

# Second Order Perturbation of Heisenberg Hamiltonian for Non-Oriented Ultra-Thin Ferromagnetic Films

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**Abstract:** The second order perturbation of magnetic energy for ferromagnetic thin films of two and three layers has been studied using classical Heisenberg Hamiltonian. According to our model, the film with two layers is equivalent to an oriented film, when anisotropy constants do not vary inside the film. But the energy of films with three layers indicates periodic variation. Introducing second order perturbation induces some sudden overshooting of energy curves, compared with smooth energy curves obtained for oriented ferromagnetic ultra thin films in one of our previous report. After taking the fourth order anisotropy into account, the overshooting part dominates by reducing the smooth part of energy graphs. Several minimums can be observed in last 3-D graph implying that the film with  $N=3$  can be oriented in some preferred directions by applying a certain value of stress. The shape of graphs of energy variation of all sc(001), fcc(001) and bcc(001) ferromagnetic ultra thin films with second (or fourth) order anisotropy is exactly same. Easy and hard directions of these all types with the effect of second order anisotropy only are  $34.4^\circ$  and  $124.4^\circ$ , respectively. The angle between easy and hard directions is exactly  $90^\circ$  as expected. Although these simulations were given for  $\frac{J}{\omega} = 10$ ,  $\frac{D_m^{(2)}}{\omega} = 10$ ,  $\frac{K_s}{\omega} = 10$  and  $\frac{D_m^{(4)}}{\omega} = 5$  values only, this same approach can be carried out for any values of  $\frac{J}{\omega}$ ,  $\frac{D_m^{(2)}}{\omega}$ ,  $\frac{K_s}{\omega}$  and  $\frac{D_m^{(4)}}{\omega}$  or any type of ferromagnetic material. Considering the other terms such as dipole interaction and demagnetization factor really complicates the simulation.

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## 1. Introduction:

The research of exchange anisotropy has received a wide attention in last decade, due to the difficulties of physical understanding of exchange anisotropy and to its application in magnetic media technology and magnetic sensors [4] . The magnetic properties of ferromagnetic thin films and multi layers have been extensively investigated because of their

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potential impact on magnetic recording devices. The magnetic properties of thin films of ferromagnetic materials have been investigated using the Bloch spin-wave theory earlier [5]. The magnetization of some thin films shows an in plane orientation due to the dipole interaction. Due to the broken symmetry uniaxial anisotropy energies at the surfaces of the film, the perpendicular magnetization is preferential. But due to the strain induced distortion in the inner layers, bulk anisotropy energies will appear absent or very small in the ideal crystal. Very thin films indicate a tetragonal distortion resulting in stress-induced uniaxial anisotropy energy in the inner layers with perpendicular orientation of easy axis. The magnetic in-plane anisotropy of a square two-dimensional (2D) Heisenberg ferromagnet in the presence of magnetic dipole interaction has been determined earlier [6]. The long range character of the dipole interaction itself is sufficient to stabilize the magnetization in 2-D magnet. Also the easy and hard axes of the magnetization with respect to lattice frame are determined by the anisotropies. Magnetic properties of the Ising ferromagnetic thin films with alternating superlattice layers were investigated [7]. In addition to these, Monte Carlo simulations of hysteresis loops of ferromagnetic thin films have been theoretically traced [8]. Since the surfaces slightly distort the symmetry of the system under consideration, physical quantities in the vicinity of surfaces generally deviate from those in the bulk.

The second order perturbation solution of Heisenberg Hamiltonian for ultra-thin ferromagnetic films has been found without considering the effect of stress induced anisotropy and demagnetization factor in some early reports [1]. The stress of a film arises mainly due to the difference between thermal expansion coefficients of the film and the substrate. When the film is cooled down or heated after annealing or deposition, the stress takes place in the film. The effect of stress on the coercivity and anisotropy of sputtered ferromagnetic thin films has been previously studied by us [2,3]. The contribution of stress to the magnetic energy is given by  $K_s \sin 2\theta$ . Here  $K_s$  depends on the magnetization and the magnitude of stress, and  $\theta$  is the angle between the stress and the magnetization. The theoretical values of demagnetization factor within the film plane and normal to the film plane are 0 and 1 in SI units, respectively.

## 2. The Model

The Heisenberg Hamiltonian of ferromagnetic films can be formulated as following.

$$H = -\frac{J}{2} \sum_{m,n} \vec{S}_m \cdot \vec{S}_n + \frac{\omega}{2} \sum_{m \neq n} \left( \frac{\vec{S}_m \cdot \vec{S}_n}{r_{mn}^3} - \frac{3(\vec{S}_m \cdot \vec{r}_{mn})(\vec{r}_{mn} \cdot \vec{S}_n)}{r_{mn}^5} \right) - \sum_m D_{\lambda_m}^{(2)} (S_m^z)^2 - \sum_m D_{\lambda_m}^{(4)} (S_m^z)^4 - \sum_{m,n} [\vec{H} - (N_d \vec{S}_n / \mu_0)] \cdot \vec{S}_m - \sum_m K_s \sin 2\theta_m$$

Here  $\vec{S}_m$  and  $\vec{S}_n$  are two spins. Above equation can be simplified into following form [1].

