_{\parallel}} \left[2J_{\gamma_{\parallel}}^{\parallel} (\Delta - \cos(k_{\parallel} \gamma_{\parallel})) + D_{\gamma_{\parallel}} \left(\left(1 - \frac{3}{2} \left(\frac{r_{\gamma_{\parallel}}^x}{r_{\gamma_{\parallel}}} \right)^2 \right) \cos(k_{\parallel} \gamma_{\parallel}) - \left(1 - 3 \left(\frac{r_{\gamma_{\parallel}}^y}{r_{\gamma_{\parallel}}} \right)^2 \right) \right] \right. \right. \\ \left. \left. + \sum_{\gamma_{\perp}} \left(2J_{\gamma_{\perp}}^{\perp} + D_{\gamma_{\perp}} \left(3 \left(\frac{r_{\gamma_{\perp}}^x}{r_{\gamma_{\perp}}} \right)^2 - 1 \right) \right) (2 - \delta_{l,1} - \delta_{l,N}) - \alpha (\delta_{l,1} + \delta_{l,N}) \right\} \delta_{l,m} \right. \\ \left. - S \left[2 \sum_{\gamma_{\perp}} J_{\gamma_{\perp}}^{\perp} \cos(k_{\parallel} \gamma_{\perp}) - D_{\gamma_{\perp}} \left(1 - \frac{3}{2} \left(\frac{r_{\gamma_{\perp}}^x}{r_{\gamma_{\perp}}} \right)^2 \right) \cos(k_{\parallel} \gamma_{\perp}) \right] (\delta_{l,m-1} + \delta_{l,m+1}) \right] \quad (3)$$

$$B_{lm}(k) = S \left(- \frac{3}{2} \sum_{\gamma_{\parallel}} D_{\gamma_{\parallel}} \left(\frac{r_{\gamma_{\parallel}}^x}{r_{\gamma_{\parallel}}} \right)^2 \cos(k_{\parallel} \gamma_{\parallel}) + \alpha (\delta_{l,1} + \delta_{l,N}) \right) \delta_{lm} \\ - \frac{3}{2} S \sum_{\gamma_{\perp}} D_{\gamma_{\perp}} \left(\frac{r_{\gamma_{\perp}}^x}{r_{\gamma_{\perp}}} \right)^2 \cos(k_{\parallel} \gamma_{\perp}) (\delta_{l,m-1} + \delta_{l,m+1}) \quad (4)$$

$r_{\delta_{ij}} = (r_{\delta_{ij}}^x, r_{\delta_{ij}}^y, r_{\delta_{ij}}^z)$ is the vector binding a site with its first neighbors in the same plan. $r_{\gamma_{\perp}} = (r_{\gamma_{\perp}}^x, r_{\gamma_{\perp}}^y, r_{\gamma_{\perp}}^z)$ is the vector binding two sites first neighbors belonging to two different plans and $D = \frac{g^2 \mu_B^2}{(r)^3}$ is the dipolar interaction constant.

The excitation spectrum is obtained by diagonalizing the hamiltonian using the method of Green functions defined by:

$$G_{k,m} = \langle\langle a_{k,l}, a_{k,m}^+ \rangle\rangle \quad \text{and} \quad G_{k,m}' = \langle\langle a_{-k,l}^+, a_{k,m}^+ \rangle\rangle.$$

The movement equations of these Green functions lead to a 2N coupled equation system represented in matrix form by:

$$\begin{bmatrix} A-E & B \\ -B & -A-E \end{bmatrix} \begin{bmatrix} G & 0 \\ G' & 0 \end{bmatrix} = \frac{-1}{2\pi} \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \quad (5)$$

A and B are matrices whose elements are given by equations (3) and (4).

