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INVESTIGATION OF ANISOTROPY CONSTANTS DEPENDENCE OF ULTRA-THIN FERROMAGNETIC FILMS WITH SECOND ORDER PERTURBED HEISENBERG HAMILTONIAN

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ABSTRACT

The variation of energy of ferromagnetic ultra-thin films with second and fourth order anisotropy was investigated using Heisenberg Hamiltonian with second order perturbation. The study was limited to sc(001) film with three layers. Graphs indicate energy minimums at certain values of second order anisotropy, fourth order anisotropy and angle. Films with fourth order anisotropy $\frac{D_m^{(4)}}{\omega}$=4 can be easily oriented in the direction given by angle of 2.66 radians for the values of other energy terms used in this simulation. When the second order anisotropy ($\frac{D_m^{(2)}}{\omega}$) is 3.1, preferred direction is 0.754 radians. When the second order anisotropy varies at a constant value of fourth order anisotropy, the graph indicates more energy minimums.

Keywords: Heisenberg Hamiltonian, magnetic thin films, magnetic anisotropies, spin

INTRODUCTION

Earlier the energy of ferromagnetic thin films was studied using Heisenberg Hamiltonian with second order perturbation for limited number of energy terms such as exchange interaction, second order anisotropy and stress induced anisotropy

(Samarasekara, 2006). The angle between easy and hard directions was found to be 90^0 for all sc(001), fcc(001) and bcc(001) ferromagnetic lattice types. In this study, all the energy terms are considered for simulations. The anisotropy constants are assumed to be an invariant for all layers through out the film. The energy of perfectly oriented thick ferromagnetic films up to 10000 layers has been investigated earlier and reported that easy and hard directions for bcc(001) lattice were $\theta=45^0$ and 135^0, respectively (Samarasekara, 2006).

Hamiltonian for ferromagnetic thin films has been solved using 2D XY model (Zhao *et al*., 2002), two-spin mean field theory (Jensen & Dreysse, 2002), spin half Ising model (Bentaleb *et al*., 2002) and classical Heisenberg model (Shan-Ho *et al*., 2003; Usadel & Hucht, 2002) by some other researchers. In addition to this, the Hamiltonian in Heisenberg model has been solved using Green functions (Ze-Nong Ding *et al*., 1993).

MODEL AND DISCUSSION

The Heisenberg Hamiltonian of any ferromagnetic film can be generally represented by following equation (Samarasekara, 2006).

$$H= -\frac{J}{2}\sum_{m,n}\vec{S}_m.\vec{S}_n+\frac{\omega}{2}\sum_{m\neq n}\left(\frac{\vec{S}_m.\vec{S}_n}{r_{mn}{}^3}-\frac{3(\vec{S}_m.\vec{r}_{mn})(\vec{r}_{mn}.\vec{S}_n)}{r_{mn}{}^5}\right)-\sum_m D_{\lambda_m}{}^{(2)}(S_m{}^z)^2-\sum_m D_{\lambda_m}{}^{(4)}(S_m{}^z)^4$$

$$-\sum_{m,n}[\vec{H}-(N_d\vec{S}_n/\mu_0)].\vec{S}_m-\sum_m K_s Sin2\theta_m$$

For the Heisenberg Hamiltonian given in above equation, total energy can be obtained as following (Samarasekara, 2006).

$$E(\theta)=E_0+\vec{\alpha}.\vec{\varepsilon}+\frac{1}{2}\vec{\varepsilon}.C.\vec{\varepsilon}=E_0-\frac{1}{2}\vec{\alpha}.C^+.\vec{\alpha}$$

The matrix elements of above matrix C are given by

$$C_{mn}=-(JZ_{|m-n|}-\frac{\omega}{4}\Phi_{|m-n|})-\frac{3\omega}{4}\cos 2\theta\Phi_{|m-n|}+\frac{2N_d}{\mu_0}$$

$$+\delta_{mn}\{\sum_{\lambda=1}^{N}[JZ_{|m-\lambda|}-\Phi_{|m-\lambda|}(\frac{\omega}{4}+\frac{3\omega}{4}\cos 2\theta)]-2(\sin^2\theta-\cos^2\theta)D_m^{(2)}$$

$$+4\cos^2\theta(\cos^2\theta-3\sin^2\theta)D_m^{(4)}+H_{in}\sin\theta+H_{out}\cos\theta-\frac{4N_d}{\mu_0}+4K_s\sin 2\theta\}$$