$$\begin{aligned}
E(\theta) = & -\frac{1}{2} \sum_{m,n=1}^N [(JZ_{|m-n|} - \frac{\omega}{4}\Phi_{|m-n|}) \cos(\theta_m - \theta_n) - \frac{3\omega}{4}\Phi_{|m-n|} \cos(\theta_m + \theta_n)] \\
& - \sum_{m=1}^N (D_m^{(2)} \cos^2 \theta_m + D_m^{(4)} \cos^4 \theta_m + H_{in} \sin \theta_m + H_{out} \cos \theta_m) \\
& + \sum_{m,n=1}^N \frac{N_d}{\mu_0} \cos(\theta_m - \theta_n) - K_s \sum_{m=1}^N \sin 2\theta_m
\end{aligned} \tag{1}$$

Here  $J$ ,  $Z_{|m-n|}$ ,  $\omega$ ,  $\Phi_{|m-n|}$ ,  $\theta$ ,  $D_m^{(2)}$ ,  $D_m^{(4)}$ ,  $H_{in}$ ,  $H_{out}$ ,  $N_d$ ,  $K_s$ ,  $m$ ,  $n$  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  $\theta_m$ .

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 number 1, the cosine and sine terms can be expanded up to the second order of  $\varepsilon_m$  and  $\varepsilon_n$  as following.

$$E(\theta) = E_0 + E(\varepsilon) + E(\varepsilon^2) + \dots$$

If the third and higher order perturbations are neglected, then

$$E(\theta) = E_0 + E(\varepsilon) + E(\varepsilon^2) \tag{2}$$

Here

$$\begin{aligned}
E_0 = & -\frac{1}{2} \sum_{m,n=1}^N (JZ_{|m-n|} - \frac{\omega}{4}\Phi_{|m-n|}) + \frac{3\omega}{8} \cos 2\theta \sum_{m,n=1}^N \Phi_{|m-n|} \\
& - \cos^2 \theta \sum_{m=1}^N D_m^{(2)} - \cos^4 \theta \sum_{m=1}^N D_m^{(4)} - N(H_{in} \sin \theta + H_{out} \cos \theta - \frac{N_d}{\mu_0} + K_s \sin 2\theta) \\
E(\varepsilon) = & -\frac{3\omega}{8} \sin 2\theta \sum_{m,n=1}^N \Phi_{|m-n|} (\varepsilon_m + \varepsilon_n) + \sin 2\theta \sum_{m=1}^N D_m^{(2)} \varepsilon_m + 2 \cos^2 \theta \sin 2\theta \sum_{m=1}^N D_m^{(4)} \varepsilon_m \\
& - H_{in} \cos \theta \sum_{m=1}^N \varepsilon_m + H_{out} \sin \theta \sum_{m=1}^N \varepsilon_m - 2K_s \cos 2\theta \sum_{m=1}^N \varepsilon_m \\
E(\varepsilon^2) = & \frac{1}{4} \sum_{m,n=1}^N (JZ_{|m-n|} - \frac{\omega}{4}\Phi_{|m-n|}) (\varepsilon_m - \varepsilon_n)^2 - \frac{3\omega}{16} \cos 2\theta \sum_{m,n=1}^N \Phi_{|m-n|} (\varepsilon_m + \varepsilon_n)^2 \\
& - (\sin^2 \theta - \cos^2 \theta) \sum_{m=1}^N D_m^{(2)} \varepsilon_m^2 + 2 \cos^2 \theta (\cos^2 \theta - 3 \sin^2 \theta) \sum_{m=1}^N D_m^{(4)} \varepsilon_m^2 \\
& + \frac{H_{in}}{2} \sin \theta \sum_{m=1}^N \varepsilon_m^2 + \frac{H_{out}}{2} \cos \theta \sum_{m=1}^N \varepsilon_m^2 - \frac{N_d}{2\mu_0} \sum_{m,n=1}^N (\varepsilon_m - \varepsilon_n)^2 + 2K_s \sin 2\theta \sum_{m=1}^N \varepsilon_m^2
\end{aligned} \tag{3}$$

After using the constraint  $\sum_{m=1}^N \varepsilon_m = 0$ ,  $E(\varepsilon) = \vec{\alpha} \cdot \vec{\varepsilon}$

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

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

Also  $E(\varepsilon^2) = \frac{1}{2} \vec{\varepsilon} \cdot C \cdot \vec{\varepsilon}$

Here the elements of matrix C can be given as following,

$$\begin{aligned} C_{mn} = & -(JZ_{|m-n|} - \frac{\omega}{4} \Phi_{|m-n|}) - \frac{3\omega}{4} \cos 2\theta \Phi_{|m-n|} + \frac{2N_d}{\mu_0} \\ & + \delta_{mn} \left\{ \sum_{\lambda=1}^N [JZ_{|m-\lambda|} - \Phi_{|m-\lambda|} (\frac{\omega}{4} + \frac{3\omega}{4} \cos 2\theta)] - 2(\sin^2 \theta - \cos^2 \theta) D_m^{(2)} \right. \\ & \left. + 4 \cos^2 \theta (\cos^2 \theta - 3 \sin^2 \theta) D_m^{(4)} + H_{in} \sin \theta + H_{out} \cos \theta - \frac{4N_d}{\mu_0} + 4K_s \sin 2\theta \right\} \quad (5) \end{aligned}$$

