Published in: *Computer Physics Communications,* ***121-122*** *(1999) 545*

Kinetic Monte Carlo simulation of the thermal evolution of multilayers

E. Adam [1], F. Lançon and B. Rodmacq

Département de Recherche Fondamentale sur la Matière Condensée, CEA Grenoble, 38054 Grenoble Cedex 9, France.

Abstract

For special Ag layer thicknesses in NiFe/Ag multilayers, an anti-ferromagnetic coupling appears between the NiFe layers. This leads to the magneto-resistance (MR) property. This MR improves with increasing annealing temperatures and then disappears rapidly. X-rays studies have explained the improvement by an interface smoothing but have given no clue to understand the deterioration. We present a kinetic Monte Carlo study on a lattice gas with exchange dynamics between Ag and NiFe particles. We show that after the initial interface smoothing, local ferromagnetic bridges appear between the magnetic layers. They replace the anti-ferromagnetic coupling by a direct ferromagnetic one. Moreover, these defects appear at a temperature at which the multilayer structure is still well defined in agreement with the experimental results.

1 Model

We have choosen to simulate a NiFe/Ag multilayer system with simple hypotheses. In the model, only the structural properties are studied and the magnetic properties are not included. The Ni and Fe particles are both represented by $+1$ "spins" and the Ag particles by -1 "spins". The crystal structure is simple cubic and we have used an Ising Hamiltonien $\mathcal{H} = -J \sum_{<i,j>_{nn}} S_i S_j$ where the summation is done over the nearest-neighbours pairs. The interaction J is positive and then corresponds to the demixion. All the calculations are done in the canonical ensemble, *i.e.* the number of particles of each type is fixed. The choosen dynamics obey this restriction since we use exchange between nearest-neighbour Ag and NiFe particles with transition rates

$$\omega(S_i \leftrightarrow S_j; S_i \neq S_j) = \nu_0 \exp(-\max(\Delta\mathcal{H}, 0)/T) \qquad (1)$$

[1] Electronic address : Erwan.Adam@cea.fr

No energy barrier is included in these transition rates but we will see later that intermediate configurations are in fact geometrical barriers between low energy configurations.

To define completely the dynamic problem, we have chosen an initial configuration corresponding to a multilayer structure where the Ag profile at the interfaces is a Gaussian function. It is represented on figure 1 (left). The boundaries are periodic in the three directions. We have done simulations at increasing annealing temperatures

To treat this problem, we have used this quite unusual Monte Carlo algorithm [2]: (i) we choose a random number $r_1 \in]0,1]$ and increment the time by $\Delta t = -\ln(r_1)/(n(\mathcal{C})\nu_0)$; (ii) with a second random number $r_2 \in [0, n(\mathcal{C})[$, we choose a pair amongst the $n(\mathcal{C})$ ones; (iii) we exchange this pair with probability $\omega(\mathcal{C} \rightarrow \mathcal{C}')/\nu_0$. Note that this algorithm differs from the usual Metropolis algorithm by the fact that the residence time are random variables and that the number $n(\mathcal{C})$ of possible events at each step is not a constant. The detailed balance relation property is conserved by this algorithm; the way of incrementing the time compensates exactly the fact that $n(\mathcal{C})$ is variable.

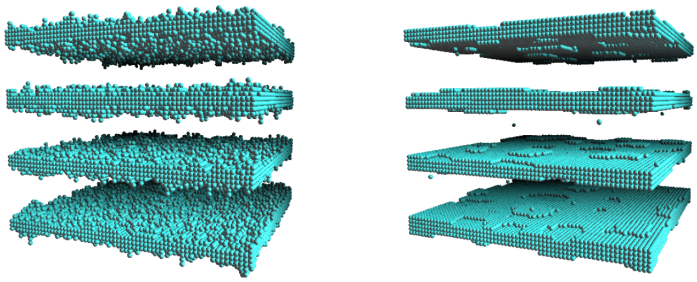

Fig. 1. Initial configuration (left) and $T = 1.2J$ (right). Only the Ag particles are shown.

2 Interface smoothing

The figure 1 (right) shows a configuration obtained at $T = 1.2J$. The interfaces are mainly composed of terraces and steps and are smoother than for the initial configuration. There are very little particles which diffuse from a layer to an adjacent one. Although there is no energy barrier, it is very difficult for the interface to relax more than shown on the figure. The reason is that when a particle arrives near a step and tries to go downwards, it has to pass trough an intermediate uncomfortable situation and then the diffusion between terraces is very limited. This effect is very similar to the Ehrlich-Schwoebel effect [3] for surfaces.

3 Ferromagnetic bridges

When the temperature increases, the diffusion at interfaces, *i.e.* on and between terraces becomes faster. The diffusion between adjacent layers is still low. In fact, it is the interfaces themselves which begin to fluctuate until a hole appears in the Ag layer as represented on the figure 3 (left). This NiFe bridge leads to a ferromagnetic coupling between the NiFe layers which is much stronger than the initial anti-ferromagnetic coupling. For a bridge as small as the figure 3 (left), the effect should be negligible. But at longer time or at higher temperature where the interfaces fluctuate more, for instance as shown on the figure 3 (right), the ferromagnetic coupling dominate over the anti-ferromagnetic one and there is no more magneto-resistance.

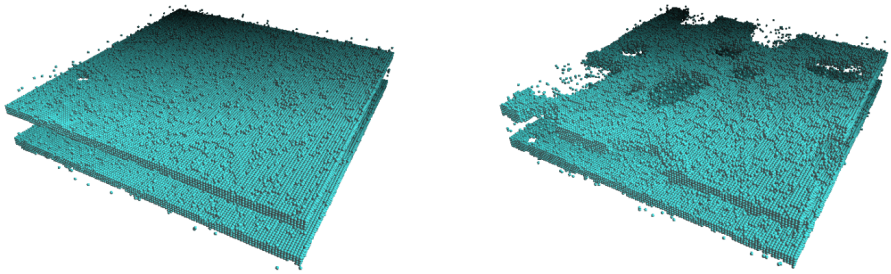

Fig. 2. Multilayers at $T = 2.2J$ (left) and $T = 2.3J$ (right). Only the Ag particles are shown. Note the hole in the Ag layer in the left picture

Note however that the density profile along the growth axis still shows a well defined multilayer structure in agreement with the X-Ray experiments. Indeed these experiments cannot detect the microscopic bridges described in this paper although they have important effects on the magnetico-transport properties.

References

[1] P. Auric, S. Bouat and B. Rodmacq, J. Phys.: Cond. Mat. **10**, 3755 (1998).

[2] E. Adam, L. Billard and F. Lançon, Submitted to Phys. Rev. E (1998).

[3] A. Pimpinelli and J. Villain in *Physics of Crystal Growth* edited by Cambridge University Press (Dec. 1998)