III- Effect of the exchange alone. Results and discussion

3-1 Excitation spectrum

In 3d transition metals like cobalt, the effect of the magnetic exchange is largely more important than that of the anisotropy and the dipolar interactions. In this paragraph, we treat the effect of the exchange alone. The correction owing to the anisotropy and dipolar will be analyzed later on. Consequently, by neglecting at once the dipolar interactions and the surface anisotropy ($D = \alpha = 0$), the hamiltonian (2) becomes:

$$\mathcal{H} = \sum_{lm} \sum_k A_{lm}(k) a_{k,l}^+ a_{k,m} \quad (6)$$

The excitation spectrum $E(k)$ is obtained by solving the equation system:

$$\text{Det}[A - EI] = 0 \quad (7)$$

A resolution of (7) similar to that we made in a former work for analogous magnetic super lattices [12-14] gives the general form of the excitation spectrum for a plan l as:

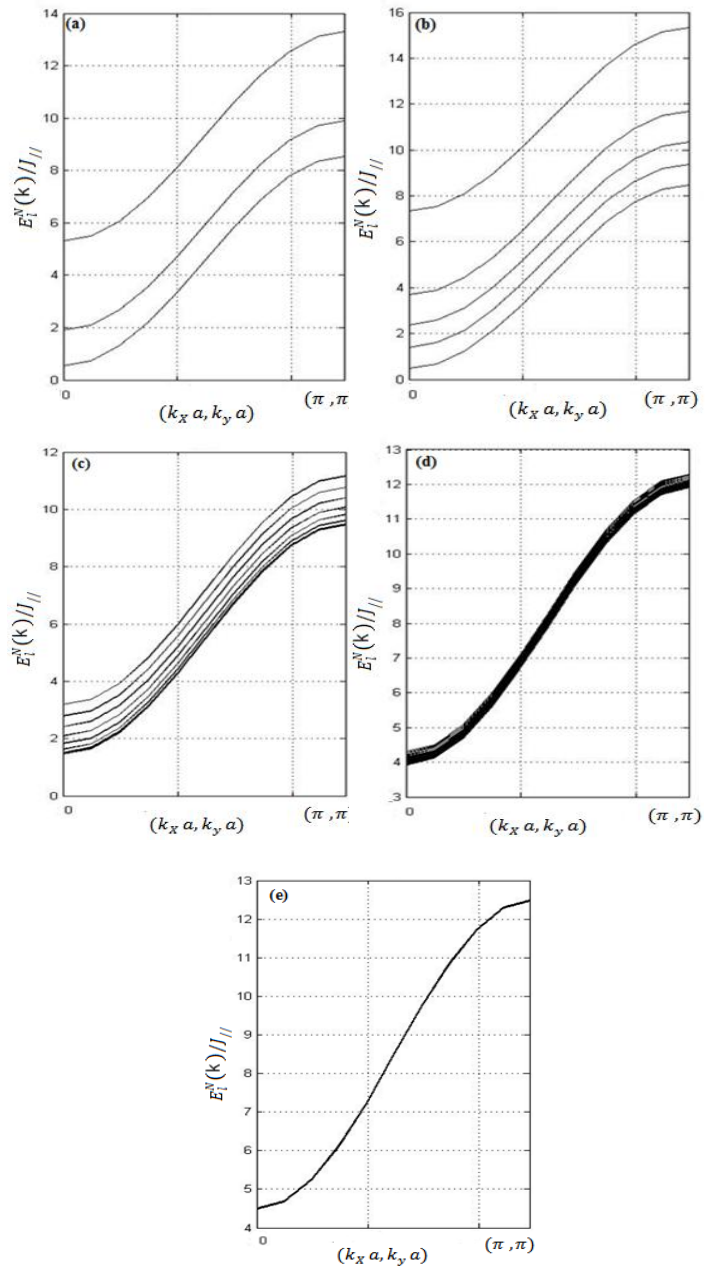
$$E_l^N(k) = A(k) + \varepsilon_l^N W(k) \quad (8)$$

with

$$A(k) = A_{11}(k) ; \quad W(k) = -A_{12}(k)$$

ε_l^N is a series of values specifying the solutions of (7). We note that for low numbers N, ε_l^N takes a number of distinct values equal to the number of plans N (see figures 1a and b) agreeing with results of former studies [12-14, 16]. This complete discernability of the magnon states by plan is probably due to the effect of the interfaces between plans which are responsible for the break of symmetry along the axis perpendicular to the film plan in the super lattice. The intrinsic differences between these interfaces lead to

discrete values of wave vector and consequently to a lifting of the $E_l^N(k)$ state degeneracy. On the other hand, more the number N of magnetic plans increases more the number of modes differs from N (figures 1c and d). In limit cases where $N \gg 1$, there is no more than only one completely degenerated mode of created magnons (figure 1e). This can be amongst other things allotted to the influence of the volume effect compared to that of the interfaces. When the number N of magnetic plans increases the volume of the sample becomes more and more dominating and at the limit of the great numbers $N \gg 1$ the effect of the intrinsic differences between interfaces is masked and the magnon states become completely degenerated.