Therefore, the total magnetic energy given in equation 2 can be deduced to [1]

$$E(\theta) = E_0 + \vec{\alpha} \cdot \vec{\varepsilon} + \frac{1}{2} \vec{\varepsilon} \cdot C \cdot \vec{\varepsilon} = E_0 - \frac{1}{2} \vec{\alpha} \cdot C^+ \cdot \vec{\alpha} \quad (6)$$

Here  $C^+$  is the pseudo-inverse given by

$$C \cdot C^+ = 1 - \frac{E}{N} \quad (7)$$

Here E is the matrix with all elements  $E_{mn}=1$ .

### 3. Results and Discussion:

First the energy will be found for a film with two layers (N=2). Since it is reasonable to assume that the anisotropy energies remain constant within an ultra-thin film with two layers,  $D_1^{(2)}=D_2^{(2)}$  and  $D_1^{(4)}=D_2^{(4)}$ .

From equation 5,  $C_{11}=C_{22}$  and  $C_{12}=C_{21}$ .

Therefore from equation 7,  $C_{12}^+ = C_{21}^+ = \frac{1}{2(C_{21}-C_{22})} = -C_{11}^+ = -C_{22}^+$

Using above results,  $\vec{\alpha} \cdot C^+ \cdot \vec{\alpha} = (\alpha_1 - \alpha_2)^2 C_{11}^+$

But from equation 4, for a film with two layers  $\alpha_1 = \alpha_2$

Therefore  $\vec{\alpha} \cdot C^+ \cdot \vec{\alpha} = 0$ , and the total energy in equation 6 is  $E_0$ . This means that the energy of a film with two layers is reduced to the energy of the oriented film.

Now if the anisotropy constants change within the film, then  $C_{12}=C_{21}$  and  $C_{22} \neq C_{11}$ .

Therefore,  $C_{11}^+ = -C_{12}^+ = \frac{C_{22}+C_{21}}{2(C_{11}C_{22}-C_{21}^2)}$  and  $C_{21}^+ = -C_{22}^+ = \frac{C_{21}+C_{11}}{2(C_{21}^2-C_{11}C_{22})}$ .

Hence,  $\vec{\alpha} \cdot C^+ \cdot \vec{\alpha} = (\alpha_1 - \alpha_2)(C_{21}^+ \alpha_2 - C_{12}^+ \alpha_1)$

Now the total energy is different from that of an oriented film. The matrix elements of  $C^+$ , which were found using equation 7 for a film with three layers (N=3), contained about 20 terms of  $C_{mn}$  elements.

The  $C_{31}^+$  has been given as an example below.

$$C_{31}^+ = \frac{A}{D}$$

$$\text{Here } A = -[(C_{22}C_{11} - C_{12}C_{21}) - 0.67(C_{11} - C_{21})(C_{12} - C_{22})]C_{31} - 0.67C_{32}(C_{11} - C_{21})^2 - 0.33(C_{22}C_{11} - C_{12}C_{21})(C_{11} - C_{21})$$

$$D = C_{31}[(C_{11}C_{23} - C_{13}C_{21})(C_{12} - C_{22}) - (C_{13} - C_{23})(C_{22}C_{11} - C_{12}C_{21})] - (C_{11}C_{23} - C_{13}C_{21})(C_{11} - C_{21})C_{32} + (C_{22}C_{11} - C_{12}C_{21})(C_{11} - C_{21})C_{33}$$

Therefore, the final result became really complicated. To avoid this problem, the matrix elements were found for special case,  $C \cdot C^+ = 1$ .

Under this condition, energy is given by equation 6 only if  $\vec{E} \cdot \vec{\alpha} = 0$ .

Therefore,  $\alpha_1 + \alpha_2 + \alpha_3 = 0$ . This implies that the average value of first perturbation ( $\frac{\alpha_1 + \alpha_2 + \alpha_3}{3}$ ) is zero under this condition. Now the  $C^+$  is the standard inverse of a matrix, given by matrix element  $C_{mn}^+ = \frac{\text{cofactor } C_{nm}}{\det C}$ . Also the matrix elements  $C_{mn}$  can be given as following according to equation 5.

$$\begin{aligned} C_{12} = C_{21} = C_{23} = C_{32} &= -JZ_1 + \frac{\omega}{4}\Phi_1(1 - 3\cos 2\theta) + \frac{2N_d}{\mu_0} \\ C_{13} = C_{31} &= -JZ_2 + \frac{\omega}{4}\Phi_2(1 - 3\cos 2\theta) + \frac{2N_d}{\mu_0} \\ C_{11} = C_{33} &= J(Z_1 + Z_2) - \frac{\omega}{4}(\Phi_1 + \Phi_2)(1 + 3\cos 2\theta) - \frac{2N_d}{\mu_0} + (2\cos 2\theta)D_m^{(2)} \\ &\quad + 4\cos^2\theta(\cos^2\theta - 3\sin^2\theta)D_m^{(4)} + H_{in}\sin\theta + H_{out}\cos\theta + 4K_s\sin 2\theta \\ C_{22} &= 2JZ_1 - \frac{\omega}{2}\Phi_1(1 + 3\cos 2\theta) - \frac{2N_d}{\mu_0} + (2\cos 2\theta)D_m^{(2)} \\ &\quad + 4\cos^2\theta(\cos^2\theta - 3\sin^2\theta)D_m^{(4)} + H_{in}\sin\theta + H_{out}\cos\theta + 4K_s\sin 2\theta \end{aligned} \quad (8)$$

