

RESEARCH ARTICLE

A COMPREHENSIVE STUDY OF MAGNETIC INTERACTIONS IN FACE CENTERED CUBIC STRUCTURED FERROMAGNETIC THIN FILMS WITH THREE SPIN LAYERS USING THE FOURTH ORDER PERTURBED HEISENBERG HAMILTONIAN*M.S.M. Farhan^{1,2} and P. Samarasekara³*¹*Department of Physical Science, Trincomalee Campus, Eastern University, Sri Lanka.*²*Postgraduate Institute of Science, University of Peradeniya, Peradeniya, Sri Lanka.*³*Department of Physics, University of Peradeniya, Peradeniya, Sri Lanka.***ABSTRACT**

Ferromagnetic thin films are crucial components in various technological applications due to their unique magnetic properties. Understanding their behavior requires sophisticated theoretical models, especially for face centered cubic (fcc) structured films with three spin layers. We investigate such films using the fourth order perturbed Heisenberg Hamiltonian, which offers a more accurate description of their magnetic interactions compared to lower order models. Our study focused on the total magnetic energy, considering factors such as magnetic energy, spin dipole interaction energy, spin exchange interaction energy, second and fourth-order anisotropy, stress-induced anisotropy, and demagnetization factor terms. Through extensive simulations using MATLAB, we analyzed the total magnetic energy of these films, plotting 3D and 2D graphs of energy versus stress induced anisotropy and azimuthal angle of spin. Our results revealed that the total magnetic energy of fcc structured films with three spin layers was significantly higher compared to simple cubic (sc) structured films with the same number of layers. We also observed that the distribution of anisotropy constants among spin layers can greatly influence the total magnetic energy. Additionally, we found that stress induced anisotropy remains consistent at certain maxima, even when the values of the second order magnetic anisotropy constant in the middle and top spin layers are interchanged. This indicates a complex interplay between stress induced and intrinsic magnetic anisotropies. Our study provided valuable insights into the magnetic properties of fcc structured ferromagnetic thin films, highlighting the importance of considering higher order interactions for a comprehensive understanding of their behavior.

Keywords: *Fourth order perturbed Heisenberg Hamiltonian, magnetic anisotropy, spin layers, stress induced anisotropy.*

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1. INTRODUCTION

Ferromagnetic thin films are thin layers of ferromagnetic material that exhibit a spontaneous magnetization, meaning they can be magnetized in the absence of an external magnetic field. These films are of great interest in various technological applications, including magnetic storage devices, magnetic sensors, and spintronic devices, due to their unique magnetic properties and potential for miniaturization.

In recent years, advancements in theoretical models and computational simulations have significantly enhanced our understanding of the complex magnetic properties exhibited by ferromagnetic thin films. By delving into the intricate interplay of factors such as exchange interactions, anisotropy constants, and magnetoelastic effects, researchers have been able to predict and comprehend the observed behaviors more accurately. These insights have not only deepened our fundamental understanding but also guided the design of novel materials tailored for specific applications.

Various models have been employed to describe ferromagnetic films, each offering unique perspectives. For instance, the quasistatic magnetic hysteresis of ferromagnetic thin films deposited on a vicinal substrate has been rigorously examined through Monte Carlo simulations [1]. Additionally, the magnetic properties of ferromagnetic thin films featuring alternating superlayers have been comprehensively studied using the Ising model [2]. Moreover, the structural and magnetic characteristics of two-dimensional FeCo ordered alloys have been precisely determined through first-principles band structure theory [3]. Lastly, the magnetic layers of Ni on Cu have been thoroughly investigated using the Korringa-Kohn-Rostoker Green's function method [4]. These diverse approaches underscore the multidimensional nature of research in this field, highlighting the need for comprehensive methodologies to unravel the intricate magnetic behaviors exhibited by ferromagnetic thin films.

The magnetic properties of ferromagnetic thin films are often described using the Heisenberg model, which is a simplified quantum mechanical model that considers the interaction between magnetic moments associated with individual atoms or ions in the material. The Heisenberg model Hamiltonian describes the energy of the system in terms of the interactions between these magnetic moments. For face-centered cubic (fcc) structure ferromagnetic thin films, the lattice structure is characterized by a cubic unit cell

with atoms located at the corners and face centers of the cube. The magnetic properties of fcc thin films are influenced by the crystal structure, layering, and interactions between atoms within and between layers.

