ISSN 1512-1461

UDC: Condensed matter physics, Solid state physics
Theoretical Condensed Matter Physics

# VARIATION OF ENERGY WITH ANISOTROPY CONSTANTS OF FERROMAGNETIC THIN FILMS WITH FOUR LAYERS

P. Samarasekara
Department of Physics, University of Peradeniya, Peradeniya, Sri Lanka

***Abstract***
*The second and fourth order anisotropy dependence of ferromagnetic thin films with four layers has been investigated using Heisenberg Hamiltonian with second order perturbation. According to energy plots, the sc(001) ferromagnetic films with four layers indicate energetically preferred directions for certain values of second and fourth order anisotropy constants, which are characteristics of magnetic materials These angles corresponding to energy minimums provide the easy directions of those magnetic materials. When the fourth order anisotropy is given by* $\frac{D_m^{(4)}}{\omega}$ *=5.3, the easy direction makes 0.6 and 2.73 radians with perpendicular line drawn to film plane. If the second order anisotropy is given by* $\frac{D_m^{(2)}}{\omega}$ *=3.8, the easy direction of film makes 0.72 radians with film normal.*

***Keywords:*** *Ferromagnetic, anisotropy, Heisenberg Hamiltonian*

## 1. Introduction:

Exchange anisotropy has been extensively investigated in recent past, because of the difficulties of understanding the behavior of exchange anisotropy and its applications in magnetic sensors and media technology [2]. Ferromagnetic films are thoroughly studied nowadays, due to their potential applications in magnetic memory devices and microwave devices. Earlier Bloch spin wave theory has been applied to study magnetic properties of ferromagnetic thin films [3]. 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 [4]. Ising model has been used to study magnetic properties of ferromagnetic thin films with alternating super layers [5].

For the first time the variation of magnetic energy of a ferromagnetic film with four layers under the influence of demagnetization factor and stress induced anisotropy has been widely studied 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 [6]. The properties of perfectly oriented thick ferromagnetic films have been investigated by classical Heisenberg model [7]. 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 number of layers. For bcc(001) lattice, the easy and hard directions calculated using both methods were exactly same. Easy and hard directions for bcc(001) lattice are $\theta=45^0$ and $135^0$, respectively [7].

## 2. Model and discussion:

Following equation represents the Heisenberg Hamiltonian of any ferromagnetic film [6, 7].

ISSN 1512-1461

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

$$-\sum_m [\vec{H} - \frac{N_d \mu_0 \mu^2}{V}\sum_n \vec{S}_n].\vec{S}_m - \sum_m K_s Sin2\theta_m$$

In this 2-D model, the spin was assumed to be in y-z plane, and the x component of the spin was considered to be zero. The angle (θ) has been measured with respect to the perpendicular line drawn to the film plane, which is the z axis of the coordinate system. The y-axis lies in the plane of the film. Since two spins ($S_m$ and $S_n$) must be taken into account in determinations of exchange interaction and dipole interactions, the azimuthal angles of $S_m$ and $S_n$ were taken as $\theta_m$ and $\theta_n$, respectively. When there is a small perturbation of angles, the azimuthal angles of spins can be given as $\theta_m = \theta + \varepsilon_m$ and $\theta_n = \theta + \varepsilon_n$. After substituting these new angles in above equation, the cosine and sine terms can be expanded up to the second order of $\varepsilon_m$ and $\varepsilon_n$. The third and higher order terms of $\varepsilon_m$ and $\varepsilon_n$ are neglected in this second order perturbation method. Because the average value of $\varepsilon_m$ (or $\varepsilon_n$) is assumed to be zero with constraint $\sum_{m=1}^{N}\varepsilon_m = 0$, the first order term of energy can be written as $E(\varepsilon)=\vec{\alpha}.\vec{\varepsilon}$ . In addition, the energy term with second order perturbation of ε and energy term without ε are taken as $\frac{1}{2}\vec{\varepsilon}.C.\vec{\varepsilon}$ and $E_0$, respectively.

The stress induced anisotropy appearing in above equation is given by [8, 9, 10, 11]

$E= -(3\lambda\sigma\sin2\phi)/2= -K_u\sin2\phi$

Here ϕ is the angle between the stress (σ) and the direction of spin, λ is the isotropic magnetostriction coefficient, and $K_u=3\lambda\sigma/2$.