Because it is reasonable to assume that second or fourth order anisotropy constants do not change inside an ultra thin film,  $D_1^{(2)} = D_2^{(2)} = D_3^{(2)}$  and  $D_1^{(4)} = D_2^{(4)} = D_3^{(4)}$ . Therefore for the convenience the matrix elements  $C_{mn}^+$  will be given in terms of  $C_{11}$ ,  $C_{22}$ ,  $C_{32}$ , and  $C_{31}$  only.

$$\begin{aligned} C_{11}^+ &= \frac{C_{11}C_{22} - C_{32}^2}{C_{11}(C_{11}C_{22} - C_{31}^2) + 2C_{32}^2(C_{31} - C_{11})} = C_{33}^+ \\ C_{12}^+ &= \frac{C_{32}C_{31} - C_{32}C_{11}}{C_{11}(C_{11}C_{22} - C_{31}^2) + 2C_{32}^2(C_{31} - C_{11})} = C_{21}^+ = C_{23}^+ = C_{32}^+ \\ C_{13}^+ &= \frac{C_{32}^2 - C_{22}C_{31}}{C_{11}(C_{11}C_{22} - C_{31}^2) + 2C_{32}^2(C_{31} - C_{11})} = C_{31}^+ \\ C_{22}^+ &= \frac{C_{11}^2 - C_{31}^2}{C_{11}(C_{11}C_{22} - C_{31}^2) + 2C_{32}^2(C_{31} - C_{11})} \end{aligned} \quad (9)$$

Both matrices  $C$  and  $C^+$  are highly symmetric about both matrix diagonals. From equation 6,

$$E(\theta) = E_0 - 0.5[C_{11}^+(\alpha_1^2 + \alpha_3^2) + C_{32}^+(2\alpha_1\alpha_2 + 2\alpha_2\alpha_3) + C_{31}^+(2\alpha_1\alpha_3) + \alpha_2^2 C_{22}^+] \quad (10)$$

Because  $C_{mn}$  terms contain sometimes about nine different terms for  $N=3$ , the product of two  $C_{mn}$  terms and hence  $C_{mn}^+$  terms will contain about 80 terms. For an example, the term  $C_{11}$  contains nine different terms, and therefore  $C_{22}^+$  will contain about 81 terms. To simplify the problem, only the magnetic exchange interaction, second order anisotropy and stress induced anisotropy terms have been considered for this simulation. For sc(001) lattice,  $Z_0=4$ ,  $Z_1=1$ ,  $Z_2=0$  [1], and from above equations number 4 and 8,

$$\alpha = \alpha_1 = \alpha_2 = \alpha_3 = D_m^{(2)} \sin 2\theta, \quad C_{12} = C_{21} = C_{23} = C_{32} = -J, \quad C_{13} = C_{31} = 0$$

$$C_{11} = C_{33} = J + (2 \cos 2\theta) D_m^{(2)} + 4K_s \sin 2\theta \quad \text{and} \quad C_{22} = 2J + (2 \cos 2\theta) D_m^{(2)} + 4K_s \sin 2\theta$$

But from equation 10,

$$E(\theta) = E_0 - 0.5\alpha^2 \frac{C_{11}(2C_{22} - 4C_{32} + C_{11}) + C_{31}(4C_{32} - 2C_{22} - C_{31})}{C_{11}(C_{11}C_{22} - C_{31}^2) + 2C_{32}^2(C_{31} - C_{11})}$$

$$E(\theta) = E_0 - \frac{1.5[D_m^{(2)}]^2 \sin^2 2\theta}{(2 \cos 2\theta) D_m^{(2)} + 4K_s \sin 2\theta}$$

From equation number 3,  $E_0 = -8J - 3[D_m^{(2)} \cos^2 \theta + K_s \sin 2\theta]$

$$\text{Therefore, } E(\theta) = -8J - 3[D_m^{(2)} \cos^2 \theta + K_s \sin 2\theta] - \frac{1.5[D_m^{(2)}]^2 \sin^2 2\theta}{(2 \cos 2\theta) D_m^{(2)} + 4K_s \sin 2\theta}$$

If  $\frac{J}{\omega} = 10$ ,  $\frac{D_m^{(2)}}{\omega} = 10$ ,  $\frac{K_s}{\omega} = 10$ , then

$$\frac{E(\theta)}{\omega} = -80 - 30[\cos^2 \theta + \sin 2\theta] - \frac{7.5 \sin^2 2\theta}{\cos 2\theta + 2 \sin 2\theta}$$

The graph between  $\frac{E(\theta)}{\omega}$  and  $\theta$  is given in figure 1. If  $K_s$  is also a variable, then

$$\frac{E(\theta)}{\omega} = -80 - 3[10 \cos^2 \theta + \frac{K_s}{\omega} \sin 2\theta] - \frac{150 \sin^2 2\theta}{20 \cos 2\theta + 4 \frac{K_s}{\omega} \sin 2\theta}$$

The 3-D plot of  $\frac{E(\theta)}{\omega}$  versus  $\frac{K_s}{\omega}$  and  $\theta$  is given in figure 2.

