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Effect of demagnetization factor on total energy of ultra-thin ferromagnetic films with three layers

P. Samarasekara
Department of Physics, University of Ruhuna, Matara, Sri Lanka
Correpondence: pubudus@phy.ruh.ac.lk

Abstract. The energy of ultra-thin sc(001) ferromagnetic film with three layers will be investigated using classical Heisenberg Hamiltonian. Energy curves show several minimums indicating that the film can be easily oriented in these directions under the influence of certain values of demagnetization factor. When the demagnetization factor is given by $\frac{N_d}{\mu_0\omega}$=8, the angle corresponding to first minimum is 0.6 radians for sc(001) ferromagnetic lattice. Under the influence of demagnetization factor of $\frac{N_d}{\mu_0\omega}$= 7.5, energy minimum can be observed at 0.6 radians for bcc(001) lattice. The energy curve of bcc(001) ferromagnetic lattice is smoother compared with that of sc(001) lattice.

Keywords: materials, thin films, Heisenberg Hamiltonian, demagnetization factor

1. Introduction:

The properties of ferromagnetic ultra-thin films have been investigated using classical model of Heisenberg Hamiltonian with limited number of terms (Usadel and Hutch 2002). Because of the difficulties of understanding the behavior of exchange anisotropy and its applications in magnetic sensors and media technology, exchange anisotropy has been extensively investigated in recent past (David et al. 2004). Ferromagnetic films are thoroughly studied nowadays, due to their potential applications in magnetic memory devices and microwave devices. Bloch spin wave theory has been used to investigate magnetic properties of ferromagnetic thin films (Martin and Robert 1951). Although the magnetization of some thin films is oriented in the plane of the film due to dipole interaction, the out of plane orientation is preferred at the surface due to the broken symmetry of uniaxial anisotropy energy. Previously two dimensional Heisenberg model has been used to explain the magnetic anisotropy in the presence of dipole interaction (Dantinzger et al. 2002). Ising model has been used to study magnetic properties of ferromagnetic thin films with alternating super layers (Bentaleb et al. 2002).

For the very first time, the variation of energy of ferromagnetic ultra-thin films with demagnetization factor will be described in this report. The energy of non-oriented ultra-thin ferromagnetic films with two and three layers has been calculated using Heisenberg Hamiltonian with second order perturbation, under the effect of limited number of energy parameters (Samarasekara 2006). The properties of perfectly oriented thick ferromagnetic films have been investigated by classical Heisenberg model (Samarasekara 2006). The variation of energy with angle and number of layers has been studied for thick films up to 10000 layers. The total magnetic energy has been calculated using two different methods depending on discrete and continuous variation of thickness. For bcc(001) lattice, the easy and hard directions calculated using both methods were exactly same.

2. Model and discussion:

The classical model of Heisenberg Hamiltonian is given as following (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 m^{th} 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

$$\frac{J}{\omega} = \frac{D_m{}^{(2)}}{\omega} = \frac{H_{in}}{\omega} = \frac{H_{out}}{\omega} = \frac{K_s}{\omega} = 10 and \frac{D_m{}^{(4)}}{\omega} = 5$$

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 and Hucht 2002),

$$\frac{C_{12}}{\omega} = \frac{C_{21}}{\omega} = \frac{C_{23}}{\omega} = \frac{C_{32}}{\omega} = -10.08 + 0.2456\cos 2\theta + \frac{2N_d}{\mu_0\omega}$$

$$\frac{C_{13}}{\omega} = \frac{C_{31}}{\omega} = \frac{2N_d}{\mu_0\omega}$$

$$\frac{C_{11}}{\omega} = \frac{C_{33}}{\omega} = 10.08 + 20.2456\cos 2\theta - \frac{2N_d}{\mu_0\omega} + 20\cos^2\theta(\cos^2\theta - 3\sin^2\theta)$$
$$+ 10\sin\theta + 10\cos\theta + 40\sin 2\theta$$

$$\frac{C_{22}}{\omega} = 20.164 + 20.49\cos 2\theta - \frac{2N_d}{\mu_0\omega} + 20\cos^2\theta(\cos^2\theta - 3\sin^2\theta)$$
$$+ 10\sin\theta + 10\cos\theta + 40\sin 2\theta$$

$$\frac{\alpha_1}{\omega} = \frac{\alpha_3}{\omega} = (3.47 + 10\cos^2\theta)\sin 2\theta$$

$$\frac{\alpha_2}{\omega} = (3.716 + 10\cos^2\theta)\sin 2\theta$$

$$\frac{E_0}{\omega} = -4.78 + 9.67\cos 2\theta$$
$$-3(10\cos^2\theta + 5\cos^4\theta + 10\sin\theta + 10\cos\theta - \frac{N_d}{\mu_0\omega} + 10\sin 2\theta)$$

