MONTE CARLO SIMULATION OF SYMMETRIC EXCHANGE SPRING IN SOFT LAYER OF DyFe₂/YFe₂ AT NEAR ZERO TEMPERATURE

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Abstract

The experimental results of bending fields and other properties of the DyFe₂/YFe₂ superlattice multilayer have been performed by many physicists around the world. So far there is no published work on computer simulation(iterative method) of this system for comparing with the experimental result before. The temperature scale that has been accessed in most laboratories today is as low as 4 K. Low temperature ferromagnetic system is advantageous in reducing thermal fluctuation that disturbs the measurement. Without the fluctuation, the system is able to show better exchange interaction and other properties resulting from it. The simulation performed here aims to show the bending field phenomena at very near zero temperature. We used Visual C++ code for the programming work. The simulation method here is Monte Carlo method with the Metropolis algorithm. At very low temperature, it could be easy for the system to fall into and struck in a metastable state. We therefore had developed a trick to escape from the metastable trap. Finally we could simulate very low temperature system with small number of moment inYFe₂ soft layer and it could render the bending field transition. The number of moment was found to be inversely proportional to the bending field strength.

Additional keywords: Monte Carlo simulation, magnetic multilayer, exchange spring, bending field transition

1.Introduction

Work on synthesising bulk rare earth intermetallic compounds (REFe₂) by Wernick and Geller (Wernick *et al.* 1960) is attractive because of some interesting features of REFe₂ materials. These REFe₂ materials are known to possess high Curie temperature due to strong Fe-Fe exchange interaction. Moreover moments of RE and Fe couple antiparallel/parallel to each other in heavy/light REFe₂ materials. Usually strong crystal field anisotropy in RE^{3+} controls dominantly direction of easy magnetisation in the hard layer (REFe₂) (Buschow 1977, Clark 1980 and Bowden *et al.* 1968) but for Y^{3+} the measured anisotropy is very low and it is not considered to be significant.

Jacobi elliptic functions could be used to express the angular dependence of the continuous 180 degrees continuous exchange spring in a hard layer substrate coated with soft Fe layer (Goto *et al.* 1965). The hard layer is assumed to be perfectly rigid and there is no anisotropy in the soft layer. Bending field, B_B was found to be proportional to $1/w^2$, where w is the thickness of the soft layer.

Experimentally the exchange spring in DyFe₂/YFe₂ was reported recently (Sawicki *et al.* 2000). They grew Laves phase multilayers [DyFe₂/YFe₂]×N by MBE on a YFe₂ seed layer in (110) growth direction (N is number of bilayer). The

measurement of magnetic properties of the materials in applied magnetic field up to 12 Tesla and temperature from 4 to 300 K shows up magnetic compensation. This compensation between hard and soft layer is the result from antiparallel orientation of soft layer's Fe moments to the direction of Dy^{3+} moments at the interfacing between soft and hard layer. This compensation breaks down when Fe thickness increases and then forms exchange spring in which soft layer Fe moments (with strong Fe-Fe ferromagnetic exchange coupling (~600 Tesla)) try to orient to the direction of the external applied field. The model of the spring is shown in figure 1. The end moment is pinned by Dy-Fe antiferromagnetic interaction.

Fullerton *et al*. (1998) and Goto *et al*. (1965) performed experiment with Sm-Co/TM (TM is Fe and Co) bilayer, they found the reversible demagnetization curves as exchange spring.They also performed the numerical simulation.The model of the simulation is given by the total energy of system;

