Influence of the interface morphology on the magnetization of Magnetic/Non-Magnetic (Fe/Cu) multilayers: a Monte Carlo investigation

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Abstract: A Monte Carlo investigation was used to study the magnetization of a Heisenberg multilayers system. Our model consists of an alternate staking of Magnetic and Non-Magnetic layers (M/NM) with disordered interfaces. The results indicate that the magnetization of multilayers M/NM depends on the atomic composition, the interface morphology and the exchange interactions at the interface.
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I. Introduction

The magnetic properties of magnetic multilayers have been the subject of numerous studies by different laboratories. Magnetic phenomena such as oscillating exchange coupling, giant magnetoresistance, and surface anisotropy have been extensively investigated. In particular, the structure and morphology of magnetic multilayers M/NM with disordered interface (M = Fe, Co, Ni or perm alloy and NM = Cu, Pd, Ag, Au noble metals) has been of growing interest within the last 20 years for both fundamental and technological reasons. Moreover, these multilayers are of prominent technological important in micro-electronic and magnetic recording devices [1-3]. Furthermore, theoretical and experimental studies have been devoted to this subject [4-8].

The effect of the interface has a critical role on the magnetic properties of multilayers as a result of the break in local symmetry, strain issuing from lattice mismatch with adjacent layers, or interface morphology (e.g surface reconstruction, roughness or interdiffusion).

On the theoretical side, many studies have shown that the spin-dependent scattering at the interface plays an important role in obtaining the new magnetic properties (giant magnetoresistance for example) [9–11]. Further study has revealed that the spin-dependent scattering is dependent largely on the electronic structure of magnetic layers, especially when they are adjacent to non-magnetic layers [12]. Therefore, establishing the relationship of interface magnetic properties to interface morphology is not only of fundamental interest but is also essential for development of new multilayers. The well orderly interface is treated in the mean of Ab initio calculation [8] in within it is shown a depend spin with interface concentration. The theoretically predicted effects will be suppressed by interface roughness and interdiffusion, which cannot be avoided in many multilayer systems, such as the Fe/Cu(001) system where intermixing is known to occur [13].

The aim of this paper is to study the dependence of magnetic properties on the interface morphology in M/NM multilayers by Monte Carlo method with Heisenberg Hamiltonian. We have chosen the Monte Carlo investigation of three-dimensional classical ferromagnetic Heisenberg model which is one of the powerful techniques to simulate complex models and has the advantage that the mean-field approximation is not made.

In the following section, we describe the model and the simulation technique. The numerical results are presented in section 3. Our conclusion and perspectives are given in section 4.

II. Models and simulation technique

II-1. Atomic model

The concept of atomically abrupt interfaces used in the theoretical studies is realized only in very few systems. In our model, the system is described with real interface in the sense that it is not really sharp but

exhibit a certain degree of defects, interdiffusion, etc. We consider a multilayers system (Figure 1) consisting of ferromagnetic Heisenberg layers with different materials M (magnetic) and NM (non magnetic) and disordered interface in between. The interface is characterized by a random arrangement of M and NM atoms so that ($M_{1-x}NM_x$) is three-dimensional stable alloy with $0 \le x \le 1$ (x = 0 or x = 1 represent on abrupt interface, $x \neq 0$ alloys). Furthermore, to describe closely a real interface, the former presented in the form of two regions. A part is beside the layer M rich in element M ($M_{k'}NM_{1-k'}$) with $0.5 \le k' \le 1$ and the other beside the layer NM rich in element NM (M_kNM_{1-k}) with $0 \le k \le 0.5$) (figure 1). For each composition x, k (or k') is related to the degree of mixture in relation with the interdiffusion at the interface and the surface roughens at the initial stage of growth process. Such configuration is observed in real samples (Fe/Cu) analyzed experimentally [14,15]. In fact in the experiment conditions, the component profiles in multilayers are growth procedure dependent [16].

In our simulation, each layer is made up four atomic planes which are L×L in cross section; all the results presented in this work are obtained from lattice size of 8×12×12. The structure of the system is [M_3/($M_{k'}NM_{1-k'}$)(M_kNM_{1-k})/NM_3]. The interface is represented by two atomic planes. For raison of simplicity we restrict our study to simple cubic with six nearest neighbors via the exchange constant.

