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BCC STRUCTURED FERROMAGNETIC ULTRATHIN FILMS WITH TWO SPIN LAYERS AS DESCRIBED BY FOURTH ORDER PERTURBED HEISENBERG HAMILTONIAN. PART 2

N.U.S. Yapa[1] and Sara N. Samarasekara[2]
[1]Department of Physics, Open University of Sri Lanka, Kandy, Sri Lanka
[2]Cullen College of engineering, University of Houston, Houston, TX77004, USA

Abstract:
Ferromagnetic films with bcc structure was investigated using fourth order perturbed Heisenberg Hamiltonian. Magnetic properties of ultrathin films with two spin layers were studied. Only spin exchange interaction, long range dipole interaction and second order magnetic anisotropy were taken into account. 3D plots of total magnetic energy versus angle and magnetic anisotropy constant of bottom spin layer were drawn for different values of magnetic anisotropy constant of top spin layer. When the magnetic anisotropy constant of top spin layer moderately increases, the total magnetic energy does not vary. On the other hand, when the magnetic anisotropy constant of top spin layer significantly increases, the total magnetic energy decreases. However, the gap between adjacent peaks does not vary with the increase of the magnetic anisotropy constant of top spin layer. In addition, 3D plot of total magnetic energy versus angle and spin exchange interaction was plotted. The peaks along the axis of the angle are closely packed in all the cases.
Keywords: *Heisenberg Hamiltonian, fourth order perturbation, bcc structure, ferromagnetic.*

1. Introduction:

Ferromagnetic ultrathin films are applied in field sensors, magnetic storage and electromagnets. Ultrathin ferromagnetic films have been investigated using various theoretical models. Theory of the extrinsic contributions to the ferromagnetic resonance in ultrathin films has been developed [1]. Two dimensional Heisenberg ferromagnets subject to uniaxial anisotropy in ultrathin films has been investigated [2]. Heisenberg Hamiltonian has been applied for EuTe films with surface elastic stresses [3]. The magnetostriction of dc magnetron sputtered FeTaN thin films has been described using De Vries theory [4]. The Korringa-Kohn-Rostoker Green’s function method has been employed to explain the magnetic layers of Ni on Cu [5]. Heisenberg model and transverse Ising model coupled with Green’s function technique have been employed to investigate the electric and magnetic properties of multiferroic thin films [6]. Ferromagnetic resonance has been used to measure the saturation magnetization of ultrathin ferromagnetic films [7]. Heisenberg Hamiltonian with terms of spin exchange interaction, magnetic dipole interaction, applied magnetic field, second and fourth order magnetic anisotropy terms has been appertained for ferromagnetic thin films [8, 9, 10]. Computer simulations have been carried out for the domain structure and Magnetization reversal in thin magnetic films [11]. In-plane dipole coupling anisotropy of square ferromagnetic Heisenberg monolayers has been investigated [12].

Variation of magnetostatic energy of domains and domain walls with film thickness has been theoretically investigated [13]. Magnetic thin films with thicknesses ranging from 2 to 4 layers have been modeled using anisotropic classical Heisenberg spins under the influence of mechanical uniaxial stresses [14]. Magnetic properties of bcc structured ultathin films have been investigated using the Monte carlo simulation [15]. Monte Carlo simulations and analytical Green’s function have been employed to find the properties of thin films made of stacked triangular layers of atoms bearing Heisenberg spins with an Ising like interaction anisotropy [16]. A Green’s function technique has been

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applied to study the influence of the magnetic surface single ion anisotropy on the spin wave spectrum including damping effects in ferromagnetic thin films [17].

According to some experimental studies, magnetic properties depend on the magnetic anisotropy [18, 19]. Ferrite thin and thick films have been elucidated using non-perturbed, second order perturbed and third order perturbed Heisenberg Hamiltonian [20-23]. Second and third order perturbed Heisenberg Hamiltonian was applied to explain ultrathin and thick ferromagnetic films [24, 25]. Furthermore, Heisenberg Hamiltonian was employed to describe the variation of magnetic easy axis orientation of experimentally deposited magnetic thin films with temperature [26, 27].