Here $\sigma=E(\alpha_f- \alpha_s)\Delta T/(1- \nu)$, where E, $\alpha_f$, $\alpha_s$, ΔT and ν are the Young's modulus of the film, thermal expansion coefficient of film, thermal expansion coefficient of substrate, difference between deposition (or annealing) temperature and Poisson ratio of film, respectively.

For the Heisenberg Hamiltonian given in above equation, total energy can be obtained as following [1].

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

The matrix elements of above matrix C are given by

$$C_{mn} = -(JZ_{|m-n|} - \frac{\omega}{4}\Phi_{|m-n|}) - \frac{3\omega}{4}\cos 2\theta\Phi_{|m-n|} + \frac{2N_d\mu_0\mu^2}{V}$$
$$+\delta_{mn}\{\sum_{\lambda=1}^{N}[JZ_{|m-\lambda|} - \Phi_{|m-\lambda|}(\frac{\omega}{4} + \frac{3\omega}{4}\cos 2\theta)] - 2(\sin^2\theta - \cos^2\theta)D_m^{(2)}$$
$$+4\cos^2\theta(\cos^2\theta - 3\sin^2\theta)D_m^{(4)} + H_{in}\sin\theta + H_{out}\cos\theta - \frac{4N_d\mu_0\mu^2}{V} + 4K_s\sin 2\theta\} \quad \mathbf{(1)}$$

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

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

Here [6]

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

ISSN 1512-1461

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

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 $\theta_m$. $E_0$ is the energy of the oriented thin ferromagnetic film. V, μ and $\mu_0$ are the volume of the sample, the magnetic moment value of electron spin and the permeability of free space, respectively.

For most ferromagnetic films, $Z_{\delta\geq 2}=\Phi_{\delta\geq 2}=0$. If the anisotropy constants do not vary within the film, then $D_m^{(2)}$ or $D_m^{(4)}$ is a constant for any layer.

From equation number 1, the matrix elements of matrix C can be given as following.

$$C_{11}=C_{44}=JZ_1-\frac{\omega}{4}\Phi_1(1+3\cos 2\theta)-2(\sin^2\theta-\cos^2\theta)D_m^{(2)}$$

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

When the difference between two indices (m, n) is 1 or -1,

$$C_{12}=C_{23}=C_{34}=C_{21}=C_{32}=C_{43}=-JZ_1+\frac{\omega}{4}\Phi_1(1-3\cos 2\theta)+\frac{2N_d\mu_0\mu^2}{V}$$

$$C_{22}=C_{33}=2JZ_1-\frac{\omega}{2}\Phi_1(1+3\cos 2\theta)-2(\sin^2\theta-\cos^2\theta)D_m^{(2)}$$

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

From equation 2, $B_1(\theta)=B_4(\theta)=-\frac{3\omega}{4}(\Phi_0+\Phi_1)+D_m^{(2)}+2D_m^{(4)}\cos^2\theta$

$$B_2(\theta)=B_3(\theta)=-\frac{3\omega}{4}(\Phi_0+2\Phi_1)+D_m^{(2)}+2D_m^{(4)}\cos^2\theta$$

Therefore, $C_{11}=C_{44}$, $C_{22}=C_{33}$, $C_{21}=C_{12}=C_{23}=C_{32}=C_{34}=C_{43}$

But $C_{13}$, $C_{14}$, $C_{24}$, $C_{31}$, $C_{41}$ and $C_{42}$ are constants, and they do not depend on angle (θ). Therefore, theses constants do not change physical properties, and they will be assumed to be zero for the convenience.

$C_{13}=C_{14}=C_{24}=C_{31}=C_{41}=C_{42}=0$

Under some special conditions [6], $C^+$ is the standard inverse of matrix C, given by matrix element $C^+_{mn}=\frac{cofactor C_{nm}}{\det C}$. For the convenience, the following matrix elements $C^+_{mn}$ will be given in terms of $C_{11}$, $C_{22}$ and $C_{12}$ only.