When the energy is minimum,  $\frac{\partial E}{\partial \theta} = 0$ .

After taking the derivative of above equation, at minimum energy the  $\frac{K_s}{\omega}$  satisfies following cubic equation.

$$2\left(\frac{K_s}{\omega}\right)^3 \cos 2\theta + 10\left(\frac{K_s}{\omega}\right)^2 [\cos^2 2\theta - \sin 2\theta] + 25\left(\frac{K_s}{\omega}\right) \cot 2\theta [2 \cos 2\theta - \sin^2 2\theta] + 125[-2 \cos 2\theta + 2 \cos^2 2\theta - \sin^2 2\theta] = 0$$

Using above equation, the preferential direction of orientation for different values of stress can be calculated.

For bcc(001) lattice  $Z_0=0$ ,  $Z_1=4$  and  $Z_2=0$  [1], and hence  $C_{12} = C_{21} = C_{23} = C_{32} = -4J$ ,  $C_{13} = C_{31} = 0$ ,

$$C_{11} = C_{33} = 4J + (2 \cos 2\theta) D_m^{(2)} + 4K_s \sin 2\theta, \quad C_{22} = 8J + (2 \cos 2\theta) D_m^{(2)} + 4K_s \sin 2\theta.$$

$E_0$  of this lattice is exactly same as that of sc(001). Finally, we can show that energy  $E(\theta)$  of bcc(001) lattice is exactly same as that of sc(001) lattice. Using  $Z_0=4$ ,  $Z_1=4$  and  $Z_2=0$  for fcc(001) lattice [1]

$$C_{12} = C_{21} = C_{23} = C_{32} = -4J, \quad C_{13} = C_{31} = 0,$$

$$C_{11} = C_{33} = 4J + (2 \cos 2\theta) D_m^{(2)} + 4K_s \sin 2\theta,$$

$$C_{22} = 8J + (2 \cos 2\theta) D_m^{(2)} + 4K_s \sin 2\theta.$$

But  $E_0 = -14J - 3[D_m^{(2)} \cos^2 \theta + K_s \sin 2\theta]$

Therefore,  $E(\theta) = -14J - 3[D_m^{(2)} \cos^2 \theta + K_s \sin 2\theta] - \frac{1.5[D_m^{(2)}]^2 \sin^2 2\theta}{(2 \cos 2\theta)D_m^{(2)} + 4K_s \sin 2\theta}$

Using  $\frac{J}{\omega} = 10$ ,  $\frac{D_m^{(2)}}{\omega} = 10$ ,  $\frac{K_s}{\omega} = 10$  for this simulation,

$$\frac{E(\theta)}{\omega} = -140 - 30[\cos^2 \theta + \sin 2\theta] - \frac{7.5 \sin^2 2\theta}{\cos 2\theta + 2 \sin 2\theta}$$

The graph between  $\frac{E(\theta)}{\omega}$  and  $\theta$  in this case is similar to the graph given in figure 1.

According to graph, the easy and hard directions of this film are  $34.4^\circ$  and  $124.4^\circ$ , respectively. These angles are higher than those of oriented ferromagnetic thin films investigated in one of our early report. Therefore, introducing second order perturbation has increased the angles corresponding to easy and hard directions. Also these angles of easy and hard directions are valid for all three type of ferromagnetic materials described in this report. The separation between any two consecutive minimums or maximums is  $180^\circ$ , similar to regular sine or cosine curve.

When  $K_s$  is also a variable,

$$\frac{E(\theta)}{\omega} = -140 - 3[10 \cos^2 \theta + \frac{K_s}{\omega} \sin 2\theta] - \frac{150 \sin^2 2\theta}{20 \cos 2\theta + 4 \frac{K_s}{\omega} \sin 2\theta}$$

The 3-D plot of  $\frac{E(\theta)}{\omega}$  versus  $\frac{K_s}{\omega}$  and  $\theta$  in this case is similar to the graph given in figure 2. This graph indicates a slow variation of energy with the variation of the stress or the angle. The graph corresponding to the minimum energy of bcc(001) and fcc(001) are exactly same as that of sc(001). Taking dipole interaction into account will give an energy equation with at least fifty terms, and therefore the effect of dipole interaction will not be discussed in this report.