2. Model:

Heisenberg Hamiltonian of ferromagnetic thin films can be expressed in terms of spin exchange interaction, long range dipole interaction and second order magnetic anisotropy as follows [20-25].

$$H= -\frac{J}{2}\sum_{m,n}\vec{S}_m.\vec{S}_n+\frac{\omega}{2}\sum_{m\neq n}\left(\frac{\vec{S}_m.\vec{S}_n}{r_{mn}^{\ 3}}-\frac{3(\vec{S}_m.\vec{r}_{mn})(\vec{r}_{mn}.\vec{S}_n)}{r_{mn}^{\ 5}}\right)-\sum_m D_{\lambda_m}^{(2)}(S_m^{\ z})^2 \qquad \textbf{(1)}$$

This equation can be deduced to following form for a unit spin [16-24]

$$E(\theta)= -\frac{1}{2}\sum_{m,n=1}^{N}[(JZ_{|m-n|}-\frac{\omega}{4}\Phi_{|m-n|})\cos(\theta_m-\theta_n)-\frac{3\omega}{4}\Phi_{|m-n|}\cos(\theta_m+\theta_n)]$$

$$-\sum_{m=1}^{N}D_m^{(2)}\cos^2\theta_m \qquad \textbf{(2)}$$

All the terms in above equation have been defined in our previous publications [20-25]. For a ferromagnetic thin film with only two spin layers, *N* changes from 1 to 2.

$$E(\theta)=E_0+E(\varepsilon)+E(\varepsilon^2)+E(\varepsilon^3)+E(\varepsilon^4) \qquad \textbf{(3)}$$

Where

$$E_0=-JZ_0+\frac{\omega\phi_0}{4}-JZ_1+\frac{\omega\phi_1}{4}+\frac{3\omega}{8}(2\phi_0+2\phi_1)\cos 2\theta-D_1^{(2)}\cos^2\theta-D_2^{(2)}\cos^2\theta$$

$$E(\varepsilon)=-\frac{3\omega}{4}[(\phi_0+\phi_1)(\varepsilon_1+\varepsilon_2)]\sin 2\theta+2\cos\theta\sin\theta\left(D_1^{(2)}\varepsilon_1+D_2^{(2)}\varepsilon_2\right)$$

$$E(\varepsilon^2)=\left(JZ_1-\frac{\omega\phi_1}{4}\right)\left(\frac{\varepsilon_1^{\ 2}+\varepsilon_2^{\ 2}-2\varepsilon_1\varepsilon_2}{2}\right)-\frac{3\omega}{8}\cos 2\theta\left(2\phi_0(\varepsilon_1^{\ 2}+\varepsilon_2^{\ 2}\right)$$

$$+\left(\varepsilon_1^{\ 2}+\varepsilon_2^{\ 2}+2\varepsilon_1\varepsilon_2\right)\phi_1)$$

$$+\varepsilon_1^{\ 2}\left(D_1^{(2)}\cos^2\theta-D_1^{(2)}\sin^2\theta\right)+\varepsilon_2^{\ 2}\left(D_2^{(2)}\cos^2\theta-D_2^{(2)}\sin^2\theta\right)$$

$$E(\varepsilon^3)=\frac{\omega}{8}\left(4\phi_0(\varepsilon_1^{\ 3}+\varepsilon_2^{\ 3})+\phi_1(\varepsilon_1^{\ 3}+3\varepsilon_1\varepsilon_2^{\ 2}+3\varepsilon_1^{\ 2}\varepsilon_2+\varepsilon_2^{\ 3})\right)\sin 2\theta$$

$$-\frac{4\cos\theta\sin\theta}{3}\left(D_1^{(2)}\varepsilon_1^{\ 3}+D_2^{(2)}\varepsilon_2^{\ 3}\right)$$

$$E(\varepsilon^4)=-\left(JZ_1-\frac{\omega\phi_1}{4}\right)\left(\frac{\varepsilon_1^{\ 4}+\varepsilon_2^{\ 4}+6\varepsilon_1^{\ 2}\varepsilon_2^{\ 2}-4\varepsilon_1^{\ 3}\varepsilon_2-4\varepsilon_1\varepsilon_2^{\ 3}}{24}\right)$$

$$+\frac{\omega}{8}\left[2\phi_0(\varepsilon_1^{\ 4}+\varepsilon_2^{\ 4})+\phi_1\left(\frac{\varepsilon_1^{\ 4}+\varepsilon_2^{\ 4}+6\varepsilon_1^{\ 2}\varepsilon_2^{\ 2}+4\varepsilon_1^{\ 3}\varepsilon_2+4\varepsilon_1\varepsilon_2^{\ 3}}{4}\right)\right]\cos 2\theta$$

