ISSN 1512-1461

UDC: **538.9** Condensed matter physics. Solid state Theoretical Condensed Matter Physics

EXPLANATION OF EASY AXIS ORIENTATION OF FERROMAGNETIC FILMS USING HEISENBERG HAMILTONIAN

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Abstract
For the first time, the easy axis orientation of some experimentally synthesized ferromagnetic thin films has been investigated using the second order perturbed Heisenberg Hamiltonian with stress induced anisotropy, demagnetization factor and fourth order anisotropy terms. The variation of average value of out of plane spin component with the temperature was plotted in order to explain the easy axis orientation. The temperature, at which the average value of out of plane of spin component becomes zero, was determined. The experimental values of temperatures corresponding to the in plane orientation of easy axis of ferromagnetic materials could be explained using our model. The deposition temperatures corresponding to in plane orientation of $CoPt_3$ films deposited on WSe_2 substrates and Fe-rich germanide films grown on Ge(001) substrates by some other researchers could be verified using this model. According to our model, the spin re-orientation temperature solely depends on the perpendicular component of internal magnetic field and the stress induced anisotropy.

Keywords*: Heisenberg Hamiltonian, spin, ferromagnetic thin films, easy axis*

1. Introduction:

Ferromagnetic materials are prime candidates in electric motors, generators, transformers, telephones, and loudspeakers, --- etc. In addition, almost all the permanent magnets are fabricated using the ferromagnetic materials. Because the in plane or out of plane easy axis oriented ferromagnetic materials find potential applications, the preparation of easy axis oriented ferromagnetic samples is really important [1-3]. Although the deposition conditions such as the type of sputtering gas, gas pressure, the separation between the target material and substrate, rate of sputtering, the material and the orientation of the substrate govern the easy axis orientation of ferromagnetic materials, the orientation of easy axis mainly depends on the substrate temperature [4-6]. Even in other deposition techniques, the orientation of easy axis is highly sensitive to the deposition temperature. In some cases, the films are annealed at higher temperatures after deposition. Therefore, a theoretical investigation of easy axis orientation of ferromagnetic films was carried out.

Previously, the magnetic properties of ferromagnetic ultra-thin and thick films have been studied using the second and third order and perturbed Heisenberg Hamiltonian by us [7-9]. In this report, the second order perturbed Heisenberg Hamiltonian was employed to investigate the easy axis orientation of ferromagnetic films. Some experimental values obtained for the easy axis orientation of ferromagnetic films by some other researches were described using our model [12, 13, 15]. MATLAB software package was employed to plot all the 2-D and 3-D graphs.

2. Model:

The spin was assumed to have only two components in this 2-D model. The spin component in the plane of the film and the spin component perpendicular to the film plane were taken as S_y and S_z, respectively. The energy of a ferromagnetic film per unit spin derived using the second order perturbed Heisenberg Hamiltonian can be given as following [9].

$$\begin{aligned}
E(\theta) = {} & -\frac{J}{2}[NZ_0 + 2(N-1)Z_1] + \{N\Phi_0 + 2(N-1)\Phi_1\}(\frac{\omega}{8} + \frac{3\omega}{8}\cos 2\theta) \\
& - N(\cos^2\theta D_m^{(2)} + \cos^4\theta D_m^{(4)} + H_{in}\sin\theta + H_{out}\cos\theta - \frac{N_d}{\mu_0} + K_s\sin 2\theta) \\
& - \frac{[-\frac{3\omega}{4}(\Phi_0 + 2\Phi_1) + D_m^{(2)} + 2D_m^{(4)}\cos^2\theta]^2 (N-2)\sin^2 2\theta}{2C_{22}} \\
& - \frac{1}{C_{11}}[-\frac{3\omega}{4}(\Phi_0 + \Phi_1) + D_m^{(2)} + 2D_m^{(4)}\cos^2\theta]^2 \sin^2 2\theta \qquad \textbf{(1)}
\end{aligned}$$

Here matrix elements C_{11} and C_{22} are given by

$$\begin{aligned}
C_{11} = {} & JZ_1 - \frac{\omega}{4}\Phi_1(1 + 3\cos 2\theta) - 2(\sin^2\theta - \cos^2\theta)D_m^{(2)} \\
& + 4\cos^2\theta(\cos^2\theta - 3\sin^2\theta)D_m^{(4)} + H_{in}\sin\theta + H_{out}\cos\theta - \frac{2N_d}{\mu_0} + 4K_s\sin 2\theta
\end{aligned}$$

$$\begin{aligned}
C_{22} = {} & 2JZ_1 - \frac{\omega}{2}\Phi_1(1 + 3\cos 2\theta) - 2(\sin^2\theta - \cos^2\theta)D_m^{(2)} \\
& + 4\cos^2\theta(\cos^2\theta - 3\sin^2\theta)D_m^{(4)} + H_{in}\sin\theta + H_{out}\cos\theta - \frac{2N_d}{\mu_0} + 4K_s\sin 2\theta
\end{aligned}$$