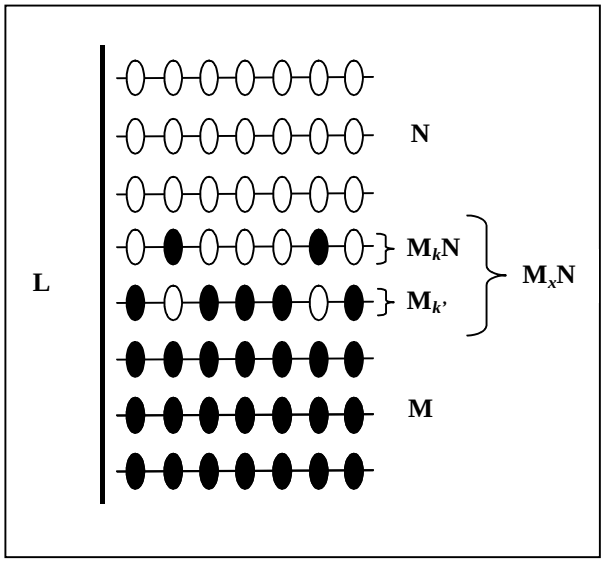

Figure 1: Part of the two dimensional cross through the multilayers system consisting of magnetic (M) and non magnetic (NM) materials with disordered interface ((M_kNM_{1-k})($M_{k'}NM_{1-k'}$), k and k' are the mixture parameter in the interface $0 \le k \le 0.5$ and $0.5 \le k' \le 1$).

II-2. Energetic model and simulation procedure

We describe the system by an isotropic Heisenberg model in absence of magnetic fields outside and by neglecting the effects of anisotropy; the Hamiltonian $\mathcal{H}$ is given by:

$$\mathcal{H} = -\sum_{\langle i,j \rangle} J_{ij} S_i S_j$$

Were S_i is a classical Heisenberg spin and the sum is taken over nearest-neighbor pairs of spins. J_{ij} denotes nearest-neighbor exchange interaction and is assumed to be $J_{M\text{-}M}(J_{NM\text{-}NM})$ between different atoms. The exchange parameters are defined in temperature units.

In order to relate our results to real systems, such as M/NM multilayers, we make the assumption that element M is Curie metal (Fe), the element NM will be Copper. According to heavy M-M interaction, the J_{MM} interaction is considered to be positive (ferromagnetic material). The magnetic moment for M is related to the spin momentum S_M by:

$$m_M = g_M \mu_B S_M$$

Where we assume that Landé factor $g_M = 2.2$ and μ_B is Bohr magneton. The exchange interaction J_{MM} have been estimated by Monte Carlo simulations on pure amorphous monatomic M systems, so that the maximum at the specific heat as the magnetic susceptibility is located at Curie temperature $Tc^{Fe}_{amorphous} \approx 202K$ [17], we found $J_{MM} \approx 110$K.

Numerical simulations were performed by using the importance Monte Carlo procedure at each temperature based on the standard Metropolis algorithms based on random trial step [18]. Our results were obtained by a slow decrease of the temperature starting from the paramagnetic state. At each temperature, 5×10^3 Monte Carlo steps (MCS) have been used for discarded for equilibration before averaging the physical quantities over the following 2×10^4 MCS. This procedure allows to reach equilibrium at each temperature when the Hamiltonian of the system does not display too much frustration, wish is the case here.

The thermodynamic magnetization per atom and the specific heat were calculated from $m(T) = \left\langle \left[(\sum_i S_i^x)^2 + (\sum_i S_i^y)^2 + (\sum_i S_i^z)^2 \right]^{1/2} \right\rangle / N$ and $C_v(T) = \left(< E^2 > - < E >^2 \right) / N k_B T$, respectively, where N is the number of atomic systems, E is the total energy, k_B is the Boltzmann constant and < > is the average over the MCS, i.e thermal average at temperature T. Periodic boundary conditions have been applied along the tree-directions. Because of the finite size effects, we note that magnetization is

different from zero in the paramagnetic state of the system.

III. Results and discussion

To study the morphological effects of interface on the magnetic properties of multilayers, we take in the first time the interface in the form of an homogeneous amorphous $M_{1-x}NM_x$ films alloy with $0 \leq x \leq 1$ as reported in figure 1. The interface spin exchange (J_i) is set equal to the bulk spin exchange (J_b). We plotted the variation of magnetization per atom as function of concentration x at low temperature (25K) (figure 2). For comparison, we have reported the experimental data obtained for $Fe_{1-x}Cu_x$ disordered alloys [19]. It can be clearly seen that over the entire range of concentration, the Monte Carlo simulation results for the average magnetization per atom for this alloys are in good agreement with the experimental data. The average magnetization per atom of $M_{1-x}NM_x$ films alloys decrease as x increases. Similar tendency was also found previously in Ni_xPd_{1-x} system [20]. Analyzing the result shown in figure 2, it is reasonable to suggest that the gradual diminution of the magnetization and a long-range magnetic order with M concentration decreasing is, most likely, associated with local environmental effects. In particular, this means a variation of first neighbours' number of magnetic atoms with x.