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$$-\varepsilon_1^{\,4}\left(\frac{D_1^{(2)}\cos^2\theta}{3}-\frac{D_1^{(2)}\sin^2\theta}{3}\right)-\varepsilon_2^{\,4}\left(\frac{D_2^{(2)}\cos^2\theta}{3}-\frac{D_2^{(2)}\sin^2\theta}{3}\right)$$

First order perturbation term can be expressed as follows [20-25].

$E(\varepsilon)=\vec{\alpha}.\vec{\varepsilon}$

Here terms of row matrix are given by $\alpha_1=-\frac{3\omega}{4}(\phi_0+\phi_1)\sin 2\theta+2\cos\theta\sin\theta D_1^{(2)}$

$$\alpha_2=-\frac{3\omega}{4}(\phi_0+\phi_1)\sin 2\theta+2\cos\theta\sin\theta D_2^{(2)}$$

Second order perturbation term can be rendered as follows [20-25].

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

Elements of 2x2 matrix (C) can be expressed as

$$C_{11}=JZ_1-\frac{\omega\phi_1}{4}-\frac{3\omega}{4}(2\phi_0+\phi_1)\cos 2\theta+2(D_1^{(2)}\cos^2\theta-D_1^{(2)}\sin^2\theta)$$

$$C_{22}=JZ_1-\frac{\omega\phi_1}{4}-\frac{3\omega}{4}(2\phi_0+\phi_1)\cos 2\theta+2(D_2^{(2)}\cos^2\theta-D_2^{(2)}\sin^2\theta)$$

$$C_{12}=C_{21}=-JZ_1+\frac{\omega\phi_1}{4}-\frac{3\omega\phi_1}{4}\cos 2\theta$$

Third order perturbation can be expressed in terms of a two by two matrix, a row matrix and a column matrix as following.

$E(\varepsilon^3)=\varepsilon^2\beta.\vec{\varepsilon}$

Elements of two by two matrix (β) are given by

$$\beta_{11}=\frac{\omega}{8}(4\phi_0+\phi_1)\sin 2\theta-\frac{4D_1^{(2)}\cos\theta\sin\theta}{3}$$

$$\beta_{22}=\frac{\omega}{8}(4\phi_0+\phi_1)\sin 2\theta-\frac{4D_2^{(2)}\cos\theta\sin\theta}{3}$$

$$\beta_{12}=\beta_{21}=\frac{3\omega}{8}\phi_1\sin 2\theta$$

Fourth order perturbation can be expressed in terms of two by two matrices, row matrices and column matrices as following.

$E(\varepsilon^4)=\varepsilon^3F.\vec{\varepsilon}+\varepsilon^2G\varepsilon^2$

Elements of two by two matrices (F and G) are delineated by

$$F_{11}=-\frac{1}{24}\left(JZ_1-\frac{\omega\phi_1}{4}\right)+\frac{\omega}{8}\left(2\phi_0+\frac{\phi_1}{4}\right)\cos 2\theta-\frac{D_1^{(2)}\cos^2\theta}{3}+\frac{D_1^{(2)}\sin^2\theta}{3}$$

$$F_{12}=F_{21}=\frac{1}{6}\left(JZ_1-\frac{\omega\phi_1}{4}\right)+\frac{\omega}{8}\phi_1\cos 2\theta$$

$$F_{22}=-\frac{1}{24}\left(JZ_1-\frac{\omega\phi_1}{4}\right)+\frac{\omega}{8}(2\phi_0+\frac{\phi_1}{4})\cos 2\theta-\frac{D_2^{(2)}\cos^2\theta}{3}+\frac{D_2^{(2)}\sin^2\theta}{3}$$

$$G_{11}=G_{22}=0$$

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$$G_{12} = G_{21} = -\frac{1}{8}\left(JZ_1 - \frac{\omega\phi_1}{4}\right) + \frac{3\omega}{32}\phi_1 \cos 2\theta$$