For sc(001), 3-D plot of energy versus angle and $\frac{N_d}{\mu_0\omega}$ is given in figure 1. The graph indicates several energy minimums at different values of angle and demagnetization factor. Under the influence of these demagnetization factors, the sample can be easily oriented in certain directions corresponding to energy minimums. For example, one minimum can be observed at $\frac{N_d}{\mu_0\omega}$=8, and the angle corresponding to this demagnetization factor can be obtained from figure 2. Angle corresponding to first minimum is 0.6 radians.

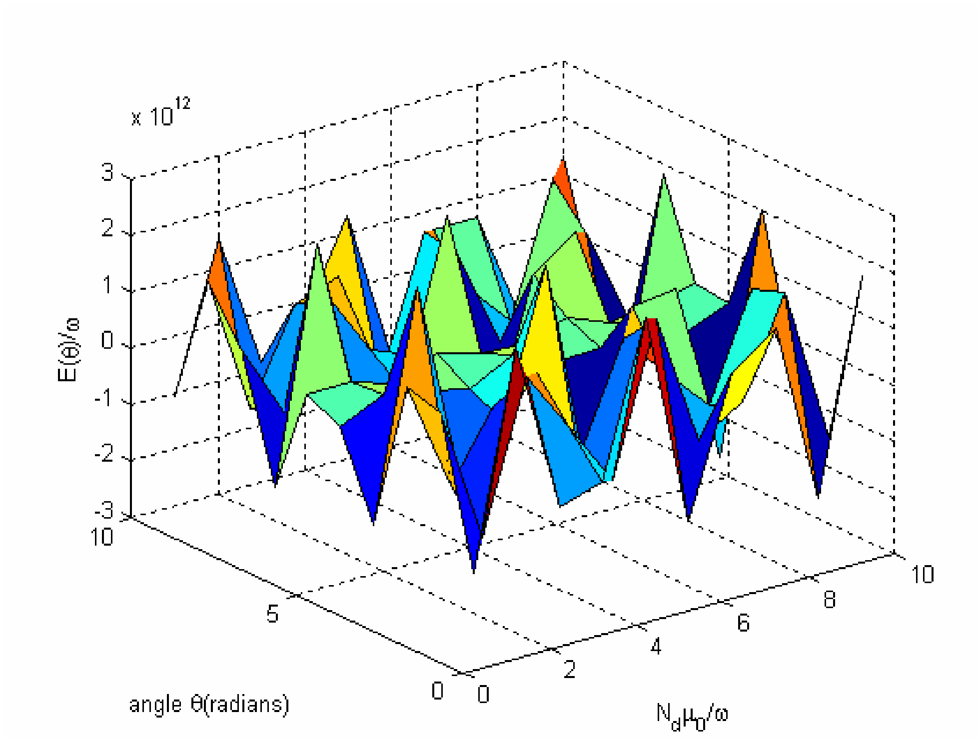

Figure 1: 3-D plot of energy versus angle and $\frac{N_d}{\mu_0\omega}$ for sc(001) ferromagnetic lattice