Figures 1: Excitation spectra calculated for the super lattices $[\text{Co}(\text{t}_{\text{Co}})/\text{Ag}]$ with:

(a) $t_{Co} = 6 \text{ \AA}$ ($N=3$); (b) $t_{Co} = 10 \text{ \AA}$ ($N=5$); (c) $t_{Co} = 32 \text{ \AA}$ ($N=16$); (d) $t_{Co} = 57 \text{ \AA}$ ($N=30$) and (e) a thick magnetic layer $N(\text{Co}) \gg 1$. The silver thickness t_{Ag} is of 50 \AA .

We in addition notice that for all the values of magnetic layer thickness t_{Co} (i.e. of N), there is an energy threshold E_{Thres}^N corresponding to the lower energy level in the spectra. We define this threshold as a creation gap of magnons which we noted as E_g . This gap depends on the anisotropy and it is responsible for the existence of a long rang magnetic order. A quantitative analysis of the gap level according to the parameters (Δ and J_{\perp}/J_{\parallel}) in the vicinity of $k_{//} = (0, 0)$, leads to build a phase diagram $E_g = E(k) = 0$ which is represented on the figure (2) with:

$$E_g = A_{11}(k) - W = 8J_{\square} S(\Delta - 1) - 2J_{\perp} S \quad (9)$$

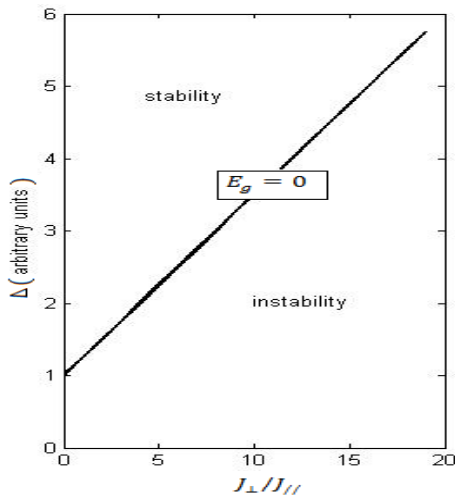


Figure 2: Phase diagram representing the variation of magneto-crystalline anisotropy Δ according to the J_{\perp}/J_{\parallel} ratio corresponding to a gap equal to zero.

The curve $E_g = 0$ represents an equilibrium situation. It corresponds to a statistical ensemble of micro-states where one can consider that the super lattice consists of an inhomogeneous collection of micro domains or clusters where the number of clusters with a stable magnetic order is equal to that of the other clusters with an unstable magnetic order. According to the ratio of the numbers of these two cluster types, the system is stable or unstable. We also note that in absence of anisotropy ($\Delta = 1$) the long range magnetic order is unstable in the super lattice for any value of the exchange. Whereas, as soon as $\Delta > 1$, there is appearance of a field of stability whose expanse increases more and more that Δ increases. When the ratio of exchange J_{\perp}/J_{\parallel} increases, the stability of the macro-

state is obtained only if the magneto-crystalline anisotropy increases too. This is coherent with the fact that in the two-dimensional systems, it is the anisotropy which is responsible for the long range magnetic order and not the exchange alone [17-19].

We also tried an exploitation of the existence of a magnon creation gap E_g in the studied super lattices [Co/Ag] in order to estimate a relaxation time τ of the magnetic elementary excitation states following the same reasoning as we had made before for similar super lattices [M/Cu] with $M = \text{Ni, Fe, Co}$ and Ni-Fe binary alloys [12-14]. The obtained τ values are gathered on table 1.

Table 1. Relaxation time of the created magnon states.

t(Co)	6Å	10Å	32Å	57Å
τ (s)	$8 \cdot 10^{-13}$	$7 \cdot 10^{-13}$	$2 \cdot 10^{-13}$	$9 \cdot 10^{-14}$

The reduction in the length of life τ with increasing magnetic thickness t_{Co} suggests that the contribution of magnons to the system properties is more important for super lattices with finer magnetic layers. Very fast decrease of the $\tau(t_{Co})$ function for thick magnetic layers gives a measurement of the impact of volume effect compared with the interface one. Surfaces and interfaces seem to support the created magnon states in these super lattices.