Determinant of 4x4 matrix= det C = $(C_{11}C_{22}-C_{12}^2)^2-C_{12}^2C_{11}^2$

$$C_{11}^+=C_{44}^+=\frac{C_{22}(C_{22}C_{11}-C_{12}^2)-C_{12}^2C_{11}}{\det C}$$

ISSN 1512-1461

$$C_{12}^{+}=C_{21}^{+}=C^{+}34=C^{+}43=-\frac{C_{12}(C_{22}C_{11}-C_{12}^{2})}{\det C}$$

$$C_{13}^{+}=C_{31}^{+}=C^{+}24=C^{+}42=\frac{C_{12}^{2}C_{11}}{\det C}$$

$$C_{14}^{+}=C_{41}^{+}=-\frac{C_{12}^{3}}{\det C}$$

$$C_{22}^{+}=C_{33}^{+}=\frac{C_{11}(C_{22}C_{11}-C_{12}^{2})}{\det C}$$

$$C_{23}^{+}=C_{32}^{+}=-\frac{C_{12}C_{11}^{2}}{\det C}$$

Total energy=$E(\theta)=E_0-\alpha_1^2(C_{11}^{+}+C_{14}^{+})-2\alpha_1\alpha_2(C_{12}^{+}+C_{13}^{+})-\alpha_2^2(C_{22}^{+}+C_{23}^{+})$ **(3)**

For sc(001) lattice, $Z_0=4$, $Z_1=1$, $Z_2=0$, $\Phi_0=9.0336$, $\Phi_1=-0.3275$ and $\Phi_2=0$ [1].

First simulation will be performed for

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

$$\frac{C_{11}}{\omega}=\frac{C_{44}}{\omega}=-9.92+20.2456\cos 2\theta+4\cos^2\theta(\cos^2\theta-3\sin^2\theta)\frac{D_m^{(4)}}{\omega}$$
$$+10\sin\theta+10\cos\theta+40\sin 2\theta$$

$$\frac{C_{22}}{\omega}=\frac{C_{33}}{\omega}=0.164+20.49\cos 2\theta+4\cos^2\theta(\cos^2\theta-3\sin^2\theta)\frac{D_m^{(4)}}{\omega}$$
$$+10\sin\theta+10\cos\theta+40\sin 2\theta$$

$$\frac{\alpha_1}{\omega}=\frac{\alpha_4}{\omega}=(3.47+2\frac{D_m^{(4)}}{\omega}\cos^2\theta)\sin 2\theta$$

$$\frac{\alpha_2}{\omega}=\frac{\alpha_3}{\omega}=(3.716+2\frac{D_m^{(4)}}{\omega}\cos^2\theta)\sin 2\theta$$

$$\frac{C_{12}}{\omega}=\frac{C_{21}}{\omega}=\frac{C_{23}}{\omega}=\frac{C_{32}}{\omega}=\frac{C_{34}}{\omega}=\frac{C_{43}}{\omega}=9.92+0.2456\cos 2\theta$$

$$\frac{E_0}{\omega}=-65.73+12.81\cos 2\theta-4(10\cos^2\theta+\frac{D_m^{(4)}}{\omega}\cos^4\theta+10\cos\theta+10\sin\theta+10\sin 2\theta)$$

Because the equations of matrix elements ($C_{mn}$) were given earlier, elements of inverse matrix ($C_{mn}^{+}$) can be found from above equations. Then the total energy can be determined from equation number 3. The 3-D plot of energy versus $\frac{D_m^{(4)}}{\omega}$ and angle is given in figure 1. According to this graph, the energy

