Monte Carlo study of magnetic properties and hysteresis behavior of the square Ising nanowire with core-shell structure

E.M. Jalal[1,2], A. Hasnaoui[2], H. Saadi[1], A. Lafhal[1], N. Hachem[1], M. El Bouziani[1]

[1] Equipe de Physique Théorique, Laboratoire L.P.M.C, Faculté des Sciences, Université Chouaib Doukkali, El Jadida, Morocco

[2] Laboratoire LS3M, faculté polydisciplinaire, université sultan moulay slimane, 25000 Khouribga, Morocco.

جامعة السلطان مولاي سليمان
Université Sultan Moulay Slimane

Aim of the work: investigate the effects of the crystal fields, the exchange couplings, and the longitudinal magnetic field on the magnetization, the internal energy, the specific heat, and hysteresis loops of the square Ising nanowire, within the framework of Monte Carlo Simulation.

The Model and Calculation

We consider a Square Ising Nanowire (SIN) consisting of a spin-3/2 core which is surrounded by a spin-1 shell layer. This nanowire is composed of N Square layers, and each layer contains four spins: one spin 3/2 in the core and four spins 1 in the shell (Fig)

$$H = -J_C \sum_{\langle ij \rangle} \sigma_i \sigma_j - J_S \sum_{\langle kl \rangle} S_k S_l - J_{in} \sum_{\langle ik \rangle} \sigma_i S_k - D_C \sum_{i=1}^{N} \sigma_i^2 - D_S \sum_{i=1}^{N} S_k^2$$

where J_C is the ferromagnetic exchange interaction between two nearest-neighbor spins in the core, J_S is the ferromagnetic exchange interaction between two nearest-neighbor spins in the surface shell and Jin denotes the ferrimagnetic exchange interaction between the spins S in the surface shell and the spins in the core. D_C represents the crystal field acting on the spins S=3/2 of the core sublattice. Our choice in this study is to consider J_C as a unit of energy.

The simulation of the Hamiltonion is carried by the Monte Carlo methode based on the algorithm of metropolis [3]. Starting from a random initial configuration of spins, the configurations are generated by attempting to spin flips which are accepted or rejected according to a specific probability founded on the Boltzmann statistics. For the boundary conditions, we apply free conditions in both x and y directions, but periodic conditions are imposed along the z direction. At each temperature, the averages of different physical quantities are calculated using 10^5 MC steps per site after discarding the first 2×10^4 steps per site for equilibrating the system.

We define some important physical quantities that our program can calculate:

The sublattice magnetizations per site m_A and m_B:

$$m_C = \frac{2}{N_T} \sum_{i \in (A)} \sigma_i \quad \text{and} \quad m_S = \frac{2}{N_T} \sum_{j \in (B)} \sigma_j$$

the total magnetization per site M_T : $M_T = \frac{m_C + m_S}{2}$

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Methods of Effective Field Theory and Lattice Field Theory

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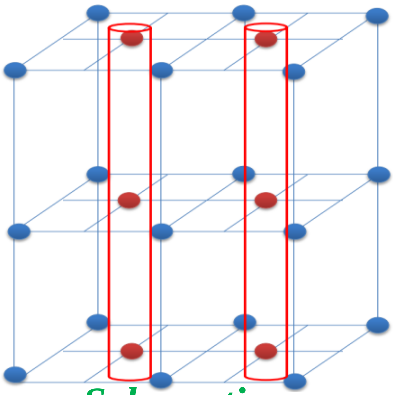
and the total susceptibility per site χT:

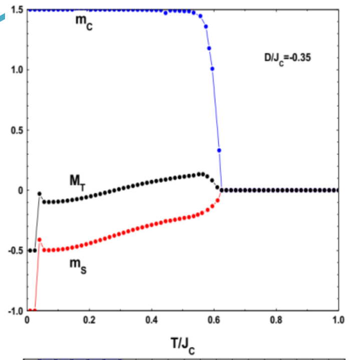
$$\chi_T = \beta N_T \left(\langle M_T^2 \rangle - \langle M_T \rangle^2 \right)$$

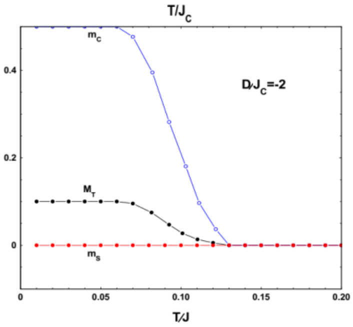
Where the total number of spins in the nanowire is N_T=N×N×L with L=500 and N=10; L is the length wire and N×N is the number of spins at each nanowire cross section, and $\beta=(K_B T)^{-1}$ with K_B the Boltzmann constant and T the absolute temperature. In the following and for simplicity, we take K_B=1.