After substituting above terms in the equation 3,

$$E(\theta) = E_0 + \vec{\alpha}.\vec{\varepsilon} + \frac{1}{2}\vec{\varepsilon}.C.\vec{\varepsilon} + \varepsilon^2 \beta.\vec{\varepsilon} + \varepsilon^3 F.\vec{\varepsilon} + \varepsilon^2 G \varepsilon^2 \quad \textbf{(4)}$$

For the minimum energy of the second order perturbed term [24, 25],

$$\vec{\varepsilon} = -C^{+}.\vec{\alpha} \quad \textbf{(5)}$$

Here C^+ is the pseudo inverse of matrix C, and C^+ can be found using

$$C.C^{+} = 1 - \frac{E}{N} \quad \textbf{(6)}$$

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

3. Results and discussion:

C^+_{11}, C^+_{12}, C^+_{21} and C^+_{22} can be found from equation 6,

$$C^{+}_{11} = -C^{+}_{12} = \frac{C_{22} + C_{21}}{2(C_{11}C_{22} - C_{21}^{\ 2})} \text{ and } C^{+}_{21} = -C^{+}_{22} = \frac{C_{21} + C_{11}}{2(C_{21}^{\ 2} - C_{11}C_{22})}.$$

ε_1 and ε_2 can be found using above equation (5). After substituting ε in equation 4, total energy can be found.

From equation 5, $\varepsilon_1 = (\alpha_2 - \alpha_1)C_{11}^{\ +}$ and $\varepsilon_2 = (\alpha_2 - \alpha_1)C_{21}^{\ +}$

$\varepsilon_1 = 2\cos\theta \sin\theta (D_2^{(2)} - D_1^{(2)})C_{11}^{\ +}$ and $\varepsilon_2 = 2\cos\theta \sin\theta (D_2^{(2)} - D_1^{(2)})C_{21}^{\ +}$

All the simulations were carried out for a film with two different magnetic anisotropy constants in two spin layers.

For bcc (001) structured ferromagnetic thin films, $Z_0=0$, $Z_1=4$, $Z_2=0$, $\Phi_0 = 5.8675$ and $\Phi_1 = 2.7126$ [8-10].

Figure 1 shows the 3D plot of $\frac{E(\theta)}{\omega}$ versus angle and $\frac{D_1^{(2)}}{\omega}$ for $\frac{D_2^{(2)}}{\omega} = 100$ and $\frac{J}{\omega}$ = 10. Energy maximums can be seen at $\frac{D_1^{(2)}}{\omega}$ = 6, 10. 14, ---- etc. Energy minimums can be seen at $\frac{D_1^{(2)}}{\omega}$ = 9, 13. 17. ---- etc. The peaks along the axis of angle are closely packed in that graph. Order of energy decreases from 10^{20} to 10^{10}, when the second order magnetic anisotropy constant of top layer increases from 50 to 100. This implies that when the second order magnetic anisotropy dominates the spin exchange interaction the energy required for rotating the magnetic moments decreases. The spin exchange interaction depends on the interaction between two adjacent spins. The anisotropy constant depends on the energy required for rotating magnetic moments from easy direction to any particular direction. Shape of this 3D plot is different from previous two 3D plots. However, changing the second order magnetic anisotropy constant of top layer does not make any influence on the gap between peaks.