3-2. Magnetization per spin

3-2-1. The results of calculations

The expression of the spin wave contribution to the average magnetization per site of the super lattice is written:

$$\begin{aligned} m(T) &= \frac{\langle S_z \rangle}{S} = 1 - \frac{1}{S} \frac{1}{N} \frac{s}{(2\pi)^2} \sum_{l=1}^N \int_{BZ} \langle a_{k,l}^+ a_{k,l} \rangle dk_x dk_y \\ &= 1 - \frac{1}{S} \frac{1}{N} \frac{s}{(2\pi)^2} \sum_{l=1}^N \int \frac{1}{\exp\left(\frac{E_l^N(k)}{k_B T}\right) - 1} dk_x dk_y \end{aligned} \quad (10)$$

s is the surface of the elementary cell, k_B is the Boltzmann constant and $\langle a_{k,l}^+, a_{k,l} \rangle$ is the average number of magnons. The excitation spectrum $E_l^N(k)$ for a plane l is given by the equation (8).

The integral of the equation (10) can be calculated analytically in the range of the low temperatures ($T \leq T_c/3$). Indeed the principal contribution of the spin waves to the super-lattice properties comes primarily from the modes with weak wave vectors ($k = 2\pi/\lambda \ll 1$) making it possible to develop $E_l^N(k)$ in the vicinity of

$k_{//} = (0, 0)$. Let us put $\xi = k_x a \ll 1$ and $\eta = k_y a \ll 1$ such as :

$$1 - \cos \frac{k_x a}{2} \approx \frac{1}{2} (\xi/2)^2 ;$$

$$1 - \cos \frac{k_y a}{2} \approx \frac{1}{2} (\eta/2)^2 \text{ and} \quad (11a)$$

$$\rho^2 = \xi^2 + \eta^2 \quad (11b)$$

By carrying out a transformation to polar coordinates (11b), the preceding development leads to an expression of the excitation spectrum as:

$$E_l(k) = 8S J_{\square} (\Delta - 1) + J_{\square} S \rho^2 + 2J_{\perp} S (1 + \varepsilon_l) \quad (12)$$

By incorporating the formula (12) in the equation (10) one obtains:

$$m(T) = 1 - \frac{1}{4\pi} \frac{1}{N} \frac{k_B T}{2JS} \sum_{i=1}^N \text{Ln} \left\{ 1 - \exp \left[-(\Delta' + 2J_{\perp} S (1 + \varepsilon_l)) / k_B T \right] \right\} \quad (13)$$

$$\Delta' = 8S J_{\square} (\Delta - 1).$$

For a great atomic plan number ($N \rightarrow \infty$), the super lattice becomes voluminal and continuous. Consequently,

the summation $\frac{1}{N} \sum_{i=1}^N$ is replaced by $\frac{a}{2\pi} \int_{-\pi/a}^{\pi/a} dk_z$ and

the term $2J_{\perp} S (1 + \varepsilon_l)$ describing the interactions between plans takes the form $4J_{\perp} S (1 - \cos k_z a) \approx 2J_{\perp} S (k_z a)^2$ for $k_z a \ll 1$

By analyzing the relative importance of the excited magnon number fluctuations in connection with the width of the thermal fluctuation spectrum, we obtained as for the previously studied super-lattices M/Cu and in the low temperature range $k_B T \ll \varepsilon_l^N(k)$:

$$m(T) = 1 - \frac{1}{2NS J_{\square}} \left(\frac{k_B}{2\pi} \right)^{3/2} \frac{1}{(2SJ_{\perp})^{1/2}} g_{3/2}(z) T^{3/2} \quad (14)$$

Where $g_{3/2}(z)$ is Bose's function and $z = e^{\frac{\Delta'}{k_B T}}$ is the magnon gas fugacity whose significant contribution to the super lattice properties is obtained at the limit $g_{3/2}(z \rightarrow 1)$. The expression (14) thus obtained corresponds well to the usual Bloch-law for the systems in volume (3D).