Here N, J, $Z_{|m-n|}, \Phi_{|m-n|}$, ω, θ, $D_m^{(2)}$, $D_m^{(4)}$, H_{in}, H_{out}, N_d and K_s are total number of layers in ferromagnetic film, spin exchange interaction, number of nearest spin neighbors, constants arisen from partial summation of dipole interaction, strength of long range dipole interaction, azimuthal angles of spins, second order anisotropy, fourth order anisotropy, in plane internal field, out of plane internal field, demagnetization factor and the stress induced anisotropy factor, respectively. In this case, the second order anisotropy constant and the fourth order anisotropy constants were assumed to be constants for the whole ferromagnetic film.

3. Results and discussion:

The average value of out of plane spin component ($\overline{S}_z$) is given by

$$\overline{S}_z = \frac{\int_0^{\pi} e^{-\frac{E}{kT}} \cos\theta d\theta}{\int_0^{\pi} e^{-\frac{E}{kT}} d\theta} \qquad \textbf{(2)}$$

After substituting C_{11} and C_{22} in equation (1), the total energy of the ferromagnetic film was found. Then this total energy (E) was substituted in equation (2) to derive an equation for $\overline{S}_z$. Here k and T are the Boltzmann’s constant and the temperature in Kelvin, respectively.

ISSN 1512-1461

The variation of $\overline{S}_z$ with the temperature of the ferromagnetic film was plotted in order to study the orientation of magnetic easy axis. $\overline{S}_z$ gradually decreases with the temperature, and becomes zero (or negligible) at one particular temperature (T_s). At this particular temperature, only the in plane spin component survives. So the magnetic easy axis of the film will be in the plane of the ferromagnetic film. According to our model, T_s is highly sensitive to H_{out} and K_s as given in figure 1 and 2.

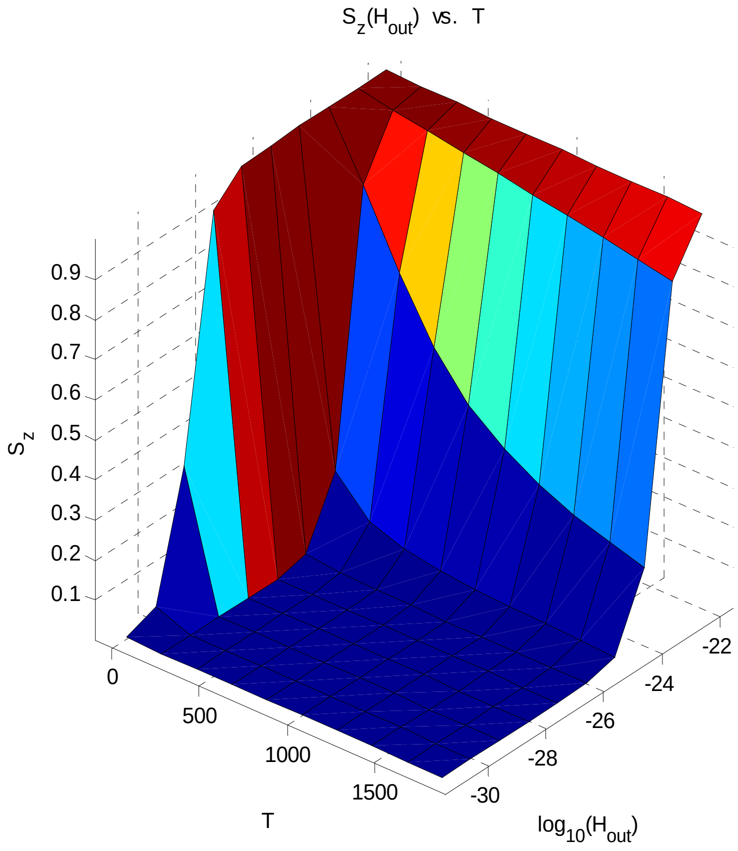

Figure1. 3-D plot of $\overline{S}_z$ versus $\log_{10}(H_{out})$ and temperature.