The fourth-order perturbed Heisenberg Hamiltonian for fcc structure ferromagnetic thin films with three spin layers is a theoretical framework used to describe the magnetic interactions in these systems with greater accuracy than the basic Heisenberg model. This Hamiltonian includes terms that account for higher-order interactions between magnetic moments, beyond the nearest-neighbor interactions considered in the basic Heisenberg model. These higher-order interactions can play a significant role in determining the magnetic properties of thin films, particularly in systems with complex layering and crystal structures.

In this study, we investigate the total energy of ferromagnetic thin films with three spin layers by solving the classical Heisenberg Hamiltonian. This approach considers various energy terms, including magnetic energy, spin dipole interaction energy, spin exchange interaction energy, second and fourth-order anisotropy, stress-induced anisotropy, and demagnetization factor terms. Specifically, we focus on the face-centered cubic (fcc) structure and employ the fourth-order perturbed Heisenberg Hamiltonian, which includes all seven magnetic energy parameters.

MATLAB computer software was used to plot 3D and 2D graph of energy versus stress induced anisotropy and azimuthal angle of spin.

2. MODEL

The Heisenberg Hamiltonian of ferromagnetic films can be formulated as following [5-7].

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

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

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

Here N , m (or n), J , $Z_{|m-n|}$, ω , $\Phi_{|m-n|}$, θ_m (θ_n), $D_m^{(2)}$, $D_m^{(4)}$, H_{in} , H_{out} , N_d and K_s are total number of layers, layer index, spin exchange interaction, number of nearest spin neighbors, strength of long range dipole interaction, partial summations of dipole interaction, azimuthal angles of spins, second and fourth order anisotropy constants, in plane and out of plane applied magnetic fields, demagnetization factor and stress induced anisotropy constants respectively.

The spin structure is considered to be slightly disoriented. Therefore, the spins could be considered to have angles distributed about an average angle θ . By choosing azimuthal angles as

$$\theta_m = \theta + \varepsilon_m \text{ and } \theta_n = \theta + \varepsilon_n$$

Where the ε 's are small positive or negative angular deviations.

Then, $\theta_m - \theta_n = \varepsilon_m - \varepsilon_n$ and $\theta_m + \theta_n = 2\theta + \varepsilon_m + \varepsilon_n$. After substituting these new angles in above equation number (1), the cosine and sine terms can be expanded up to the fourth order of ε_m and ε_n as following.

$$E(\theta) = E_0 + E(\varepsilon) + E(\varepsilon^2) + E(\varepsilon^3) + E(\varepsilon^4) + \dots$$

If the fifth and higher order perturbations are neglected, then

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

Here

$$E_0 = -\frac{1}{2} \sum_{m,n=1}^N \left(JZ_{|m-n|} - \frac{\omega}{4} \Phi_{|m-n|} \right) + \frac{3\omega}{8} \cos 2\theta \sum_{m,n=1}^N \Phi_{|m-n|} - \cos^2 \theta \sum_{m=1}^N D_m^{(2)}$$

$$-\cos^4\theta \sum_{m=1}^N D_m^{(4)} - N(H_{in}\sin\theta + H_{out}\cos\theta + K_s\sin 2\theta) + \frac{N_d N^2}{\mu_0} \quad (3)$$

$$E(\varepsilon) = -\frac{3\omega}{8}\sin 2\theta \sum_{m,n=1}^N \Phi_{|m-n|}(\varepsilon_m + \varepsilon_n) + \sin 2\theta \sum_{m=1}^N D_m^{(2)}\varepsilon_m + 2\cos^2\theta\sin 2\theta \sum_{m=1}^N D_m^{(4)}\varepsilon_m \\ -H_{in}\cos\theta \sum_{m=1}^N \varepsilon_m + H_{out}\sin\theta \sum_{m=1}^N \varepsilon_m - 2K_s\cos 2\theta \sum_{m=1}^N \varepsilon_m \quad (4)$$