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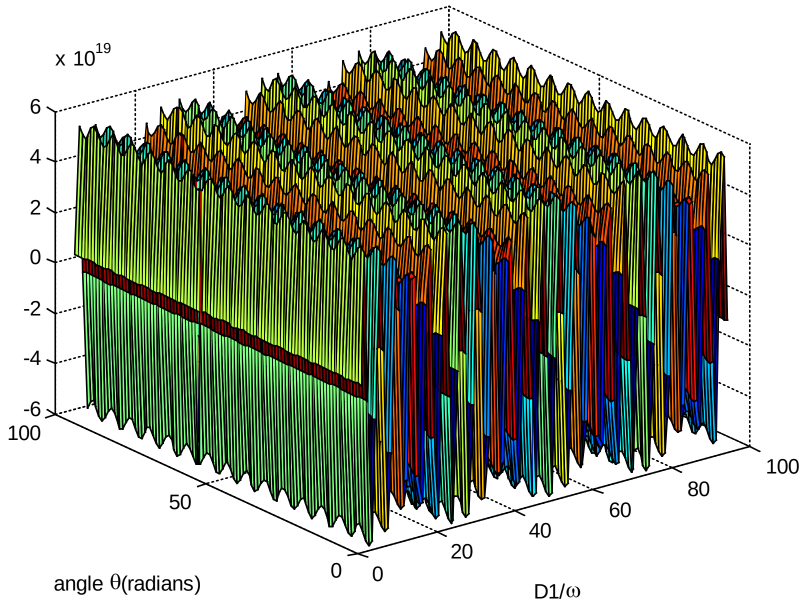

Figure 1: 3D plot of $\frac{E(\theta)}{\omega}$ versus angle and $\frac{D_1^{(2)}}{\omega}$ for $\frac{D_2^{(2)}}{\omega}=100$ and $\frac{J}{\omega}$ = 10.

Figure 2 displays the 3D plot of $\frac{E(\theta)}{\omega}$ versus angle and $\frac{J}{\omega}$ for $\frac{D_1^{(2)}}{\omega}=10$ and $\frac{D_2^{(2)}}{\omega}=5$. The shape of this 3D plot is entirely different from the previous 3D plots. Order of energy (10^6) is less than the order of energy in previous 3D plots. Energy maximums can be found at $\frac{J}{\omega}$ = 13, 17, 21, ----- etc. The bottom side of the plot is almost flat without any noticeable minimums.

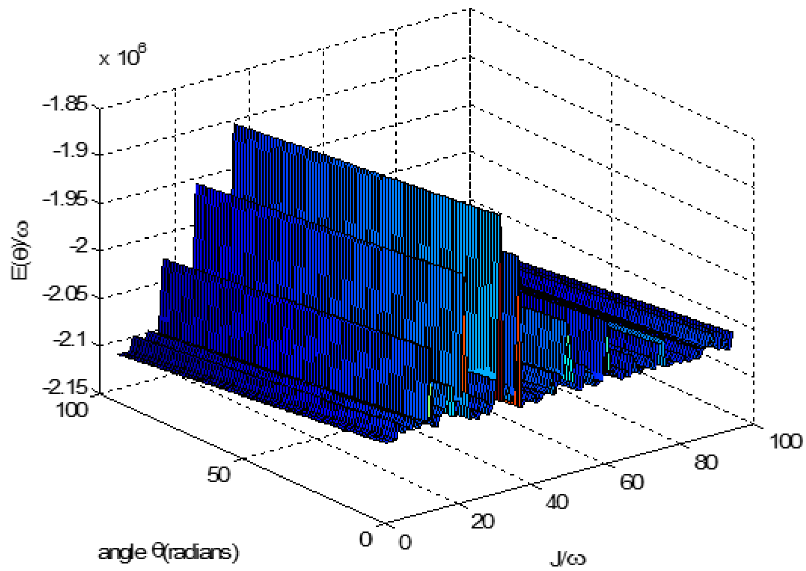

Figure 2: 3D plot of $\frac{E(\theta)}{\omega}$ versus angle and $\frac{J}{\omega}$ for $\frac{D_1^{(2)}}{\omega}=10$ and $\frac{D_2^{(2)}}{\omega}=5$.

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4. Conclusion:

As described in part1, when the second order magnetic anisotropy dominates the spin exchange interaction, the total magnetic energy decreases. Shape of each plot is different from shape of other plots. The bottom of the 3D plot of energy versus angle and spin exchange interaction is flat. According to 3D plot of total magnetic energy versus angle and magnetic anisotropy constant of bottom of spin layer for $\frac{D_2^{(2)}}{\omega}=100$ and $\frac{J}{\omega}$ = 10, energy maximums appear at $\frac{D_1^{(2)}}{\omega}$ = 6, 10. 14, ---- etc., and energy minimums appear seen at $\frac{D_1^{(2)}}{\omega}$ = 9, 13. 17. ---- etc.

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