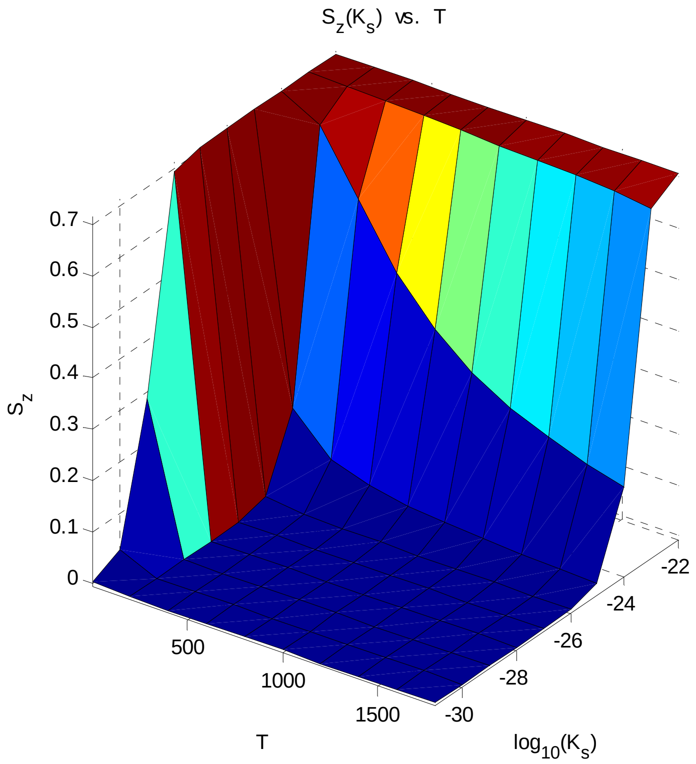

Figure2. 3-D plot of $\bar{S}_z$ versus $\log_{10}(K_s)$ and temperature.

But the temperature variation of $\bar{S}_z$ is really small for other energy parameters as given in figure 3. Although the curve in figure 3 is given only for N_d, the temperature variation of $\bar{S}_z$ with J, ω, $D_m^{(2)}$, $D_m^{(4)}$ or H_{in} is similar to the curve in figure 3. According to some of our previous experimental data of ferrite thin films, the magnetic anisotropy mainly depends on the stress induced anisotropy [10, 11].

Above model was employed to investigate the easy axis orientation of fcc structured ferromagnetic $CoPt_3$ films synthesized on WSe_2 substrates using electron gun deposition method in a ultra high vacuum by some other researchers [12, 13].

For fcc structure, $Z_0=4$, $Z_1=4$, $\Phi_0=9.0336$, and $\Phi_1=1.4294$ [14].

Because it is difficult to find the exact experimental values of J, ω, $D_m^{(2)}$, $D_m^{(4)}$, H_{in}, H_{out}, N_d and K_s for this particular $CoPt_3$ film, the simulations have been performed for the following set of above energy parameters. As given in figure 4, the $\bar{S}_z$ gradually decreases toward zero with temperature. At 423 K, $\bar{S}_z$ drops down to 10% of its initial value, when K_s and H_{out} are set to 10^{-22} Joules and $10^{-23}Am^{-1}$, respectively. Also as H_{out} increases, $\bar{S}_z$ at 423 K increases. Because the temperature variation of $\bar{S}_z$ solely depends on K_s and H_{out} according to our model, the other energy parameters such as J, ω, $D_m^{(2)}$, $D_m^{(4)}$, H_{in} and N_d are assumed to be negligible. Number of layers (N) is