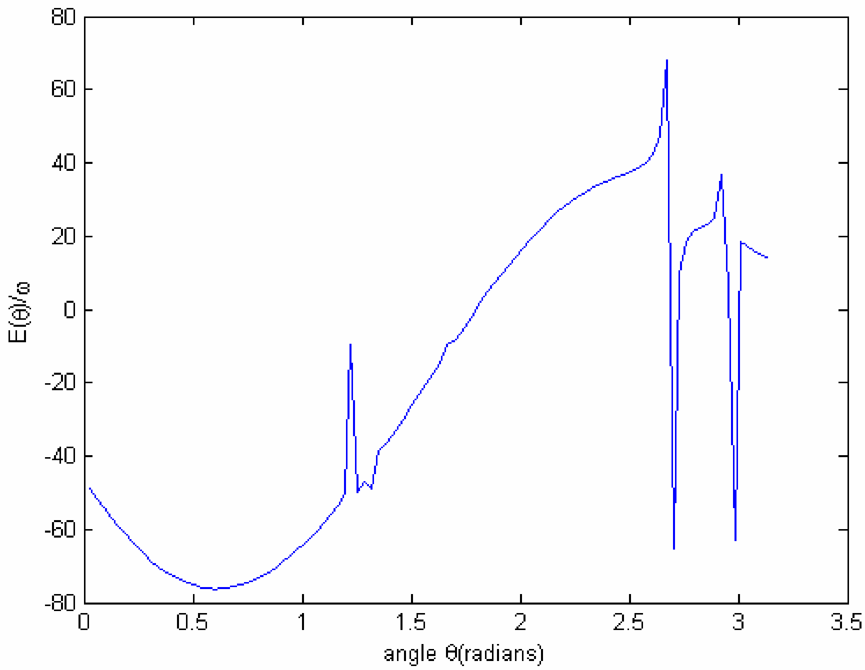

Figure 2: Energy versus angle at $\frac{N_d}{\mu_0\omega}$=8 for sc (001) lattice

For bcc(001) lattice, Z_0=0, Z_1=4, Z_2=0, Φ_0=5.8675 and Φ_1=2.7126 (Usadel and Hucht 2002),

$$\frac{C_{12}}{\omega}=\frac{C_{21}}{\omega}=\frac{C_{23}}{\omega}=\frac{C_{32}}{\omega}=-39.32-2.03\cos 2\theta+\frac{2N_d}{\mu_0\omega}$$

$$\frac{C_{13}}{\omega}=\frac{C_{31}}{\omega}=\frac{2N_d}{\mu_0\omega}$$

$$\frac{C_{11}}{\omega}=\frac{C_{33}}{\omega}=39.32-2.03\cos 2\theta-\frac{2N_d}{\mu_0\omega}+20\cos^2\theta(\cos^2\theta-3\sin^2\theta)$$
$$+10\sin\theta+10\cos\theta+40\sin 2\theta$$

$$\frac{C_{22}}{\omega}=78.64-4.07\cos 2\theta-\frac{2N_d}{\mu_0\omega}+20\cos^2\theta(\cos^2\theta-3\sin^2\theta)$$
$$+10\sin\theta+10\cos\theta+40\sin 2\theta$$

$$\frac{\alpha_1}{\omega}=\frac{\alpha_3}{\omega}=(3.565+10\cos^2\theta)\sin 2\theta$$

$$\frac{\alpha_2}{\omega}=(1.53+10\cos^2\theta)\sin 2\theta$$

$$\frac{E_0}{\omega} = -76.44 + 10.67\cos 2\theta$$
$$-3(10\cos^2\theta + 5\cos^4\theta + 10\sin\theta + 10\cos\theta - \frac{N_d}{\mu_0\omega} + 10\sin 2\theta)$$

3-D plot of energy versus angle and $\frac{N_d}{\mu_0\omega}$ for bcc(001) ferromagnetic lattice is given in figure 3. This graph also indicates several energy minimums. Energy is minimum at $\frac{N_d}{\mu_0\omega}$ = 7.5. The figure 4 has been drawn to find the easy directions corresponding to this energy minimum at $\frac{N_d}{\mu_0\omega}$ = 7.5. Energy minimum can be observed at 0.6 radians, and this angle gives the easy direction at $\frac{N_d}{\mu_0\omega}$ = 7.5. This graph is smoother compared with the energy curve given in figure 2.