At fixed concentration x, the interface morphology presents several configurations with different atomic arrangement. Such configurations will affect the magnetic properties of the system. In the following, we purpose a rough interface with a particular distribution of different atoms with the same concentration of these elements as described below (Figure 1). The particular case treated is corresponding to x = 0.5 then we consider the variation of the concentration at each region of the interface represented by the parameter k.

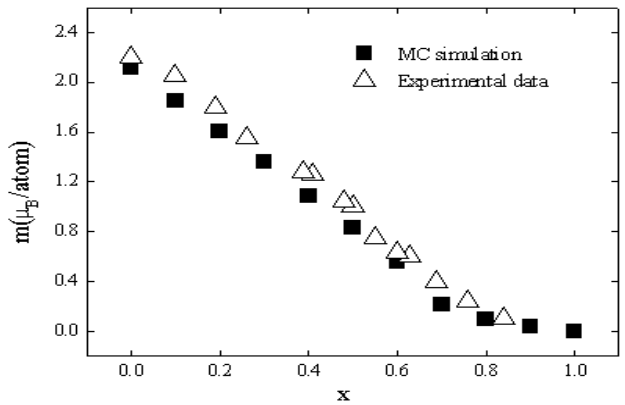

Figure 2: Concentration dependences of magnetization per atom of ($M_{1-x}NM_x$) interface with $0 \leq x \leq 1$ at T = 25K. Δ indicates the experimental data of the $Fe_{1-x}Cu_x$ alloys given by Ushida et al [19]. ■ indicates the value simulated by MC.

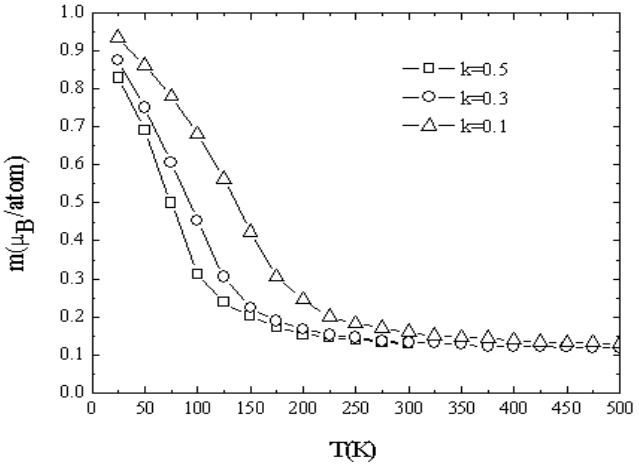

Figure 3: The thermal variation of the magnetization per atom of the interface in the case M_kNM_{1-k} with $0 \leq k \leq 0.5$ for k = 0.1, 0.3, and 0.5.

Figure 3 shows the effects of concentration k on the thermal evolution of the magnetization per atom of the interface. For the reason of clarity, only the curves of some values of k are drawn. The interface magnetization decreases with increasing interface mixture for all temperatures. The alloy magnetization decreases as much as 50% at some temperatures, as the degree of mixture increases towards the formation of a perfect alloy ($M_{0.5}NM_{0.5}$) with complete mixture. In terms of local magnetic ordering, the magnetization is the morphology interface dependant. Small values of k are corresponding to interfaces with long terraces, so that we obtain a long-rang magnetic order. But when k is close to 0.5, it presents the formation of clusters what are favourable for the formation of different magnetic domains.