$\vec{\alpha}(\varepsilon)=\vec{B}(\theta)\sin 2\theta$ are the terms of matrices with

$$B_\lambda(\theta)=-\frac{3\omega}{4}\sum_{m=1}^{N}\Phi_{|\lambda-m|}+D_\lambda^{(2)}+2D_\lambda^{(4)}\cos^2\theta \qquad \textbf{(1)}$$

Here (Samarasekara, 2006)

$$E_0=-\frac{J}{2}[NZ_0+2(N-1)Z_1]+\{N\Phi_0+2(N-1)\Phi_1\}(\frac{\omega}{8}+\frac{3\omega}{8}\cos 2\theta)$$

$$-N(\cos^2\theta D_m^{(2)}+\cos^4\theta D_m^{(4)}+H_{in}\sin\theta+H_{out}\cos\theta-\frac{N_d}{\mu_0}+K_s\sin 2\theta)$$

E_0 is the energy of the oriented thin ferromagnetic film. Here J, $Z_{|m-n|}$, ω, $\Phi_{|m-n|}$, θ, $D_m^{(2)}, D_m^{(4)}, H_{in}, H_{out}, N_d, K_s$, m, n and N are spin exchange interaction, number of nearest spin neighbors, strength of long range dipole interaction, constants for partial summation of dipole interaction, azimuthal angle of spin, second and fourth order anisotropy constants, in plane and out of plane applied magnetic fields, demagnetization factor, stress induced anisotropy constant, spin plane indices and total number of layers in film, respectively. When the stress applies normal to the film plane, the angle between mth spin and the stress is θ_m.

Matrix elements for a film with three layers (N=3) can be given as following (Samarasekara, 2006),

$$C_{12}=C_{21}=C_{23}=C_{32}=-JZ_1+\frac{\omega}{4}\Phi_1(1-3\cos 2\theta)+\frac{2N_d}{\mu_0}$$

$$C_{13}=C_{31}=-JZ_2+\frac{\omega}{4}\Phi_2(1-3\cos 2\theta)+\frac{2N_d}{\mu_0}$$

$$C_{11} = C_{33} = J(Z_1 + Z_2) - \frac{\omega}{4}(\Phi_1 + \Phi_2)(1 + 3\cos 2\theta) - \frac{2N_d}{\mu_0} + (2\cos 2\theta)D_m^{(2)}$$

$$+ 4\cos^2\theta(\cos^2\theta - 3\sin^2\theta)D_m^{(4)} + H_{in}\sin\theta + H_{out}\cos\theta + 4K_s\sin 2\theta$$

$$C_{22} = 2JZ_1 - \frac{\omega}{2}\Phi_1(1 + 3\cos 2\theta) - \frac{2N_d}{\mu_0} + (2\cos 2\theta)D_m^{(2)}$$

$$+ 4\cos^2\theta(\cos^2\theta - 3\sin^2\theta)D_m^{(4)} + H_{in}\sin\theta + H_{out}\cos\theta + 4K_s\sin 2\theta$$

If the second or fourth order anisotropy constants are invariants inside an ultra thin film, then $D_1^{(2)}=D_2^{(2)}=D_3^{(2)}$ and $D_1^{(4)}=D_2^{(4)}=D_3^{(4)}$. Under some special conditions (Samarasekara, 2006), C^+ is the standard inverse of a matrix, given by matrix element $C^+_{mn} = \frac{cofactor C_{nm}}{\det C}$. For the convenience, the matrix elements C^+_{mn} will be given in terms of C_{11}, C_{22}, C_{32}, and C_{31} only.