After taking fourth order anisotropy term into account for sc(001)

$$C_{12} = C_{21} = C_{23} = C_{32} = -J, \quad C_{13} = C_{31} = 0,$$

$$C_{11} = C_{33} = J + (2 \cos 2\theta)D_m^{(2)} + 4 \cos^2 \theta (\cos^2 \theta - 3 \sin^2 \theta)D_m^{(4)} + 4K_s \sin 2\theta$$

$$C_{22} = 2J + (2 \cos 2\theta)D_m^{(2)} + 4 \cos^2 \theta (\cos^2 \theta - 3 \sin^2 \theta)D_m^{(4)} + 4K_s \sin 2\theta$$

$E(\theta) = -8J - 3[D_m^{(2)} \cos^2 \theta + D_m^{(4)} \cos^4 \theta + K_s \sin 2\theta]$

$$- \frac{1.5[D_m^{(2)} + 2D_m^{(4)} \cos^2 \theta]^2 \sin^2 2\theta}{(2 \cos 2\theta)D_m^{(2)} + 4 \cos^2 \theta (\cos^2 \theta - 3 \sin^2 \theta)D_m^{(4)} + 4K_s \sin 2\theta}$$

If  $\frac{D_m^{(4)}}{\omega} = 5$ , then

$$\frac{E(\theta)}{\omega} = -80 - 15[2 \cos^2 \theta + \cos^4 \theta + 2 \sin 2\theta] - \frac{7.5[1 + \cos^2 \theta]^2 \sin^2 2\theta}{\cos 2\theta + \cos^2 \theta (\cos^2 \theta - 3 \sin^2 \theta) + 2 \sin 2\theta}$$

The graph between  $\frac{E(\theta)}{\omega}$  and  $\theta$  is given in figure 3. According to figure 1 and 3, introducing the fourth anisotropy has destroyed the smoothness of the curve. Sudden periodical overshooting can be observed in the graph. The separation between any adjacent minimum and maximum is very small. The first and second minimums of overshooting can be observed at  $74^\circ$  and  $160.5^\circ$ . The curved parts with smooth maximums and minimums in figure 1 have been flattened in figure 3.

If  $K_s$  is a variable,

$$\frac{E(\theta)}{\omega} = -80 - 3[10\cos^2\theta + 5\cos^4\theta + \frac{K_s}{\omega}\sin 2\theta] - \frac{150[1 + \cos^2\theta]^2 \sin^2 2\theta}{20 \cos 2\theta + 20 \cos^2\theta(\cos^2\theta - 3\sin^2\theta) + 4\frac{K_s}{\omega}\sin 2\theta}$$

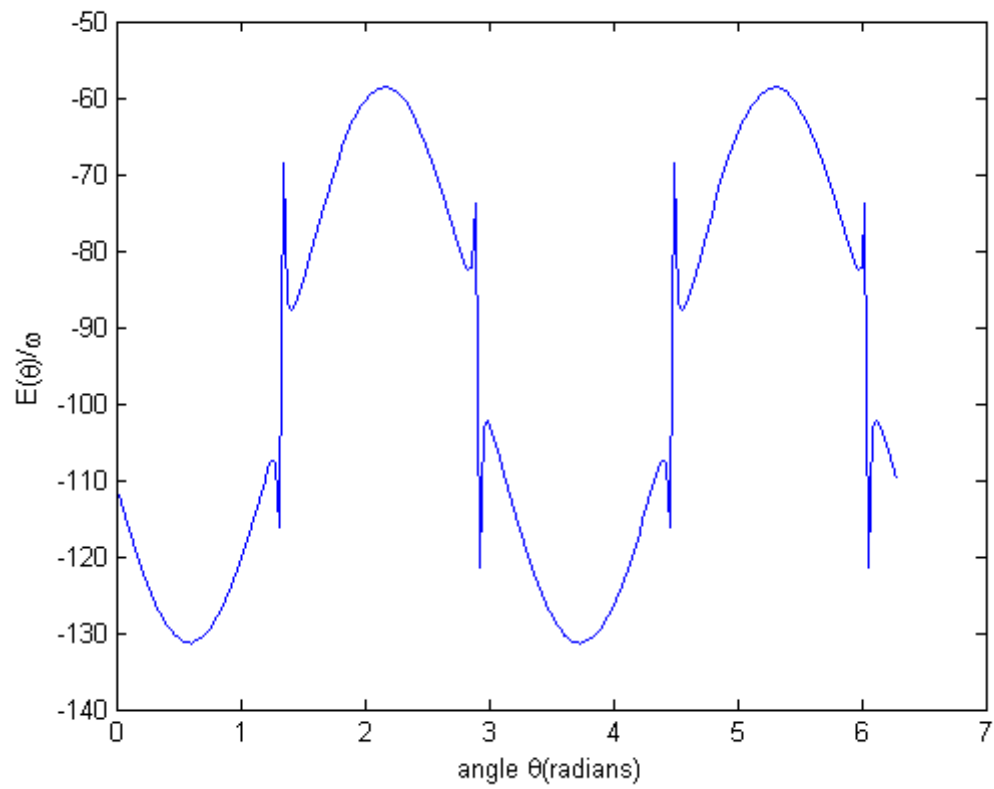
The 3-D plot of  $\frac{E(\theta)}{\omega}$  versus  $\frac{K_s}{\omega}$  and  $\theta$  is given in figure 4. According to this graph, the energy varies rapidly with angle and stress after taking the effect of fourth order anisotropy into account. Several minimums of energies can be observed at different angles and stresses. The stresses corresponding to the different directions of preferred orientation can be determined from this graph.