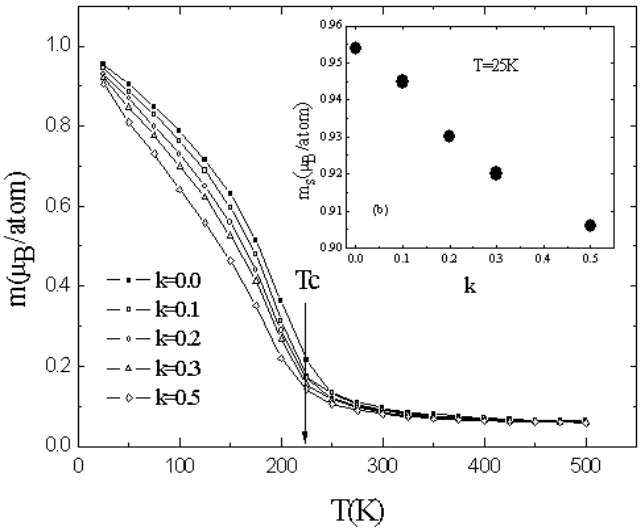

Figure 4: The thermal variation of the magnetization per atom of M/NM multilayers with abrupt (x = 0) interface and disordered interface ((M_kNM_{1-k})($M_{k'}NM_{1-k'}$), k and k' are the mixture parameter in the interface, $0 \leq k \leq 0.5$ and $0.5 \leq k' \leq 1$). The inset shows the magnetization per atom versus the concentration k at T=25K.

Figure 7 (a) shows the magnetization per atom of multilayers M/NM as function of temperature for different values of the interface concentration k with $J_i = J_b$. The magnetization per atom decreases with increasing the interface mixture (figure 4 (b)). This variation reaches as much 20% at some temperatures when the interface concentration k increases from 0.0 to 0.5. For all the cases, the specific heat present a maximum at the same position, then the Curie temperature T_C of multilayers M/NM does not vary with the interface mixture and its value remains around of the bulk Curie temperature.

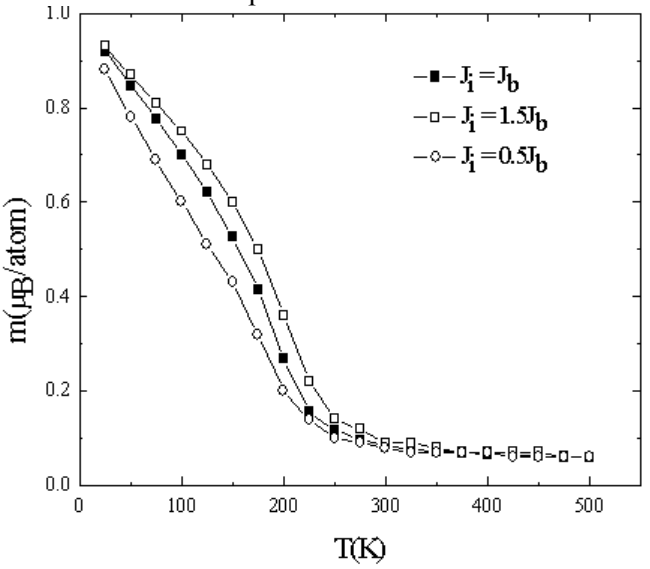

Figure 5: The thermal variation of the magnetization per atom of M/NM multilayers with disordered interface ((M_kNM_{1-k}) ($M_{k'}NM_{1-k'}$), k = 0.3 and k' = 0.7) using $J_i = J_b$, $J_i = 0.5J_b$ and $J_i = 1.5J_b$.

When J_i differs from J_b, the behavior of the multilayer magnetization with changing interface morphology is much more complex and interesting. J_i may be larger or smaller than J_b. The reduced atomic coordination at the interface produces a narrower band width and hence a larger magnetic moment [21-23] favoring $J_i \rangle J_b$. On the other hand, the interface lattice spacing can be larger than the bulk lattice spacing, leading to a weaker spin-spin interaction and favoring $J_i \langle J_b$. We therefore consider both possibilities. The figure 5 shows an example of the dependence of magnetization on temperature for M/NM multilayers with disordered interface ((M_kNM_{1-k})($M_{k'}NM_{1-k'}$)) with x = 0.5 and k = 0.3 using $J_i = 0.5J_b$ and $J_i = 1.5J_b$. The magnetizations always decrease with decreasing the ratio J_i/J_b in saturation zone and the temperature of Curie T_C remains constant and does not present a remarkable variation compared to that of bulk. This result can be explained by the reduction of the interaction spin-spin at the interface and consequently a reduction in the total magnetization of multilayers.

IV. Conclusion

In summary, we have studied the dependence of magnetic properties on the interface morphology in the Heisenberg multilayers M/NM by using Monte Carlo simulations. Our simulations confirm that the form of distribution of the atoms in interface i.e. morphology interface and the exchange interactions, modify its magnetic proprieties and by consequence the magnetic properties of the multilayers.

In near future, we planned to investigate the influence of different parameters like layer thicknesses and the stepped interface in order to compare Carlo Monte data with experimental results in M/NM multilayers, such as Fe/Cu, Ni/Cu or Co/Cu systems.

V. References

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