$$E_{tot} = -\sum_{i=1}^{n-1}(A_{i,i+1}/d^2)\,cos(\theta_i - \theta_{i+1}) \ - \sum_{i=1}^{n} K_i\,cos^2(\theta_i) - \sum_{i=1}^{n} HM_i\,cos(\theta_i - \theta_H) \qquad (1)$$
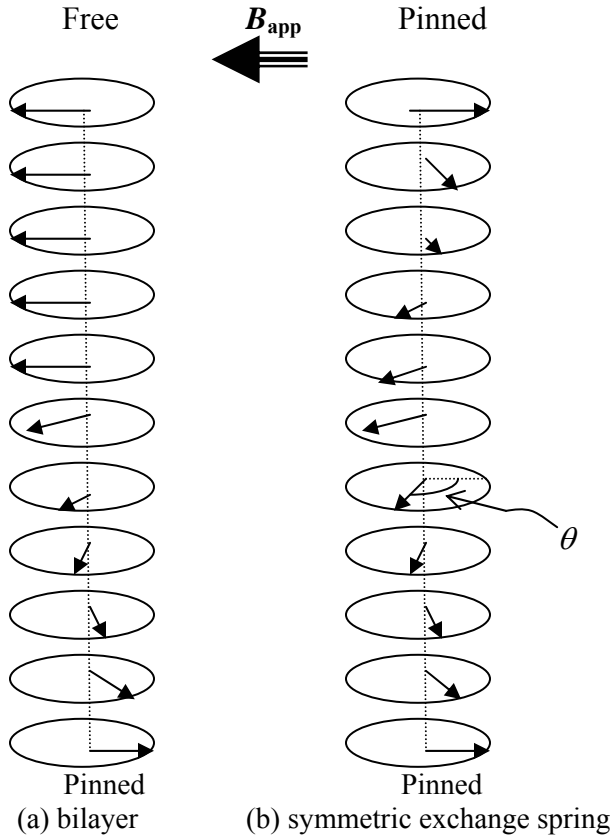

Figure 1: Schematic drawing of bilayer and symmetric multilayer exchange spring

This model is a classical model which considers bilayer as sum of each atomic layer. The atomic layers are treated as a one-dimensional chain of atomic moments normal to bilayer. The model was used successfully before in different system (Mibu *et al.* 1996 and Wüchner *et al.* 1997). Expressions for the notations in equation (1) are as follow;

M_i: magnetic moment of each Fe atom;

K_i: uniaxial anisotropy constant;

θ_i: in-plane angle measured relative to the easy axis direction of hard layer;

θ_H: angle of external applied field with respect to the easy axis;

H: magnitude of external applied magnetic field;

$A_{i,i+1}$: exchange couple constant;

d: spacing between moments.

According to the work of Fullerton (Fullerton *et al* 1998 and 1999), the simulation starts from letting all moments in the soft layer point at $\theta_i \sim \Pi$ radians and $\theta_H = 0$ radian. Moments in soft layer then start to rotate with the applied magnetic field. They used iterative method outlined by Camley (Camley 1987 and Camley *et al.* 1988). The moments are chosen randomly and their directions are also updated randomly until reaching their equilibrium state. Typically for 200 spins, (in soft layer) 10^5 to 10^6 iterations are needed to thermalize the system.

In this work, the procedure of symmetric exchange spring simulation is described in details and the simulation is applied for $DyFe_2/YFe_2$ multilayers at $T \sim 0$ K.

2.Model

The classical X-Y chain model is used here. It can be drawn schematically in figure 1 (Bowden *et al.* 2000). In the figure, both bilayer magnetic exchange spring and symmetric multilayer magnetic exchange spring are presented. We consider here that the exchange interaction between Dy^{3+} and Fe^{3+} is very strong in both figure 1a and 1b. This results from very strong anisotropy in the hard layer $DyFe_2$. We consider the symmetric exchange spring in soft layer YFe_2 (figure 1b) which has both ends pinned by very strong antiferromagnetic Dy-Fe exchange interaction Therefore we will assume that there is no spring penetration into the hard layers. Soft layer Hamiltonian for the model ignores very small Y^{3+} anisotropy. All interactions are nearest neighbouring interaction. The energy of. each lattice site (moment) is (Fullerton *et al.* 1998 and 1999, Bowden *et al.* 2000)

$$E_i \ = \ - \mu_{Fe}B_{app} \ cos \ (\theta_i - \theta_B) \ - \ (1/2) \ \mu_{Fe}B_{ex} \ (\ cos(\theta_i - \theta_{i+1}) \ + \ cos(\theta_{i-1} - \theta_i)) \qquad (2)$$