ISSN 1512-1461

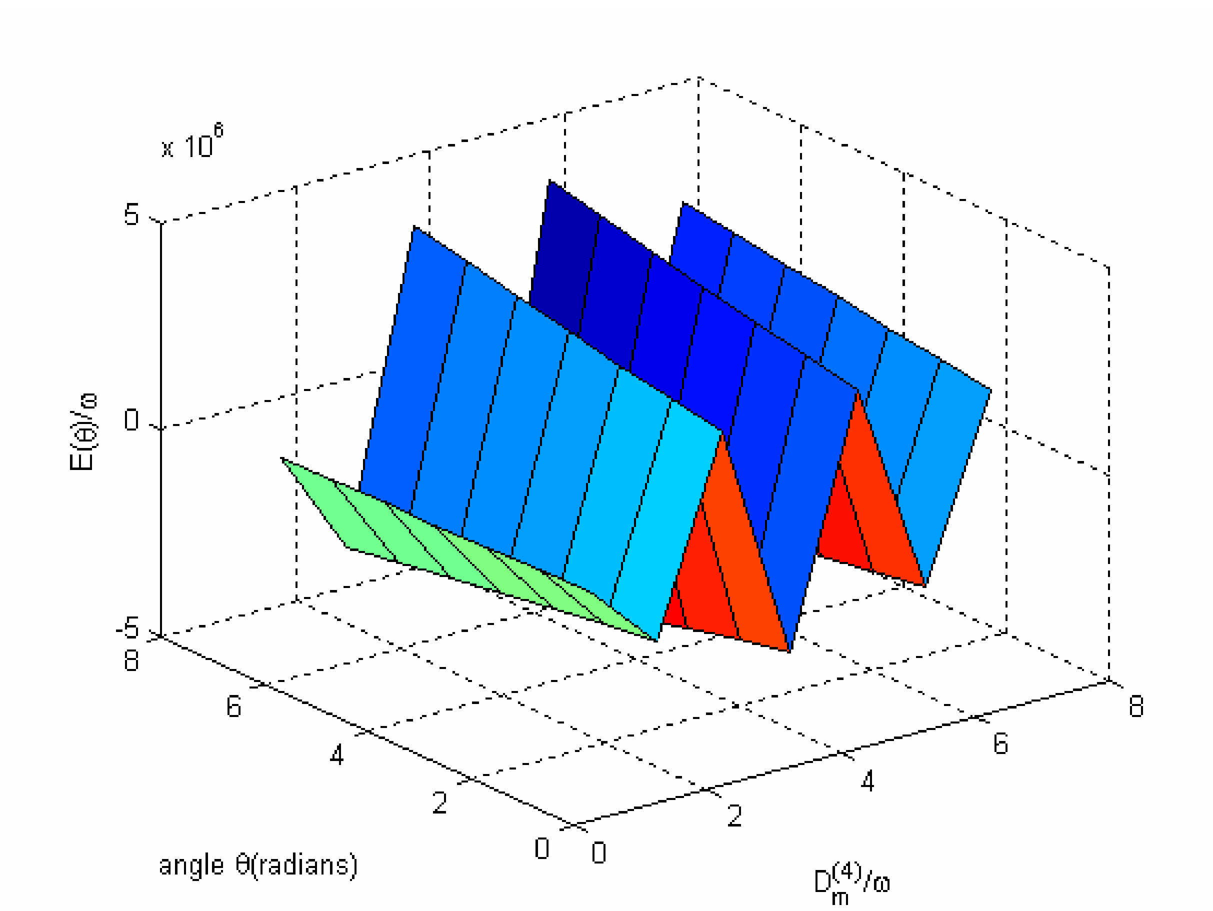


Figure 1. 3-D plot of energy versus $\frac{D_m^{(4)}}{\omega}$ and angle, for sc(001) lattice with four layers

is a minimum at certain values of angles and fourth order anisotropy. The graph between angle and energy was drawn in order to determine easy direction corresponding to $\frac{D_m^{(4)}}{\omega}$ =5.3, as shown in figure 2. Energy is a minimum at 0.6 and 2.73 radians.