$$E(\varepsilon^2) = \frac{1}{4} \sum_{m,n=1}^N \left(JZ_{|m-n|} - \frac{\omega}{4}\Phi_{|m-n|} \right) (\varepsilon_m - \varepsilon_n)^2 - \frac{3\omega}{16}\cos 2\theta \sum_{m,n=1}^N \Phi_{|m-n|}(\varepsilon_m + \varepsilon_n)^2 \\ + \cos 2\theta \sum_{m=1}^N D_m^{(2)}\varepsilon_m^2 + 2\cos^2\theta(\cos^2\theta - 3\sin^2\theta) \sum_{m=1}^N D_m^{(4)}\varepsilon_m^2 + \frac{H_{in}}{2}\sin\theta \sum_{m=1}^N \varepsilon_m^2 \\ + \frac{H_{out}}{2}\cos\theta \sum_{m=1}^N \varepsilon_m^2 - \frac{N_d}{2\mu_0} \sum_{m,n=1}^N (\varepsilon_m - \varepsilon_n)^2 + 2K_s\sin 2\theta \sum_{m=1}^N \varepsilon_m^2 \quad (5)$$

$$E(\varepsilon^3) = \frac{\omega}{16}\sin 2\theta \sum_{m,n=1}^N \Phi_{|m-n|}(\varepsilon_m + \varepsilon_n)^3 - \frac{4}{3}\sin\theta\cos\theta \sum_{m=1}^N D_m^{(2)}\varepsilon_m^3 \\ -4\sin\theta\cos\theta \left(\frac{5}{3}\cos^2\theta - \sin^2\theta \right) \sum_{m=1}^N D_m^{(4)}\varepsilon_m^3 + \frac{H_{in}}{6}\cos\theta \sum_{m=1}^N \varepsilon_m^3 - \frac{H_{out}}{6}\sin\theta \sum_{m=1}^N \varepsilon_m^3 \\ + \frac{4}{3}K_s\cos 2\theta \sum_{m=1}^N \varepsilon_m^3 \quad (6)$$

$$E(\varepsilon^4) = -\frac{1}{48} \sum_{m,n=1}^N \left(JZ_{|m-n|} - \frac{\omega}{4}\Phi_{|m-n|} \right) (\varepsilon_m - \varepsilon_n)^4 + \frac{\omega}{64}\cos 2\theta \sum_{m,n=1}^N \Phi_{|m-n|}(\varepsilon_m + \varepsilon_n)^4 \\ -\frac{1}{3}\cos 2\theta \sum_{m=1}^N D_m^{(2)}\varepsilon_m^4 - \left(\frac{5}{3}\cos^4\theta - 8\cos^2\theta\sin^2\theta + \sin^4\theta \right) \sum_{m=1}^N D_m^{(4)}\varepsilon_m^4 \\ -\frac{H_{in}}{24}\sin\theta \sum_{m=1}^N \varepsilon_m^4 - \frac{H_{out}}{24}\cos\theta \sum_{m=1}^N \varepsilon_m^4 + \frac{N_d}{24\mu_0} \sum_{m,n=1}^N (\varepsilon_m - \varepsilon_n)^4 \\ -\frac{2}{3}K_s\sin 2\theta \sum_{m=1}^N \varepsilon_m^4 \quad (7)$$

For films with three spin layers, $N = 3$. Therefore, m and n change from 1 to 3.

$$E_0 = -\frac{3}{2}\left(JZ_0 - \frac{\omega}{4}\Phi_0\right) - 2\left(JZ_1 - \frac{\omega}{4}\Phi_1\right) + \frac{3\omega}{8}\cos 2\theta(3\Phi_0 + 4\Phi_1) - \cos^2\theta(D_1^{(2)} + D_2^{(2)} + D_3^{(2)}) - \cos^4\theta(D_1^{(4)} + D_2^{(4)} + D_3^{(4)}) - 3(H_{in}\sin\theta + H_{out}\cos\theta + K_s\sin 2\theta) + 9\frac{N_d}{\mu_0} \quad (8)$$

$$E(\varepsilon) = -\frac{3\omega}{4}\sin 2\theta[\Phi_0(\varepsilon_1 + \varepsilon_2 + \varepsilon_3) + \Phi_1(\varepsilon_1 + 2\varepsilon_2 + \varepsilon_3)] + \sin 2\theta(D_1^{(2)}\varepsilon_1 + D_2^{(2)}\varepsilon_2 + D_3^{(2)}\varepsilon_3) + 2\cos^2\theta\sin 2\theta(D_1^{(4)}\varepsilon_1 + D_2^{(4)}\varepsilon_2 + D_3^{(4)}\varepsilon_3) - H_{in}\cos\theta(\varepsilon_1 + \varepsilon_2 + \varepsilon_3) + H_{out}\sin\theta(\varepsilon_1 + \varepsilon_2 + \varepsilon_3) - 2K_s\cos 2\theta(\varepsilon_1 + \varepsilon_2 + \varepsilon_3) \quad (9)$$