Schematic representation of Square Ising nanowire.

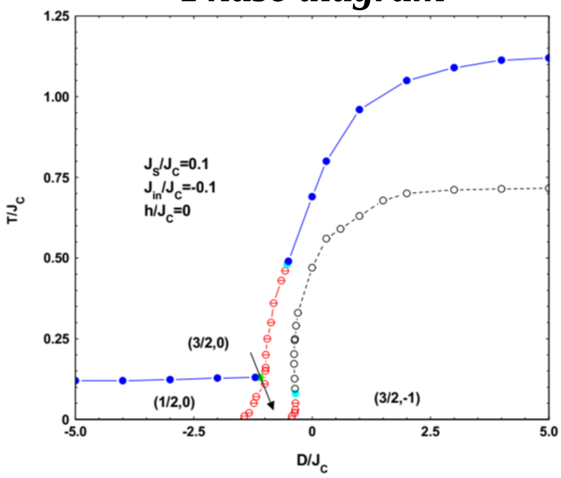
Results



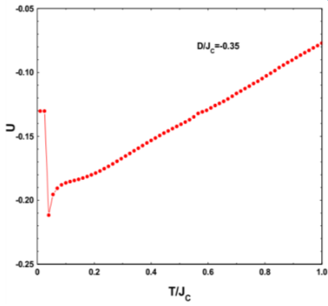


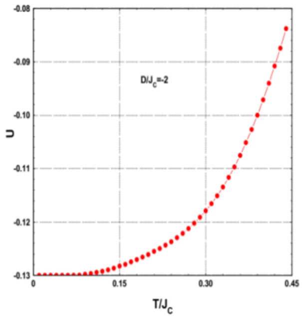
Magnetisation

Phase diagram

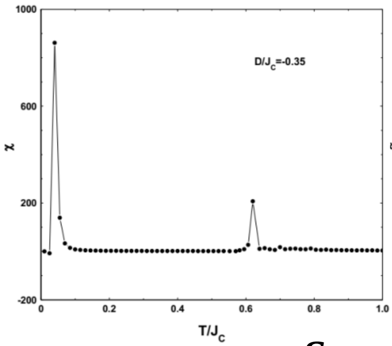


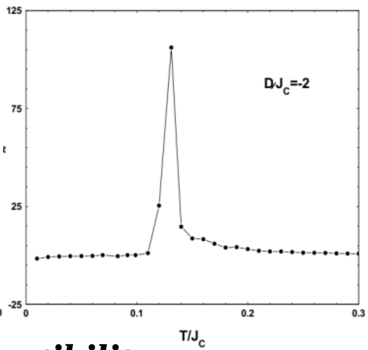
Effect of the crystal field D/J_C.