#### 4. Conclusion:

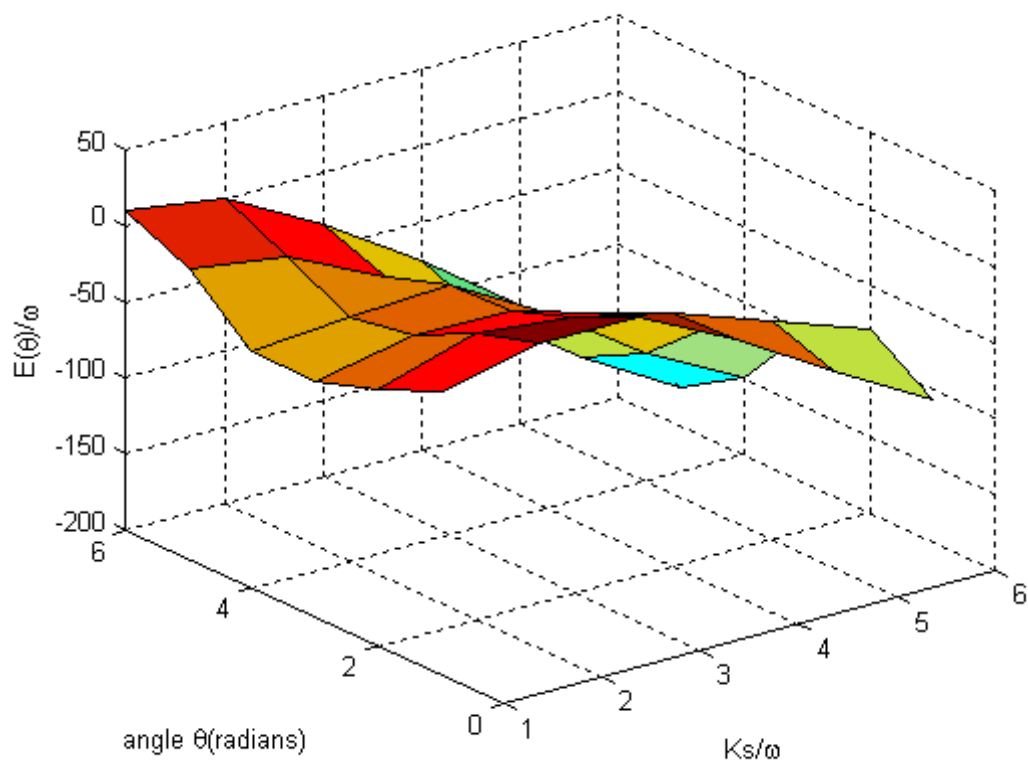
Although the ultra-thin ferromagnetic film with two layers behaves as an oriented film when anisotropy constants remain same for both layers, the energy of film with three layers indicates periodic variation. Some sudden overshooting of energies can be observed after taking second order perturbation into consideration, compared with energy curves of oriented ferromagnetic ultra thin films described in one of our previous report. The way of energy variation of all sc(001), fcc(001) and bcc(001) ferromagnetic ultra thin films with second (or fourth) order anisotropy are exactly same. Easy and hard directions of these sc(001), fcc(001) and bcc(001) ferromagnetic ultra thin films with the effect of second order anisotropy only are  $34.4^\circ$  and  $124.4^\circ$ , respectively. Here these angles have been measured with respect to the normal drawn to the film. The angle between easy and hard directions is exactly  $90^\circ$  as expected. These angles corresponding to easy and hard directions are higher than those of oriented ultra ferromagnetic thin films studied in our early report. Introducing the fourth order anisotropy reduces the smoothness of energy graphs, and indicates several minimums in 3-D graph. Although these details were given for  $\frac{J}{\omega} = 10$ ,  $\frac{D_m^{(2)}}{\omega} = 10$ ,  $\frac{K_s}{\omega} = 10$  and  $\frac{D_m^{(4)}}{\omega} = 5$  values only, all these simulations can be performed for any values of  $\frac{J}{\omega}$ ,  $\frac{D_m^{(2)}}{\omega}$ ,  $\frac{K_s}{\omega}$  and  $\frac{D_m^{(4)}}{\omega}$  or any other type of ferromagnetic material than sc(001), fcc(001) and bcc(001). Since tedious simulations have to be carried out after considering all the terms, above few terms have been taken into account. According to graph 4, the film can be preferentially oriented in some certain directions by applying some certain stresses.