$$E(\varepsilon^2) = \frac{1}{2}\left(JZ_1 - \frac{\omega}{4}\Phi_1\right)(\varepsilon_1^2 + 2\varepsilon_2^2 + \varepsilon_3^2 - 2\varepsilon_1\varepsilon_2 - 2\varepsilon_2\varepsilon_3) - \frac{3\omega}{8}\cos 2\theta[2\Phi_0(\varepsilon_1^2 + \varepsilon_2^2 + \varepsilon_3^2) + \Phi_1(\varepsilon_1^2 + 2\varepsilon_2^2 + \varepsilon_3^2 + 2\varepsilon_1\varepsilon_2 + 2\varepsilon_2\varepsilon_3)] + \cos 2\theta(D_1^{(2)}\varepsilon_1^2 + D_2^{(2)}\varepsilon_2^2 + D_3^{(2)}\varepsilon_3^2) + 2\cos^2\theta(\cos^2\theta - 3\sin^2\theta)(D_1^{(4)}\varepsilon_1^2 + D_2^{(4)}\varepsilon_2^2 + D_3^{(4)}\varepsilon_3^2) + \frac{H_{in}}{2}\sin\theta(\varepsilon_1^2 + \varepsilon_2^2 + \varepsilon_3^2) + \frac{H_{out}}{2}\cos\theta(\varepsilon_1^2 + \varepsilon_2^2 + \varepsilon_3^2) - 2\frac{N_d}{\mu_0}(\varepsilon_1^2 + \varepsilon_2^2 + \varepsilon_3^2 - \varepsilon_1\varepsilon_2 - \varepsilon_1\varepsilon_3 - \varepsilon_2\varepsilon_3) + 2K_s\sin 2\theta(\varepsilon_1^2 + \varepsilon_2^2 + \varepsilon_3^2) \quad (10)$$

$$E(\varepsilon^3) = \frac{\omega}{8}\sin 2\theta[4\Phi_0(\varepsilon_1^3 + \varepsilon_2^3 + \varepsilon_3^3) + \Phi_1(\varepsilon_1^3 + 3\varepsilon_1^2\varepsilon_2 + 3\varepsilon_1\varepsilon_2^2 + 2\varepsilon_2^3 + 3\varepsilon_2^2\varepsilon_3 + 3\varepsilon_2\varepsilon_3^2 + \varepsilon_3^3)] - \frac{4}{3}\sin\theta\cos\theta(D_1^{(2)}\varepsilon_1^3 + D_2^{(2)}\varepsilon_2^3 + D_3^{(2)}\varepsilon_3^3) - 4\sin\theta\cos\theta\left(\frac{5}{3}\cos^2\theta - \sin^2\theta\right)(D_1^{(4)}\varepsilon_1^3 + D_2^{(4)}\varepsilon_2^3 + D_3^{(4)}\varepsilon_3^3) + \frac{H_{in}}{6}\cos\theta(\varepsilon_1^3 + \varepsilon_2^3 + \varepsilon_3^3) - \frac{H_{out}}{6}\sin\theta(\varepsilon_1^3 + \varepsilon_2^3 + \varepsilon_3^3) + \frac{4}{3}K_s\cos 2\theta(\varepsilon_1^3 + \varepsilon_2^3 + \varepsilon_3^3) \quad (11)$$