Here i labels the ith moment and it takes the value from 2 to n-1. n is the total number of moments (monolayers) in this soft layer. The energy of both end moments are

$$E_1 \ = \ - \mu_{Fe}B_{app} \ cos \ (\theta_1 - \theta_B) \ - \ \mu_{Fe}B_{ex}(cos(\theta_1 - \theta_2)) \qquad (3)$$

$$E_n \ = \ - \mu_{Fe}B_{app} \ cos \ (\theta_n - \theta_B) \ - \ \mu_{Fe}B_{ex}(cos(\theta_{n-1} - \theta_n)) \qquad (4)$$

Here, the angle of easy axis is 0 radian and all notations are described as follow;

μ_{Fe}: magnetic moment of Fe^{3+},

B_{app}: external applied magnetic field,

B_{ex}: exchange magnetic field (approximated value is 600 Tesla),

θ_i : angle of ith moment (with respect to the easy axis),

θ_{i+1}: angle of $(i+1)^{th}$ moment (with respect to the easy axis),

θ_{i-1}: angle of $(i-1)^{th}$ moment (with respect to the easy axis),

θ_B: angle of B_{app} direction (with respect to the easy axis),

θ_1, θ_2: angle of 1st and 2nd moment (with respect to the easy axis),

θ_{n-1}, θ_n: angle of $(n-1)^{th}$ and n^{th} moment (with respect to the easy axis).

The value of μ_{Fe} is approximately $1.5\mu_B$. Bohr magneton, $\mu_B = 9.27401 \times 10^{-24}$ J/Tesla. The first term is Zeeman energy term and the second term is Fe-Fe ferromagnetic exchange interaction term. The factor (1/2) comes from the fact that we have added together two exchange energy terms (both interaction with upper and lower moments) at particular i index. The total energy of the exchange spring is then given by

$$E_{tot} \ = \ E_1 + \sum_{i=2}^{n-1} (E_i) \ + \ E_n \qquad (5)$$

3.Monte Carlo Simulation

In the simulation, θ_B is set precisely to be Л radians and all initial moments orient to the opposite direction i.e. 0 radian. This procedure is different from the work of Fullerton (Fullerton *et al.* 1998) that applied magnetic field direction is not set to be slightly different from the easy axis as it was in their paper. E_{tot} of this initial moment configuration is evaluated. One of moments $i=2$ to $i=n$-1 is selected randomly. Both end moments are not selected since they are pinned. We change direction of the chosen moment slightly. Our procedure of changing the direction of each moment is by setting a maximum value of angle change that will be allowed ($\delta\theta_{max}$). This maximum angle change should be small. Then a pseudo-random number is generated in the range [-0.5,0.5) for obtaining the random angle change:

$$\delta\theta_i \quad = \quad \delta\theta_{max} \, (2r_i \text{-}1) \tag{6}$$

r_i is the random number in the range [0,1). This random angle change will be in the range [-($\delta\theta_{max}$/2) , ($\delta\theta_{max}$/2)). Therefore new angle for moment i[th] is

$$\theta_{i\,new} \quad = \quad \theta_{i\,old} \; + \; \delta\theta_i \tag{7}$$

Hence Hamiltonian of the system is changed just "a little".

After this moment has been selected and changed, we now have the second configuration (apart from initial configuration which has all $\theta_i = 0$). New E_{tot} of the second configuration is calculated for comparing with the E_{tot} of the previous configuration. The energy difference between new and old configuration is

$$dE \quad = \quad E_{tot(new\ config.)} - E_{tot(previous\ config.)} \tag{8}$$

Using Metropolis algorithm for updating the system, negative dE value is accepted to be our configuration for the further step. Zero or positive dE value is accepted in the probability $\exp(-dE/k_BT)$.