## References

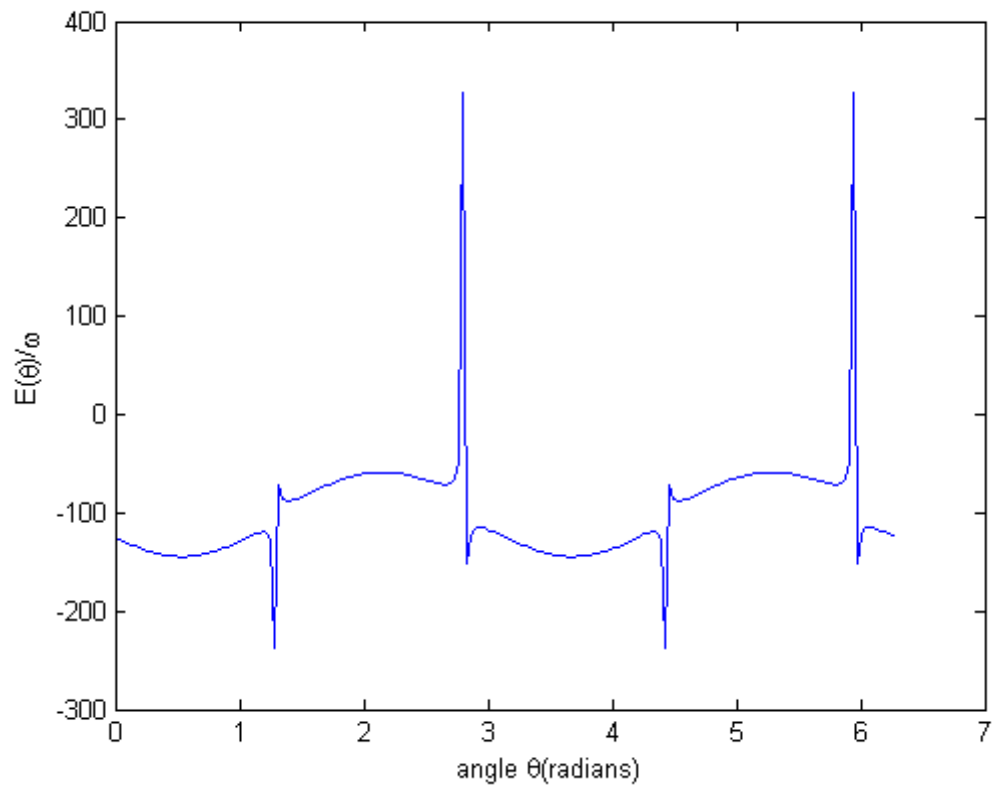
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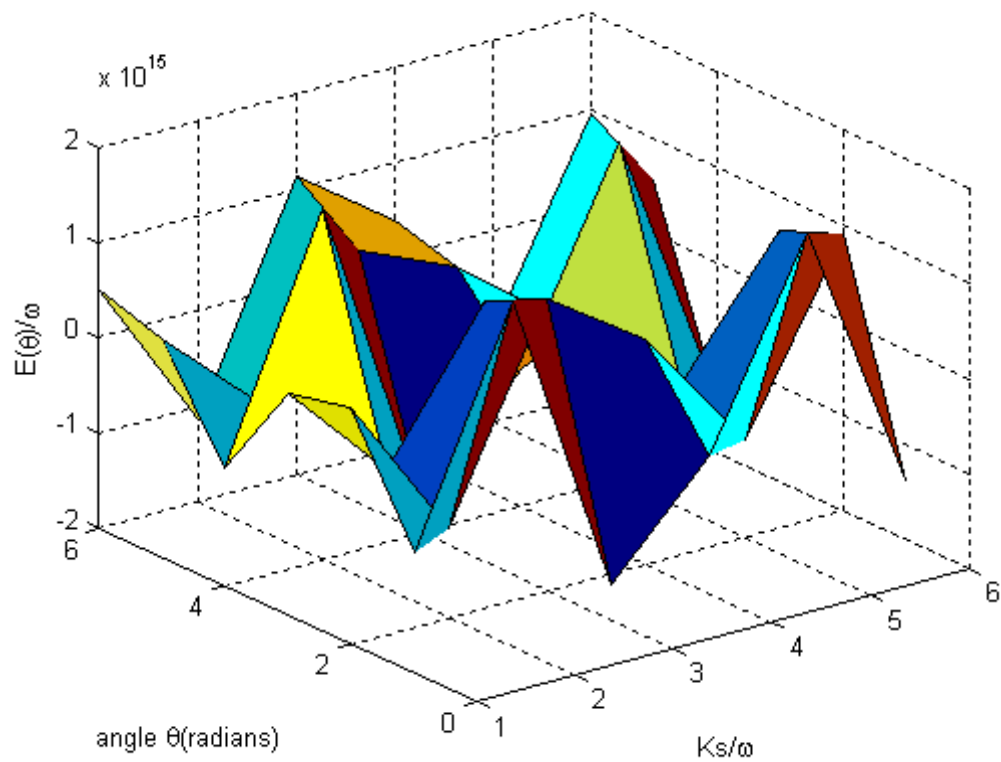
**Fig. 1** Graph between  $\frac{E(\theta)}{\omega}$  and  $\theta$ s for  $\frac{K_s}{\omega}=10$  with the effect of second order anisotropy



**Fig. 2** 3-D plot of  $\frac{E(\theta)}{\omega}$  versus  $\frac{Ks}{\omega}$  and  $\theta$ s with the effect of second order anisotropy



**Fig. 3** Graph between  $\frac{E(\theta)}{\omega}$  and  $\theta$ s for  $\frac{K_s}{\omega}=10$  with the effect of second and fourth order anisotropy



**Fig. 4** 3-D plot of  $\frac{E(\theta)}{\omega}$  versus  $\frac{Ks}{\omega}$  and  $\theta$ s with the effect of second and fourth order anisotropy