$$E(\varepsilon^4) = -\frac{1}{24}\left(JZ_1 - \frac{\omega}{4}\Phi_1\right)(\varepsilon_1^4 - 4\varepsilon_1^3\varepsilon_2 + 6\varepsilon_1^2\varepsilon_2^2 - 4\varepsilon_1\varepsilon_2^3 + 2\varepsilon_2^4 - 4\varepsilon_2^3\varepsilon_3 + 6\varepsilon_2^2\varepsilon_3^2 - 4\varepsilon_2\varepsilon_3^3 + \varepsilon_3^4) + \frac{\omega}{32}\cos 2\theta[8\Phi_0(\varepsilon_1^4 + \varepsilon_2^4 + \varepsilon_3^4) + \Phi_1(\varepsilon_1^4 + 4\varepsilon_1^3\varepsilon_2 + 6\varepsilon_1^2\varepsilon_2^2 + 4\varepsilon_1\varepsilon_2^3 + 2\varepsilon_2^4 + 4\varepsilon_2^3\varepsilon_3 + 6\varepsilon_2^2\varepsilon_3^2 + 4\varepsilon_2\varepsilon_3^3 + \varepsilon_3^4)] - \frac{1}{3}\cos 2\theta(D_1^{(2)}\varepsilon_1^4 + D_2^{(2)}\varepsilon_2^4$$

$$\begin{aligned}
 & +D_3^{(2)}\varepsilon_3^4) - \left(\frac{5}{3}\cos^4\theta - 8\cos^2\theta\sin^2\theta + \sin^4\theta\right) \left(D_1^{(4)}\varepsilon_1^4 + D_2^{(4)}\varepsilon_2^4 + D_3^{(4)}\varepsilon_3^4\right) \\
 & - \frac{H_{in}}{24}\sin\theta(\varepsilon_1^4 + \varepsilon_2^4 + \varepsilon_3^4) - \frac{H_{out}}{24}\cos\theta(\varepsilon_1^4 + \varepsilon_2^4 + \varepsilon_3^4) + \frac{N_d}{6\mu_0}(\varepsilon_1^4 - 2\varepsilon_1^3\varepsilon_2 \\
 & + 3\varepsilon_1^2\varepsilon_2^2 - 2\varepsilon_1\varepsilon_2^3 + \varepsilon_2^4 - 2\varepsilon_1^3\varepsilon_3 + 3\varepsilon_1^2\varepsilon_3^2 - 2\varepsilon_1\varepsilon_3^3 + \varepsilon_3^4 - 2\varepsilon_2^3\varepsilon_3 + 3\varepsilon_2^2\varepsilon_3^2 \\
 & - 2\varepsilon_2\varepsilon_3^3) - \frac{2}{3}K_s\sin 2\theta(\varepsilon_1^4 + \varepsilon_2^4 + \varepsilon_3^4)
 \end{aligned} \tag{12}$$

First order perturbation term can be expressed in terms of a row and column matrix with all seven terms in each as following.

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

Here terms of α are given by α_1 , α_2 and α_3 .

$$\begin{aligned}
 \alpha_1 = & -\frac{3\omega}{4}\sin 2\theta(\Phi_0 + \Phi_1) + \sin 2\theta D_1^{(2)} + 2\cos^2\theta\sin 2\theta D_1^{(4)} - H_{in}\cos\theta + H_{out}\sin\theta \\
 & - 2K_s\cos 2\theta
 \end{aligned} \tag{13}$$

$$\begin{aligned}
 \alpha_2 = & -\frac{3\omega}{4}\sin 2\theta(\Phi_0 + \Phi_1) + \sin 2\theta D_2^{(2)} + 2\cos^2\theta\sin 2\theta D_2^{(4)} - H_{in}\cos\theta + H_{out}\sin\theta \\
 & - 2K_s\cos 2\theta
 \end{aligned} \tag{14}$$

$$\begin{aligned}
 \alpha_3 = & -\frac{3\omega}{4}\sin 2\theta(\Phi_0 + \Phi_1) + \sin 2\theta D_3^{(2)} + 2\cos^2\theta\sin 2\theta D_3^{(4)} - H_{in}\cos\theta + H_{out}\sin\theta \\
 & - 2K_s\cos 2\theta
 \end{aligned} \tag{15}$$

Second order perturbation term can be expressed in terms of a two-by-two matrix. A row matrix and a column matrix as following.