In the range of higher temperatures such as: $E_l^N(k) \square k_B T \leq k_B T_C / 3$, $m(T)$ is written:

$$m(T) = 1 - \frac{k_B}{4\pi N 2 J_{\square} S} T \text{Ln} \left\{ \frac{2k_B}{(\Delta' + 2SJ_{\perp}) \left[1 + \left[1 - (4SJ_{\perp} / (\Delta' + 4SJ_{\perp}))^2 \right]^{1/2} \right]} T \right\} \quad (15)$$

The expression (15) then described a behavior known for quasi-bidimensional systems (2D). The logarithmic factor is a consequence of the coupling between the atomic plans. In absence at once of this coupling ($J=0$) and anisotropy ($\Delta=1$) this factor diverges for any non-zero value of the temperature T. This confirms the suggestion deduced from the analysis above concerning the existence of a gap of magnon creation and that in this type of systems a ferromagnetic order can exist only in the presence of the anisotropy.

3-3-2. Comparison between $m(T)$ calculated and measurement results

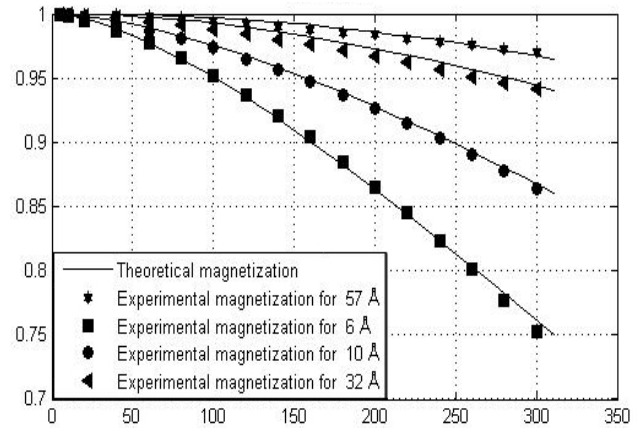


Figure 3: Comparison of the thermal evolution of magnetization per spin calculated $m_{calc}(T)$ (continuous line) with the experimental values $m_{mes}(T)$ (symbols) for various thicknesses of the magnetic layer.

We reported on figure 3 the evolution of the measured values of magnetization per spin $m_{mes}(T)$ (symbols), for various thicknesses of the cobalt layer and for a fixed silver thickness layer $t_{Ag} = 50 \text{ \AA}$, compared with those calculated $m_{calc}(T)$ starting from the expression (10) above (continuous lines).

It arises thus from the adjustment of $m_{calc}(T)$ with $m_{mes}(T)$ the existence of a very good agreement. What enabled us to deduce from the values of the exchange integral J presented on table 2. These values thus obtained are coherent with the values of J usually found for this type of super lattices containing 3d- transition metals like cobalt. What would suggest that the exchange in this type of super lattices is owing to the mixture of the

s and d states of the transition metal with prevalence of d character at the Fermi level. The d states of these metals are indeed located enough, which could explain this agreement with computed values within the framework of the Heisenberg model designed at the origin for localized moments. Moreover, this agreement between $m_{calc}(T)$ and $m_{mes}(T)$ confirm the existence of a dimensionality crossover (3D-2D) in the behavior of the super lattices [Co/Ag]. Indeed, when the temperature of the samples increases, $m(T)$ pass from an evolution in a $T^{3/2}$ - law for the low temperatures (eq. (14)) as for the 3-dimension systems to a quasilinear evolution in $T \ln T$ (eq. (15)) known for the 2-dimension systems. This behavior of dimensionality crossover was also observed for similar magnetic super lattices [M/Cu] previously studied [12-14].