ISSN 1512-1461

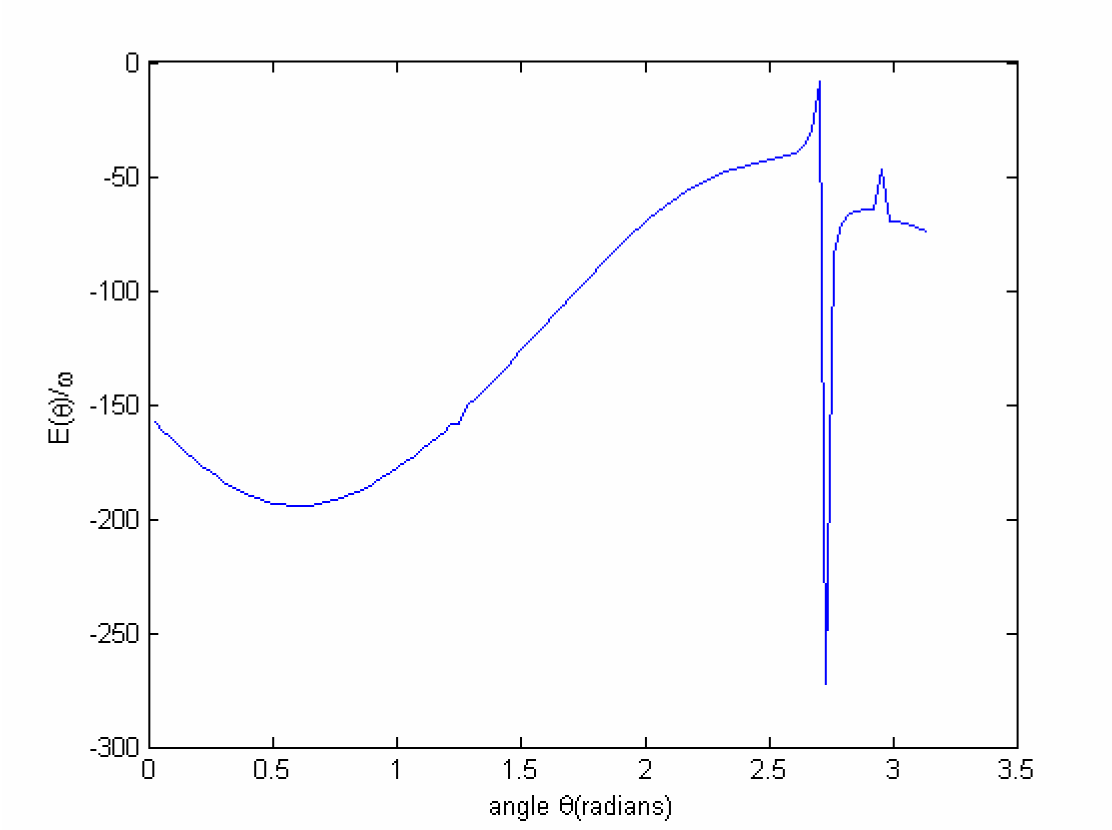


Figure 2. Energy versus angle at $\frac{D_m^{(4)}}{\omega}$ =5.3

When $\frac{J}{\omega} = \frac{H_{in}}{\omega} = \frac{H_{out}}{\omega} = \frac{N_d \mu_0 \mu^2}{V\omega} = \frac{K_S}{\omega} = 10$ and $\frac{D_m^{(4)}}{\omega}$ =5

$$\frac{C_{11}}{\omega} = \frac{C_{44}}{\omega} = -9.92 + 0.2456\cos 2\theta + 2\frac{D_m^{(2)}}{\omega}\cos 2\theta + 20\cos^2\theta(\cos^2\theta - 3\sin^2\theta) + 10\sin\theta + 10\cos\theta + 40\sin 2\theta$$

$$\frac{C_{22}}{\omega} = \frac{C_{33}}{\omega} = 0.164 + 0.49\cos 2\theta + 2\frac{D_m^{(2)}}{\omega}\cos 2\theta + 20\cos^2\theta(\cos^2\theta - 3\sin^2\theta) + 10\sin\theta + 10\cos\theta + 40\sin 2\theta$$

$$\frac{\alpha_1}{\omega} = \frac{\alpha_4}{\omega} = (-6.53 + \frac{D_m^{(2)}}{\omega} + 10\cos^2\theta)\sin 2\theta$$

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

ISSN 1512-1461

$\frac{E_0}{\omega} = -65.73 + 12.81\cos 2\theta - 4(\frac{D_m^{(2)}}{\omega}\cos^2\theta + 5\cos^4\theta + 10\cos\theta + 10\sin\theta + 10\sin 2\theta)$ 3-D plot of energy versus angle and $\frac{D_m^{(2)}}{\omega}$ is given in figure 3. At $\frac{D_m^{(2)}}{\omega}$ =3.8, energy minimum can be observed. The angles of easy directions corresponding to this energy minimum can be found from figure 4. The energy is a minimum at 0.72 radians.