The same process is reperformed to the other moments. The new (updated) configuration must be used if it was accepted in the previous selection. Each moment must be chosen only once. When all moments have already been chosen, that is to say the first sweep (or iteration) is completed, we calculate the *Acceptance* by

$$Acceptance \quad = \quad (accept) \,/\, (n\text{-}2) \tag{9},$$

where *accept* is times that new configurations are accepted. Fine tuning technique is performed here by controlling the *Acceptance* to be closed to ~0.50. For the chain of 17 moments, 1×10^5 iterations over all process mentioned above is fine enough to ensure thermalization of the simulation. In the simulation at zero temperature, it is easy for the system to be trapped in some metastable states. Like equilibrium state,

these metastable states are characterised from $dE/d\theta_i = 0$. This would be problem. To avoid this problem, we need some trick. The trick is to start the simulation from some finite low temperature (10 K). At this temperature, thermal fluctuation is able to shake the system out of metastable trap. The system is gradually cooled down with iteration to a temperature that is very closed to zero finally.

4.Results and Discussion

As we run the program many times with different initial random seeds, the simulations render different medium-step configurations. Thermalization is approached in slightly different ways. At last we obtain slightly different shape of the spring. This is not to be surprised because we start from finite-temperature (10 K) system which still has thermal fluctuation. We use random numbers and regard it as probability for accepting the trials at finite temperature. Hence changing in initial random number must effect the simulation. In case that T is always fixed at zero, only negative dE is accepted and then different initial random numbers can not effect the final result. Table 1 shows the angle of the middle moment (of 17 moments chain) in 7 simulations at temperature closed to $T=0$ K i.e. 0.000247 K. (Each simulation has different initial random numbers.)   To find the more precise value of the angle of the middle moment, we need to evaluate an ensemble average of these middle moment angles at the same applied field but different initial random numbers. Table 2 shows the mean value of middle moment angles. Each value shown in the table is averaged over 30 simulations. The initial random numbers are different in each round. We can compare the mean middle angles at different B_{app} .

Simulations	Angle of the middle moment (radian)
1st simulation	-2.23270
2nd simulation	2.31065
3rd simulation	2.30316
4th simulation	-2.29419
5th simulation	-2.28249
6th simulation	-2.24988
7th simulation	2.29375

Table 1: Angle of the middle moments compared to each other at B_{app} = 25 Tesla (n = 17, B_{ex}=600 Tesla, 100,000 iterations). The program is run for 7 times, different initial random numbers are used at each time. The sign in front of each angle is not to be worried since the spring could be created in either direction.

B_{app} (Tesla)	Mean value of the middle moment angle (radian)
12.50	0.74357
12.00	0.55218
11.50	0.29715
11.00	0.05652
10.50	0.01753
10.00	0.01591
9.50	0.01389
9.00	0.01226
8.50	0.01006

Table 2: Mean middle angle magnitude at various B_{app} values (final temperature = 0.000247 K, n=17, B_{ex} = 600 Tesla)

The results in table 2 show the bending field transition at about 11.0 to 11.5 Tesla for the system of 17 moments. The exchange spring with very symmetric shape can be obtained when we average (over 30 simulations) the angle of each moment in the chain. The result is shown in table 3 and figure 2.

i^{th} moment	Mean angle(radian)
1	0.00000
2	0.10928
3	0.21190
4	0.30731
5	0.39098
6	0.46050
7	0.51148
8	0.54154
9	0.55218
10	0.54145
11	0.51011
12	0.45948
13	0.39140
14	0.30813
15	0.21306
16	0.10978
17	0.00000