Table 2: Values of the exchange integrals and the creation gap energy of magnons calculated for various thicknesses of the cobalt layer.

t(Co)	6Å	10Å	32Å	57Å
$J_{\perp}(K)$	157	190	200	205
Eg(K)	8.5	9.7	28.4	80.6

IV- Combined effect of the surface anisotropy and dipolar interaction

To study the effect of the simultaneous presence of the surface anisotropy and dipolar interactions on the properties of the super lattices [Co/Ag], we start again from the previous equation (10):

$$m(T) = \frac{\langle S_z \rangle}{S} = 1 - \frac{1}{S} \frac{1}{N} \frac{s}{(2\pi)^2} \sum_{l=1}^N \int_{BZ} \langle a_{k,l}^+ a_{k,l} \rangle dk_x dk_y$$

The average number of spin waves $\langle a_{k,l}^+, a_{k,l} \rangle$ intervening in this expression is calculated using the spectral theorem allowing a relation between this number and the Green functions $\langle\langle a_{k,l}^+, a_{k,l} \rangle\rangle$ such as:

$$\langle a_{k,l}^+ a_{k,l} \rangle = -2 \int \frac{\text{Im} \langle\langle a_{k,l}^+, a_{k,l} \rangle\rangle}{e^{\beta E_l(k)} - 1} dk_x dk_y \quad (16)$$

The Green functions $G_{l,l} = \langle\langle a_{k,l}^+, a_{k,l} \rangle\rangle$ are expressed, according to the matrices of passage P and its reverse P^{-1} allowing the resolution of the system of equations (5), by:

$$\langle a_{k,l}^+ a_{k,l} \rangle = \sum_{n=1}^N \left[\frac{P_{ln} P_{nl}^{-1} - P_{ln'} P_{n'l}^{-1}}{e^{\beta E_l(k)} - 1} - P_{ln'} P_{n'l}^{-1} \right] \quad (17)$$

with $n' = N + n$

Magnetization per spin is given then by:

$$m(T) = 1 - \frac{1}{S} \frac{1}{N} \frac{s}{(2\pi)^2} \sum_{l=1}^N \sum_{n=1}^N \int_{BZ} \left[\frac{P_{ln} P_{nl}^{-1} - P_{ln'} P_{n'l}^{-1}}{e^{\beta E_l(k)} - 1} - P_{ln'} P_{n'l}^{-1} \right] dk_x dk_y \quad (18)$$

The integration is made in Brillouin zone.

An analytical expression of magnetization is clearly more complex to obtain starting from the formula (18) than in case treated in paragraph III above where anisotropy of surface (α) and the dipolar one (D) both are considered absent ($\alpha = D = 0$). We will limit ourselves consequently to the numerical study of the combined effects of the surface anisotropy and the dipolar interactions.

On the figure (4) we present a phase diagram describing the thermal evolution of the combined relative effects of the two factors α and D on the magnetic state of the studied super lattice through a measurement of the ratio $\rho_N(T, R)$ of magnetization when these two factors contribute differently ($R = \alpha/D \neq 1$) and if they contribute with the same weight ($R = 1$) such as:

$$\rho_N(T, R) = \frac{m(T, R \neq 1)}{m(T, R = 1)}$$

Thus, in comparison with the case where $R = 1$, we note that when the anisotropy of surface dominates ($R > 1$) magnetization increases; whereas in the case where the dipolar interactions are preponderant ($R < 1$), magnetization decreases. The dipolar interactions indeed tend to align the magnetic moments parallel to the film plan, whereas the anisotropy aligns the magnetic moments perpendicular to this plan and consequently favours magnetization and reinforces the stability of the magnetic order.

V- Conclusion

The study of properties of the magnetic super lattice [Co/Ag], for fixed t_{Ag} and variable t_{Co} , was carried out within the framework of spin wave theory. The corresponding Heisenberg hamiltonian is treated by the Green function method. In the presence of the exchange alone, we calculated the excitation spectrum of magnons E (K) as well as magnetization per spin. For low values of the number N of magnetic plans, the number of modes obtained is equal to N. The existence of a gap of creation of magnons was also highlighted showing the paramount

role played by the surface anisotropy in the stability of long range magnetic order. A very good agreement between the evolution of $m(T)$ calculated and measured one is obtained leading to exchange integral values which are in concord with values usually measured for super lattices engaging 3d-transition metals. The existence of a dimensionality crossover (3D-2D) in the behavior of the super lattice [Co/Ag] is also shown. The $m(T)$ evolution pass from a $T^{3/2}$ -law, as for the systems with 3-dimensions, to a $T \ln(T)$ -law known for systems with 2-dimensions, when the temperature T increases. The study of the combined effect of the surface anisotropy and dipolar interactions confirms the paramount role of the anisotropy in the stability of the long distance order in these super lattices.

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