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

Elements of 3×3 matrix (C) are delineated by

$$\begin{aligned}
 C_{11} = & JZ_1 - \frac{\omega}{4}\Phi_1 - \frac{3\omega}{4}\cos 2\theta(2\Phi_0 + \Phi_1) + 2\cos 2\theta D_1^{(2)} + 4\cos^2\theta(\cos^2\theta - 3\sin^2\theta)D_1^{(4)} \\
 & + H_{in}\sin\theta + H_{out}\cos\theta - \frac{4N_d}{\mu_0} + 4K_s\sin 2\theta
 \end{aligned} \tag{16}$$

$$C_{12} = C_{21} = C_{23} = C_{32} = -JZ_1 + \frac{\omega}{4}\Phi_1 - \frac{3\omega}{4}\cos 2\theta\Phi_1 + \frac{2N_d}{\mu_0} \tag{17}$$

$$C_{13} = C_{31} = \frac{2N_d}{\mu_0} \quad (18)$$

$$C_{22} = 2(JZ_1 - \frac{\omega}{4}\Phi_1) - \frac{3\omega}{2}\cos 2\theta(\Phi_0 + \Phi_1) + 2\cos 2\theta D_2^{(2)} + 4\cos^2\theta(\cos^2\theta - 3\sin^2\theta)D_2^{(4)} \\ + H_{in}\sin\theta + H_{out}\cos\theta - \frac{4N_d}{\mu_0} + 4K_s\sin 2\theta \quad (19)$$

$$C_{33} = JZ_1 - \frac{\omega}{4}\Phi_1 - \frac{3\omega}{4}\cos 2\theta(2\Phi_0 + \Phi_1) + 2\cos 2\theta D_3^{(2)} + 4\cos^2\theta(\cos^2\theta - 3\sin^2\theta)D_3^{(4)} \\ + H_{in}\sin\theta + H_{out}\cos\theta - \frac{4N_d}{\mu_0} + 4K_s\sin 2\theta \quad (20)$$

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

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

Elements of 3×3 matrix (β) are specified by

$$\beta_{11} = \frac{\omega}{8}\sin 2\theta(4\Phi_0 + \Phi_1) - \frac{4}{3}\sin\theta\cos\theta D_1^{(2)} - 4\sin\theta\cos\theta\left(\frac{5}{3}\cos^2\theta - \sin^2\theta\right)D_1^{(4)} \\ + \frac{H_{in}}{6}\cos\theta - \frac{H_{out}}{6}\sin\theta + \frac{4}{3}K_s\cos 2\theta \quad (21)$$

$$\beta_{12} = \beta_{21} = \beta_{23} = \beta_{32} = \frac{3\omega}{8}\sin 2\theta\Phi_1 \quad (22)$$

$$\beta_{13} = \beta_{31} = 0 \quad (23)$$

$$\beta_{22} = \frac{\omega}{4}\sin 2\theta(2\Phi_0 + \Phi_1) - \frac{4}{3}\sin\theta\cos\theta D_2^{(2)} - 4\sin\theta\cos\theta\left(\frac{5}{3}\cos^2\theta - \sin^2\theta\right)D_2^{(4)} \\ + \frac{H_{in}}{6}\cos\theta - \frac{H_{out}}{6}\sin\theta + \frac{4}{3}K_s\cos 2\theta \quad (24)$$

$$\beta_{33} = \frac{\omega}{8}\sin 2\theta(4\Phi_0 + \Phi_1) - \frac{4}{3}\sin\theta\cos\theta D_3^{(2)} - 4\sin\theta\cos\theta\left(\frac{5}{3}\cos^2\theta - \sin^2\theta\right)D_3^{(4)} \\ + \frac{H_{in}}{6}\cos\theta - \frac{H_{out}}{6}\sin\theta + \frac{4}{3}K_s\cos 2\theta \quad (25)$$

Fourth order perturbation term can be expressed in terms of a two-by-two matrix. A row matrix and a column matrix as following.

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

Elements of 3×3 matrix (F and G) are delineated by

$$\begin{aligned} F_{11} = & -\frac{1}{24} \left(JZ_1 - \frac{\omega}{4} \Phi_1 \right) + \frac{\omega}{32} \cos 2\theta (8\Phi_0 + \Phi_1) - \frac{1}{3} \cos 2\theta D_1^{(2)} \\ & - \left(\frac{5}{3} \cos^4 \theta - 8 \cos^2 \theta \sin^2 \theta + \sin^4 \theta \right) D_1^{(4)} - \frac{H_{in}}{24} \sin \theta - \frac{H_{out}}{24} \cos \theta + \frac{N_d}{6\mu_0} - \frac{2}{3} K_s \sin 2\theta \end{aligned} \quad (26)$$