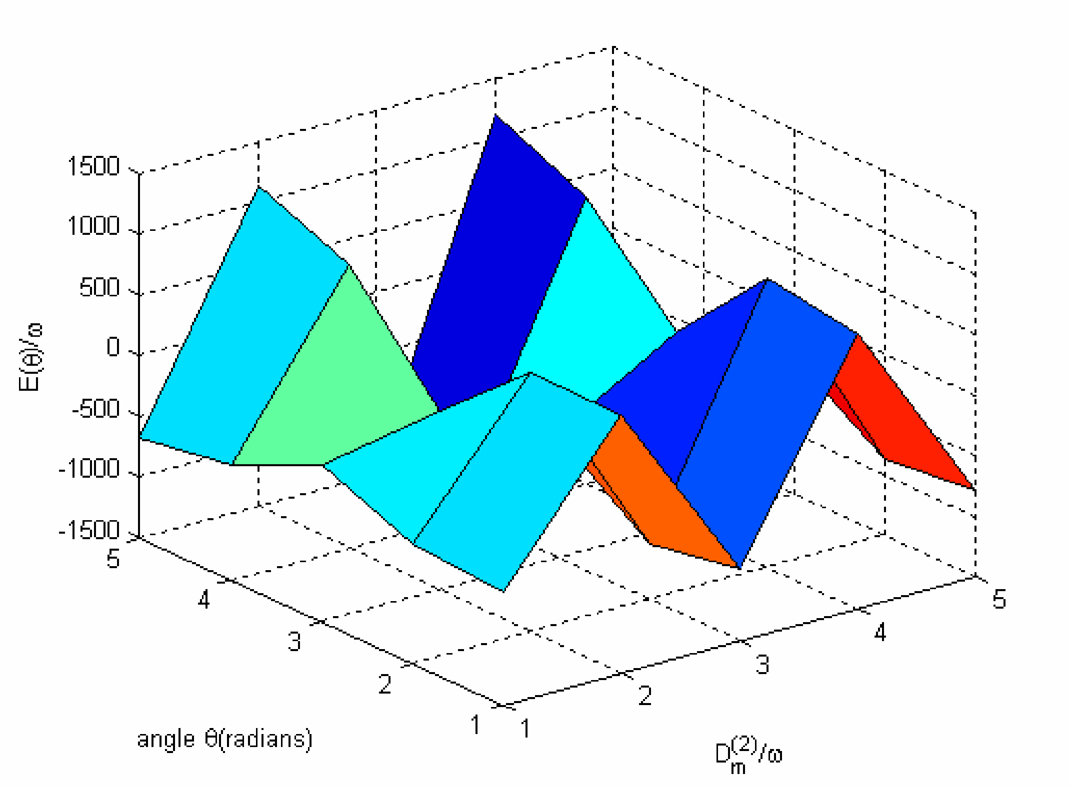


Figure 3. 3-D plot of energy versus angle and $\frac{D_m^{(2)}}{\omega}$, for sc(001) lattice with four layers