Table 3: Mean value of ith moment averaged over 30 simulations B_{app} = 12 Tesla, T approaching from 10 to 0 K (0.000247K).
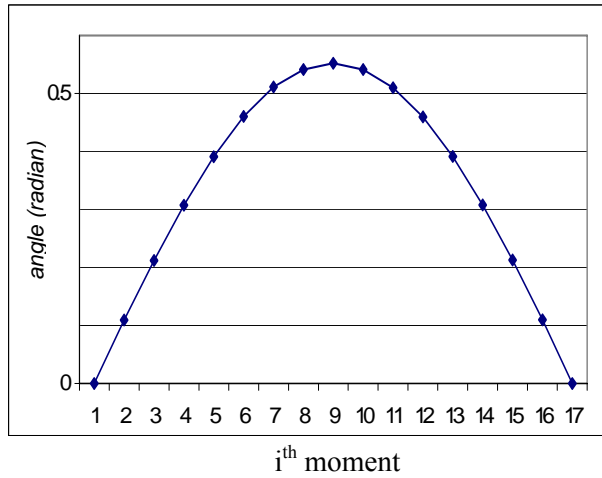
Figure 2: Mean value of ith moment averaged over 30 simulations versus i^{th} moment of the chain. B_{app} = 12 Tesla, T approaching from 10 to 0 K (0.000247K).

The bending field transition can be seen visually in figure 3. Here applied field is varied and we start each simulation with all $\theta_i = 0$. This picture we see that the bending field transition occurs at ~11.0-11.5 Tesla.
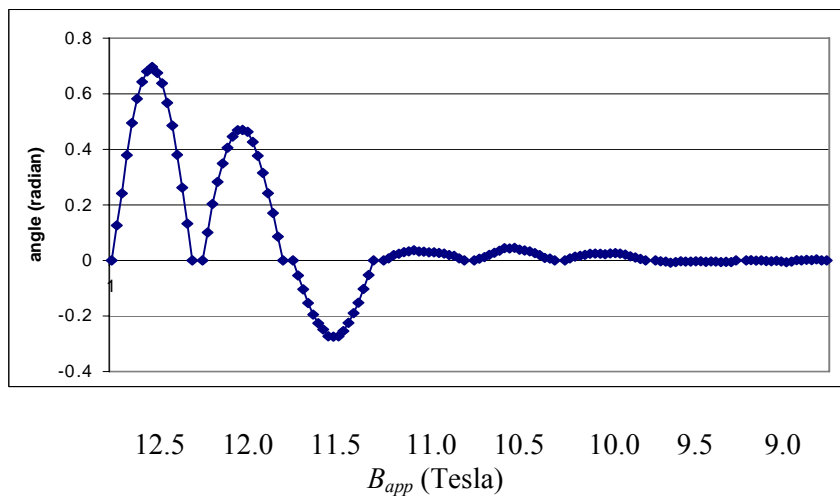

Figure 3: exchange spring configurations at various B_{app} values (100,000 sweeps, n=17, T ~ 0 K (0.000247K)

The thickness of soft layer is changed to check its relation to the bending field value. The result for n = 17, 28, 30 and 41 is shown below in table 4 where the bending field values (B_B) inversely varied with the number moment in the chain. This agrees with the result for bilayer spring at zero temperature in previous work (Goto *et al.* 1965) which employs different numerical approach.

n	B_B (Tesla)
17	~11.05{between 11.00-11.10}
28	~3.60{between 3.50-3.70}
30	~3.45{between 3.40-3.50}
41	~1.65{between 1.60-1.70}

Table 4: B_B of various n at T ~ 0 K.

5.Conclusions

The Monte Carlo simulation at zero temperature can render good exchange spring configuration result and the bending field value. It also shows obviously the bending field transition. Number of moments in the chain is inversely proportional to the bending field and this agrees with the previous work of the bilayer case (Goto *et al.* 1965). The trick we found here for simulating this system at near zero temperature is to cool the system slowly from some finite low temperature (10 K). It would be much interesting if the work by experimentalists in the near future can reached very close to zero temerature. This work is then able to provide the prediction of those experimental results. The current experiments on $DyFe_2$/YFe_2 multilayers are performed at 4 K to 300 K with soft layer thickness from 50 Å to 200 Å (Sawicki *et al.* 2000 and Bowden *et al.* 2000) and they still need the confirmation from computer simulation.

6.Acknowledgements

7. References

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