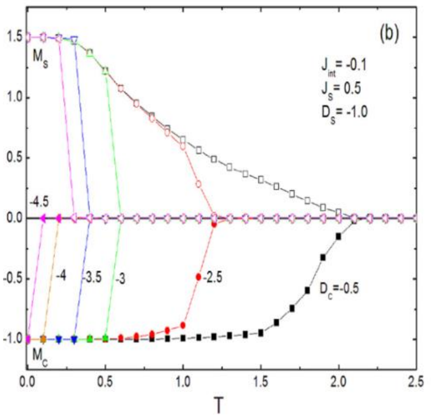
Internal enery





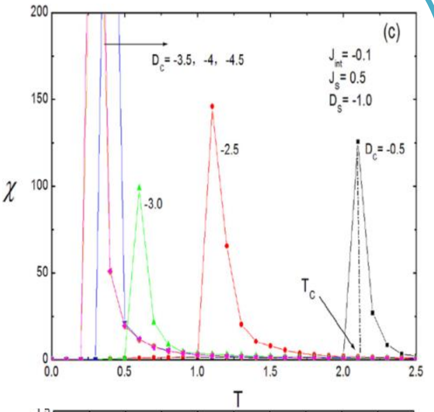
Susceptibility

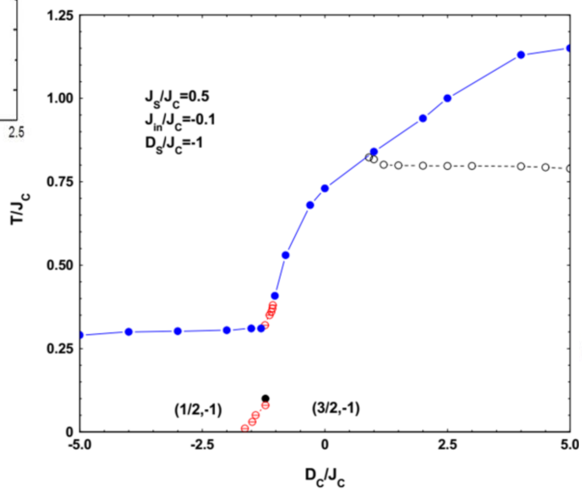
Effect of the crystal field D/J_C.



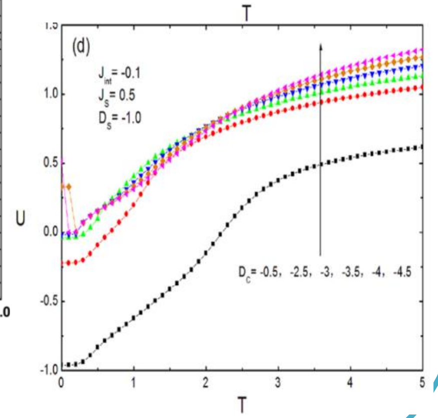
Magnetisation

Susceptibility





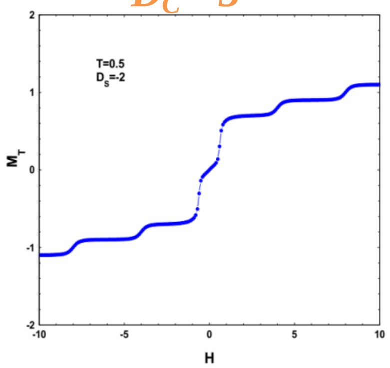
Phase diagram



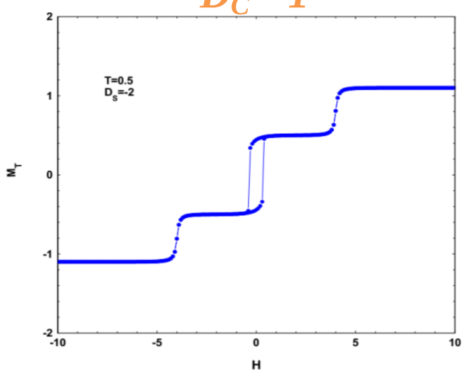
Internal enery

hysteresis loop

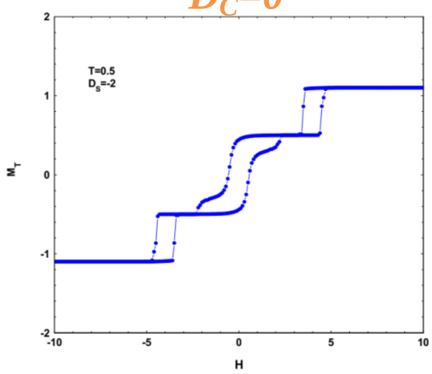
D_C=-3



D_C=-1



D_C=0



Single loops ***Triple loops***

With the increase of D_C/J_C

✓ ***Our results are in great agreement with those found both theoretically in Ising nanowire and nanotube***

Onclusion

Using MC simulation, the magnetic and thermodynamic characteristics of the ferrimagnetic square Ising nanowire have been studied. Multiple magnetization curves and saturation values have been found. Under several parameter, the phase diagrams have been presented and analyzed. The results show that the crystal field D and D_C have an opposite impact on the magnetic behavior. In addition to the single-loop, the system also can show triple loops under certain parameters. We aspire that our theoretical results may provide some assistance for the theoretical and experimental study of the nanowire.