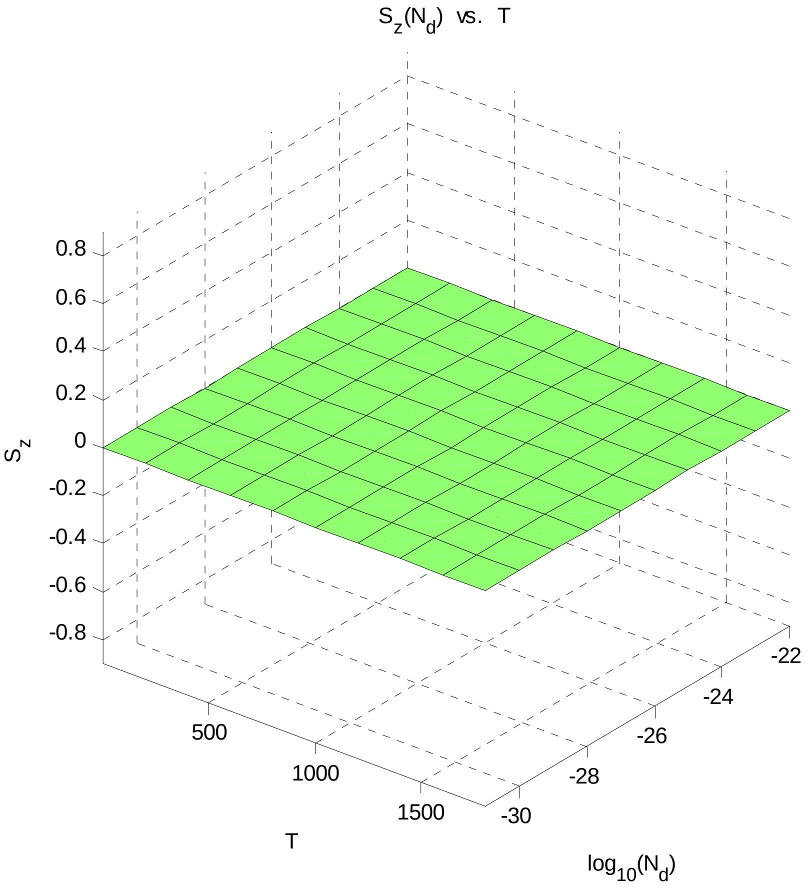

Figure3. 3-D plot of $\bar{S}_z$ versus $\log_{10}(N_d)$ and temperature.

taken as 16 for the film thickness of 6nm. In general, below 423 K most of the spins are in the out of plane direction, and beyond 423 K most of the spins are in the in-plane orientation. The easy axis of $CoPt_3$ fabricated using electron gun deposition method is oriented in the plane of the film above 150 ^{o}C experimentally [12]. Hence our theoretical evaluations are in consistence with their experimental observations.

The same simulation was carried out for bcc structured Fe-rich germanide films grown on Ge(001) substrates using magnetron sputtering by some other researchers [15] as following.

For bcc structure, $Z_0=0$, $Z_1=4$, $\Phi_0 = 5.8675$, $\Phi_1 = 2.7126$ [14].

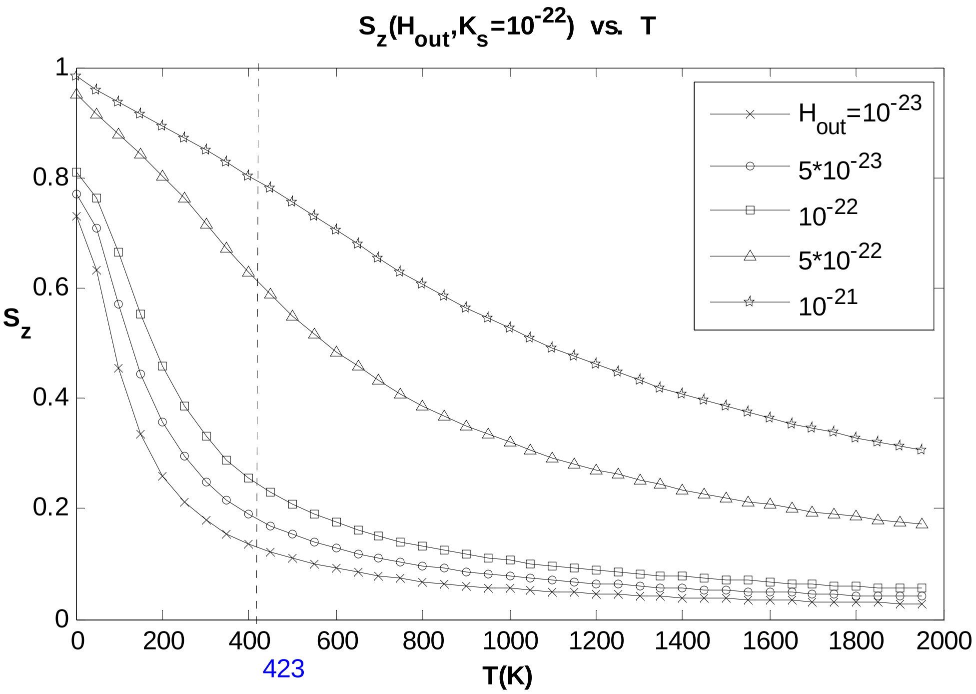

Figure4. Graph of $\bar{S}_z$ versus temperature, for $K_s=10^{-22}$ Joules and various values of H_{out}.