$$C^+_{11} = \frac{C_{11}C_{22} - C_{32}^2}{C_{11}(C_{11}C_{22} - C_{31}^2) + 2C_{32}^2(C_{31} - C_{11})} = C^+_{33}$$

$$C^+_{12} = \frac{C_{32}C_{31} - C_{32}C_{11}}{C_{11}(C_{11}C_{22} - C_{31}^2) + 2C_{32}^2(C_{31} - C_{11})} = C^+_{21} = C^+_{23} = C^+_{32}$$

$$C^+_{13} = \frac{C_{32}^2 - C_{22}C_{31}}{C_{11}(C_{11}C_{22} - C_{31}^2) + 2C_{32}^2(C_{31} - C_{11})} = C^+_{31}$$

$$C^+_{22} = \frac{C_{11}^2 - C_{31}^2}{C_{11}(C_{11}C_{22} - C_{31}^2) + 2C_{32}^2(C_{31} - C_{11})} \qquad \textbf{(2)}$$

Matrices C and C^+ are highly symmetric, and total energy can be given as (Samarasekara, 2006),

$E(\theta)=E_0-0.5[C^+_{11}(\alpha_1^2+\alpha_3^2)+C^+_{32}(2\alpha_1\alpha_2+2\alpha_2\alpha_3)+C^+_{31}(2\alpha_1\alpha_3)+\alpha_2^2C^+_{22}]$

From equation 1,

$$B_1(\theta) = B_3(\theta) = -\frac{3\omega}{4}(\Phi_0 + \Phi_1 + \Phi_2) + D_\lambda^{(2)} + 2D_\lambda^{(4)}\cos^2\theta$$

$$B_2(\theta) = -\frac{3\omega}{4}(\Phi_0 + 2\Phi_1) + D_\lambda^{(2)} + 2D_\lambda^{(4)}\cos^2\theta$$

Because in this case, $\alpha_1=\alpha_3$

$E(\theta)=E_0-0.5[2C^+_{11}\alpha_1^2+4C^+_{32}\alpha_1\alpha_2+2C^+_{31}\alpha_1^2+\alpha_2^2C^+_{22}]$ **(3)**

First simulation will be carried out for

$$\frac{J}{\omega} = \frac{D_m^{(2)}}{\omega} = \frac{H_{in}}{\omega} = \frac{H_{out}}{\omega} = \frac{N_d}{\mu_0\omega} = \frac{K_s}{\omega} = 10$$

For sc(001) lattice, $Z_0=4$, $Z_1=1$, $Z_2=0$, $\Phi_0=9.0336$, $\Phi_1= -0.3275$ and $\Phi_2=0$ (Usadel & Hucht, 2002),

$$\frac{C_{12}}{\omega} = \frac{C_{21}}{\omega} = \frac{C_{23}}{\omega} = \frac{C_{32}}{\omega} = 9.92 + 0.2456\cos 2\theta$$

$$\frac{C_{13}}{\omega} = \frac{C_{31}}{\omega} = 20$$

$$\frac{C_{11}}{\omega} = \frac{C_{33}}{\omega} = -9.92 + 20.2456\cos 2\theta + 4\cos^2\theta(\cos^2\theta - 3\sin^2\theta)\frac{D_m^{(4)}}{\omega}$$

$$+10\sin\theta + 10\cos\theta + 40\sin 2\theta$$

$$\frac{C_{22}}{\omega} = 0.164 + 20.49\cos 2\theta + 4\cos^2\theta(\cos^2\theta - 3\sin^2\theta)\frac{D_m^{(4)}}{\omega}$$

$$+10\sin\theta + 10\cos\theta + 40\sin 2\theta$$

$$\frac{\alpha_1}{\omega} = \frac{\alpha_3}{\omega} = (3.47 + 2\frac{D_m^{(4)}}{\omega}\cos^2\theta)\sin 2\theta$$

$$\frac{\alpha_2}{\omega} = (3.716 + 2\frac{D_m^{(4)}}{\omega}\cos^2\theta)\sin 2\theta$$

$$\frac{E_0}{\omega} = 25.22 + 9.67\cos 2\theta$$

$$-3(10\cos^2\theta + \frac{D_m^{(4)}}{\omega}\cos^4\theta + 10\sin\theta + 10\cos\theta + 10\sin 2\theta)$$