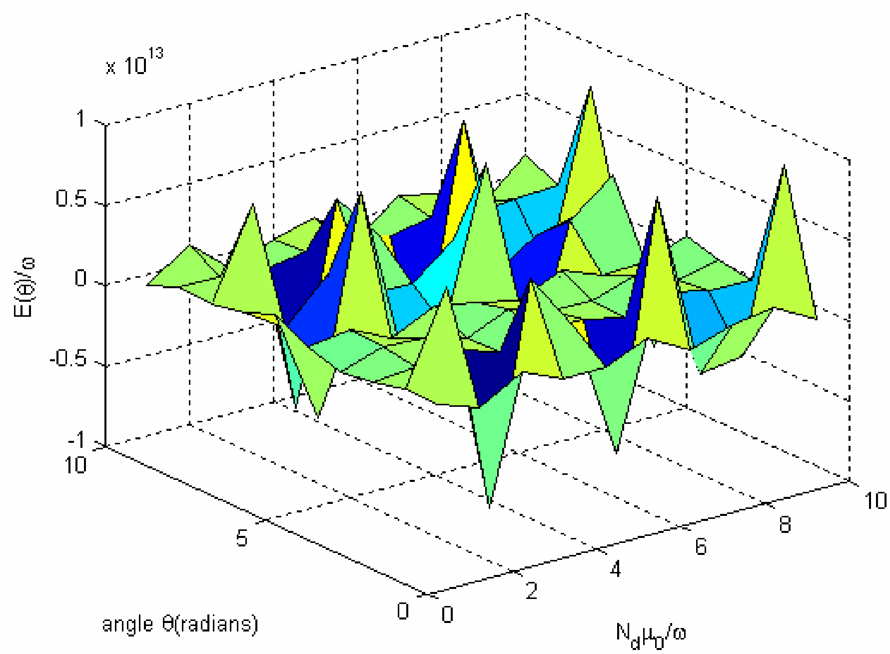

Figure 3: 3-D plot of energy versus angle and $\frac{N_d}{\mu_0\omega}$ for bcc(001) ferromagnetic lattice

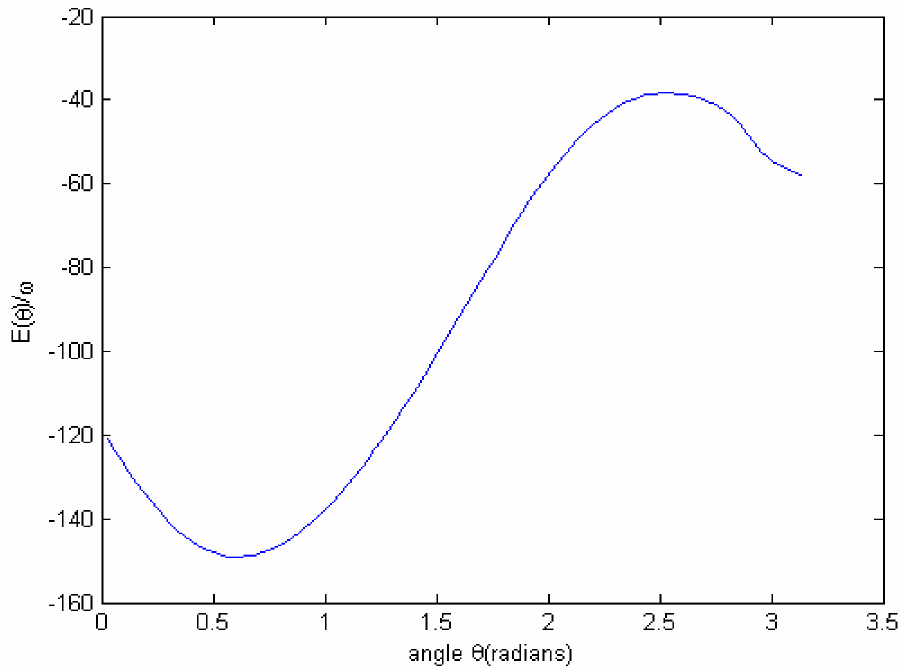

Figure 4: Energy versus angle at $\frac{N_d}{\mu_0 \omega}$ =7.5 for bcc (001) lattice

3. Conclusion:

3-D plots and 2-D plots of energy indicate several minimums implying that the film can be easily oriented in these directions given by angles corresponding to minimums under the influence of certain values of demagnetization factor. At $\frac{N_d}{\mu_0 \omega}$=8, the angle corresponding to first minimum is 0.6 radians for sc(001) ferromagnetic lattice. Under the influence of demagnetization factor given by $\frac{N_d}{\mu_0 \omega}$= 7.5, energy minimum can be observed at 0.6 radians for bcc(001) lattice. This simulation can be carried out for any other values of these energy parameters as well.

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