Thickness of the film is between 20 – 30 nm. In this experiment, spin reorientation from the out of plane to the in-plane direction has been observed at temperatures around 180^0 C (453 K). Taking the average thickness of 25 nm, the number of layers was calculated to be N=87. The curves of $\bar{S}_z$ versus temperature at $K_s=10^{-24}$ Joules for different values of H_{out} are given in figure 5. At 453 K, $\bar{S}_z$ drops down to less than 10% of initial value, when K_s and H_{out} are set to 10^{-24} Joules and 8×10^{-24} Am^{-1}, respectively. When H_{out} increases, $\bar{S}_z$ at 453 K increases. However, the decrease of $\bar{S}_z$ is less than 40% even at $H_{out}=6\times10^{-23}$ Am^{-1}. Thus as expected spin reorientation occurs around 453K. At temperatures less than 453 K, most of the spins are in the out of plane direction, and beyond 453 K most of the spins are in the in-plane orientation.

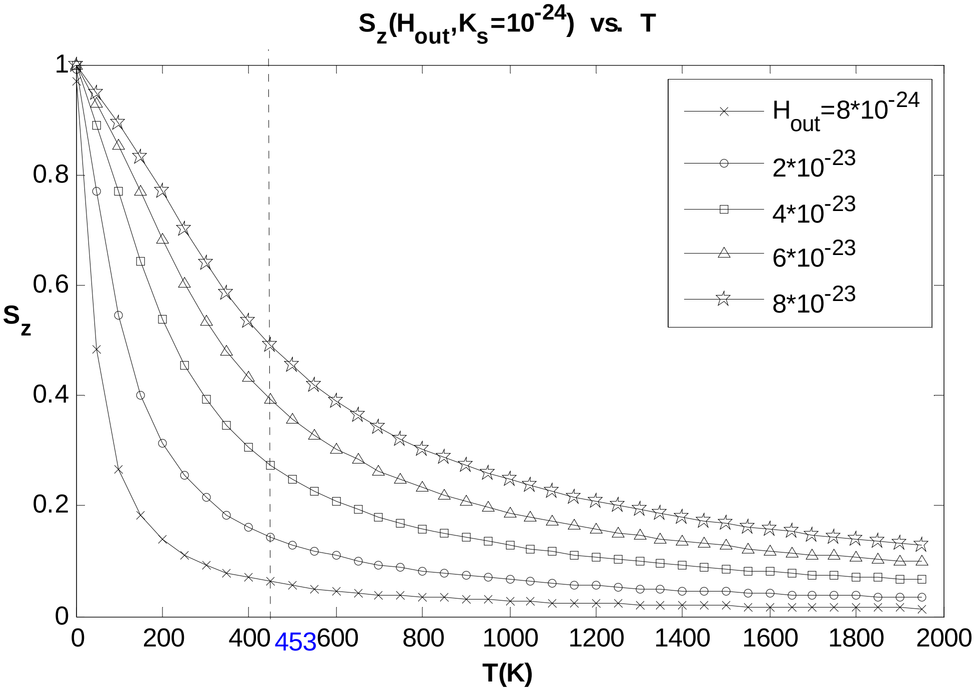

Figure5. Graph of $\overline{S}_z$ versus temperature, for $K_s=10^{-24}$ Joules and various values of H_{out}.

4. Conclusion:

The modified Heisenberg Hamiltonian with second order perturbation could be successfully employed to explain the easy axis orientation of some ferromagnetic films synthesized by some other researchers experimentally. In plane easy axis orientation of ferromagnetic $CoPt_3$ thin films with 16 layers synthesized on WSe_2 substrates using electron gun deposition method could be explained using $K_s=10^{-22}$ Joules and $H_{out}=10^{-23}$ Am^{-1} plugged in the equations of our model. Also the temperature, at which the easy axis of Fe-rich germanide film with 87 layers grown on Ge(001) substrates using magnetron sputtering orients in the plane of the film, could be explained using $K_s=10^{-24}$ Joules and $H_{out}=8\times10^{-24}$ Am^{-1}. In addition, the spin reorientation temperature mainly depends on the values of perpendicular magnetic field (H_{out}) and the stress induced anisotropy (K_s) according to our model. The average value of the out of plane spin component ($\overline{S}_z$) increases with H_{out} at one particular temperature as given in graphs of figures 4 and 5. Also the stress induced anisotropy plays a significant role in soft magnetic materials according to some of our previous experimental studies [10, 11].

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Article received: 2011-10-31