ISSN 1512-1461

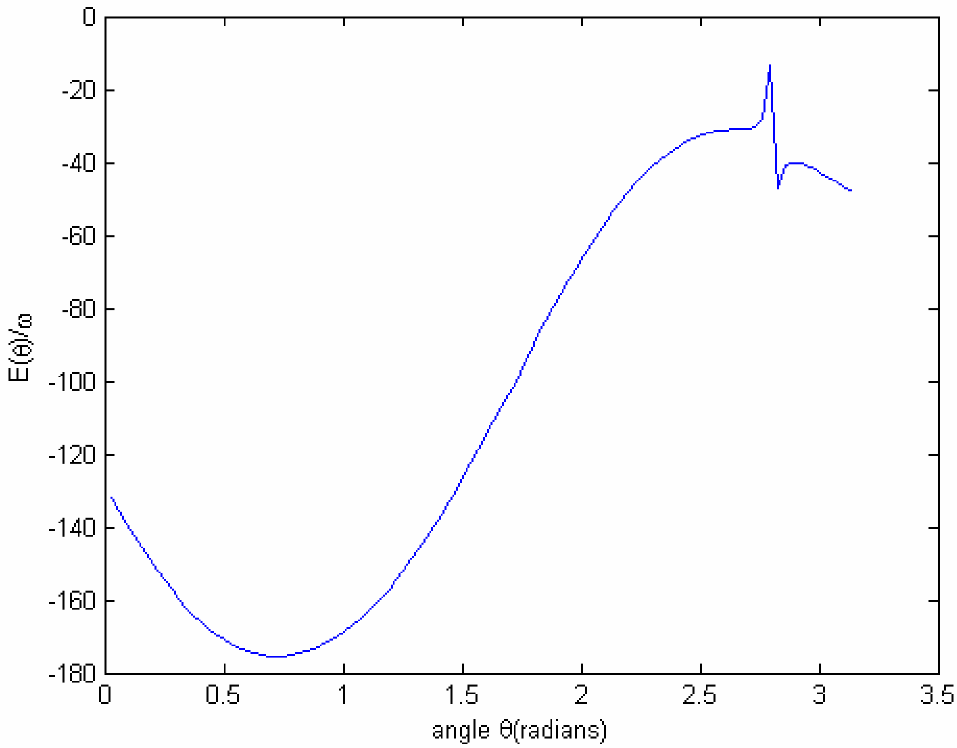


Figure 4. Graph between energy and angle at $\frac{D_m^{(2)}}{\omega}$ =3.8

**3. Conclusion:**

3-D plots indicate that the sc(001) ferromagnetic films with four layers can be easily oriented in certain directions for certain values of second and fourth order anisotropy constants. Because the anisotropy constants mostly depend on the magnetic material, these angles corresponding to energy minimums provide the easy direction of magnetization only for the parameters given in this report. If the fourth order anisotropy is given by $\frac{D_m^{(4)}}{\omega}$ =5.3, then energy is minimum at 0.6 and 2.73 radians. Under the influence of second order anisotropy $\frac{D_m^{(2)}}{\omega}$ =3.8, the film can be easily oriented along direction of 0.72 radians. Because it is difficult to find experimental values of $\frac{J}{\omega}, \frac{H_{in}}{\omega}, \frac{H_{out}}{\omega}, \frac{N_d \mu_0 \mu^2}{V\omega}, \frac{K_s}{\omega}$, $\frac{D_m^{(2)}}{\omega}$ and $\frac{D_m^{(4)}}{\omega}$, this simulation was carried out for some reasonable values of $\frac{J}{\omega}, \frac{H_{in}}{\omega}, \frac{H_{out}}{\omega}, \frac{N_d \mu_0 \mu^2}{V\omega}, \frac{K_s}{\omega}$, $\frac{D_m^{(2)}}{\omega}$ and $\frac{D_m^{(4)}}{\omega}$.

ISSN 1512-1461

**References:**

1. K.D. Usadel and A. Hucht, Phys. Rev. B (2002), **66**, 024419-1.
2. David Lederman, Ricardo Ramirez and Miguel Kiwi, Phys. Rev. B (2004), **70**, 18442.
3. Martin J. Klein and Robert S. Smith, Phys. Rev. (1951), **81**, 378.
4. M. Dantziger, B. Glinsmann, S. Scheffler, B. Zimmermann and P.J. Jensen, Phys. Rev. B (2002), **66**, 094416.
5. M. Bentaleb, N. El Aouad and M. Saber, Chinese J. Phys. (2002), **40(3)**, 307.
6. P. Samarasekara, Elec. J. Theo. Phys. (2006), **3(11)**, 71.
7. P. Samarasekara, Chinese J. Phys. (2006), **44(5)**, 377.
8. S. Chikazumi, Physics of Magnetism (John Wiley and Sons, New York, 1964)
9. M. Gomi, T. Tanida and M. Abe, J. Appl. Phys. (1985), **57 (1)**, 3888.
10. P.J.M. Vander Starten, V.V. Banderanko and R. Metselaar, J. Cryst. Growth (1981), **51**, 119.
11. P.J. Besser, J.E. Mee, P.E. Elkins and D.M. Hienz, Mater. Res. Bull. (1971), **6**, 1

**Article received: 2011-07-06**