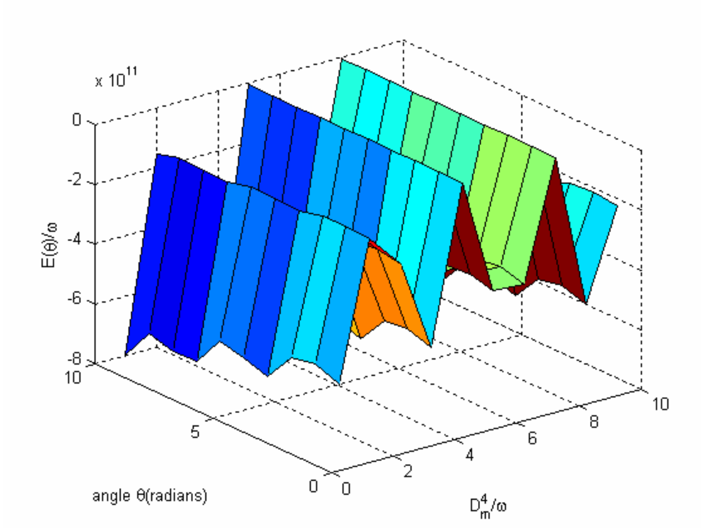

Figure 1. 3-D plot of total energy versus angle and $\frac{D_m^{(4)}}{\omega}$ for a film with three layers

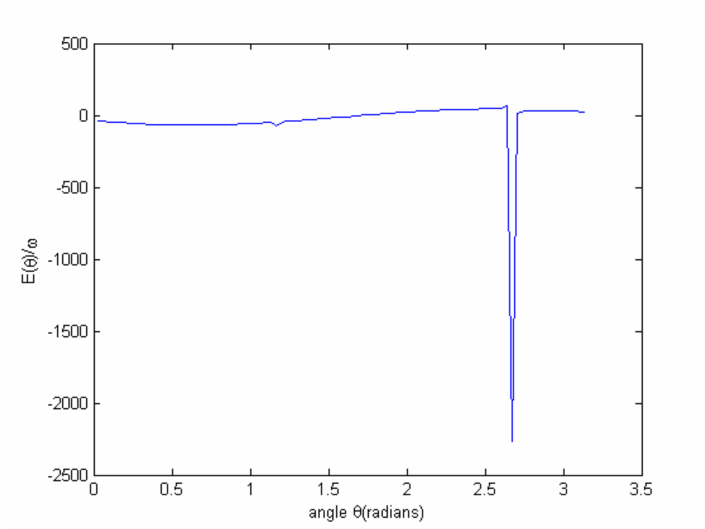

Figure 2. Plot between energy and the angle at $\frac{D_m^{(4)}}{\omega}$ =4

The total energy can be found using equation 3. 3-D plot of total energy versus angle and $\frac{D_m^{(4)}}{\omega}$ is given in Fig. 1. The energy becomes minimums at some values of angles and second order anisotropy constants by indicating that films with this second order anisotropy can be easily oriented in the directions given by these angles. The second and fourth order anisotropy constants are characteristics of magnetic materials, and they mostly depend on the type of material. For example, when $\frac{D_m^{(4)}}{\omega}$ = 4 the film can be easily oriented in some certain directions. As shown in Fig. 2, the plot between energy and the angle at $\frac{D_m^{(4)}}{\omega}$ =4 was drawn in order to find the angle corresponding to easy directions. The angle corresponding to energy minimums is 2.66 radians.

When $\frac{J}{\omega}=\frac{H_{in}}{\omega}=\frac{H_{out}}{\omega}=\frac{N_d}{\mu_0\omega}=\frac{K_s}{\omega}=10$ and $\frac{D_m^{(4)}}{\omega}$ =5

$$\frac{C_{11}}{\omega}=\frac{C_{33}}{\omega}=-9.92+0.2456\cos 2\theta$$

$$+2\frac{D_m^{(2)}}{\omega}\cos 2\theta+20\cos^2\theta(\cos^2\theta-3\sin^2\theta)$$

$$+10\sin\theta+10\cos\theta+40\sin 2\theta$$

$$\frac{C_{22}}{\omega}=0.164+0.49\cos 2\theta+2\frac{D_m^{(2)}}{\omega}\cos 2\theta+20\cos^2\theta(\cos^2\theta-3\sin^2\theta)$$

$$+10\sin\theta+10\cos\theta+40\sin 2\theta$$

$$\frac{\alpha_1}{\omega}=\frac{\alpha_3}{\omega}=(-6.53+\frac{D_m^{(2)}}{\omega}+10\cos^2\theta)\sin 2\theta$$

$$\frac{\alpha_2}{\omega}=(-6.28+\frac{D_m^{(2)}}{\omega}+10\cos^2\theta)\sin 2\theta$$

$$\frac{E_0}{\omega}=25.22+9.67\cos 2\theta$$

$$-3(\frac{D_m^{(2)}}{\omega}\cos^2\theta+5\cos^4\theta+10\sin\theta+10\cos\theta+10\sin 2\theta)$$

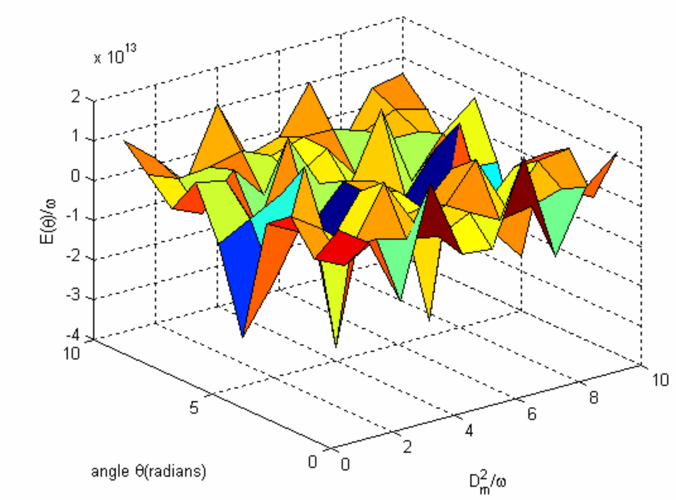

Figure 3. 3-D plot of energy versus angle and $\frac{D_m^{(2)}}{\omega}$ for a film with three layers

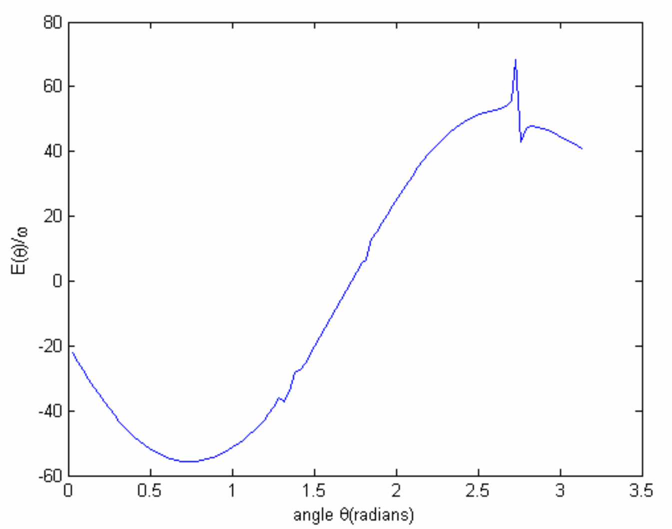

Figure 4. Graph between energy and angle at $\frac{D_m^{(2)}}{\omega}$=3.1

3-D plot of energy versus angle and $\frac{D_m^{(2)}}{\omega}$ is given in Fig. 3. This graph indicates more energy minimums and higher energy values compared with previous graph. At $\frac{D_m^{(2)}}{\omega}$ =3.1, energy is minimum. Therefore, graph between energy and angle was plotted in order to find other angles corresponding to other energy minimums at $\frac{D_m^{(2)}}{\omega}$ =3.1, as shown in Fig. 4. Energy is minimized at 0.754 radians. This graph is smoother compared with the previous graph.

CONCLUSIONS

For sc(001) films with three layers, graphs indicate several energy minimums at particular values of second order anisotropy, fourth order anisotropy and angle. When the fourth order anisotropy $\frac{D_m^{(4)}}{\omega}$ is 4, film can be easily oriented in the direction of 2.66 radians. If the second order anisotropy ($\frac{D_m^{(2)}}{\omega}$) is 3.1, energetically favorable direction is 0.754 radians. When the second order anisotropy varies at a constant value of fourth order anisotropy, the graph indicates more energy minimums and higher energy values. Although this simulation was performed for some specific values of these parameters, this same simulation can be carried out for other values of these parameters.

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