$$F_{12} = F_{21} = F_{23} = F_{32} = \frac{1}{6} \left(JZ_1 - \frac{\omega}{4} \Phi_1 \right) + \frac{\omega}{8} \cos 2\theta \Phi_1 - \frac{N_d}{3\mu_0} \quad (27)$$

$$F_{13} = F_{31} = -\frac{N_d}{3\mu_0} \quad (28)$$

$$\begin{aligned} F_{22} = & -\frac{1}{12} \left(JZ_1 - \frac{\omega}{4} \Phi_1 \right) + \frac{\omega}{16} \cos 2\theta (4\Phi_0 + \Phi_1) - \frac{1}{3} \cos 2\theta D_2^{(2)} \\ & - \left(\frac{5}{3} \cos^4 \theta - 8 \cos^2 \theta \sin^2 \theta + \sin^4 \theta \right) D_2^{(4)} - \frac{H_{in}}{24} \sin \theta - \frac{H_{out}}{24} \cos \theta + \frac{N_d}{6\mu_0} - \frac{2}{3} K_s \sin 2\theta \end{aligned} \quad (29)$$

$$\begin{aligned} F_{33} = & -\frac{1}{24} \left(JZ_1 - \frac{\omega}{4} \Phi_1 \right) + \frac{\omega}{32} \cos 2\theta (8\Phi_0 + \Phi_1) - \frac{1}{3} \cos 2\theta D_3^{(2)} \\ & - \left(\frac{5}{3} \cos^4 \theta - 8 \cos^2 \theta \sin^2 \theta + \sin^4 \theta \right) D_3^{(4)} - \frac{H_{in}}{24} \sin \theta - \frac{H_{out}}{24} \cos \theta + \frac{N_d}{6\mu_0} - \frac{2}{3} K_s \sin 2\theta \end{aligned} \quad (30)$$

$$G_{11} = G_{22} = G_{33} = 0 \quad (31)$$

$$G_{12} = G_{21} = -\frac{1}{8} \left(JZ_1 - \frac{\omega}{4} \Phi_1 \right) + \frac{3\omega}{32} \cos 2\theta \Phi_1 + \frac{N_d}{4\mu_0} \quad (32)$$

$$G_{23} = G_{32} = -\frac{1}{8} \left(JZ_1 - \frac{\omega}{4} \Phi_1 \right) + \frac{3\omega}{32} \cos 2\theta \Phi_1 + \frac{N_d}{2\mu_0} \quad (33)$$

$$G_{13} = G_{31} = \frac{N_d}{4\mu_0} \quad (34)$$

Therefore, the total magnetic energy given in equation (2) can be deduced to

$$E(\theta) = E_0 + \vec{\alpha} \cdot \vec{\varepsilon} + \frac{1}{2} \vec{\varepsilon} \cdot C \cdot \vec{\varepsilon} + \varepsilon^2 \cdot \beta \cdot \vec{\varepsilon} + \varepsilon^3 \cdot F \cdot \vec{\varepsilon} + \varepsilon^2 \cdot G \cdot \varepsilon^2 \quad (35)$$

For the minimum energy of the second order perturbed term

$$\vec{\varepsilon} = -C^+ . \alpha \quad (36)$$

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

$$C . C^+ = 1 - \frac{E}{N} \quad (37)$$

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

Therefore, from the matrix equation (36)

$$\varepsilon_1 = -(C_{11}^+ \alpha_1 + C_{12}^+ \alpha_2 + C_{13}^+ \alpha_3) \quad (38)$$

$$\varepsilon_2 = -(C_{21}^+ \alpha_1 + C_{22}^+ \alpha_2 + C_{23}^+ \alpha_3) \quad (39)$$

$$\varepsilon_3 = -(C_{31}^+ \alpha_1 + C_{32}^+ \alpha_2 + C_{33}^+ \alpha_3) \quad (40)$$

After substituting ε in equation (35), the total magnetic energy can be determined.

3. RESULTS AND DISCUSSION

All the graphs in this manuscript were plotted for ferromagnetic films with face centered cubic lattice and three spin layers. For ferromagnetic films with fcc (001) structure, $Z_0=4$, $Z_1=4$, $Z_2=0$, $\Phi_0 = 9.0336$ and $\Phi_1 = 1.4294$ [8-10]. 3D plot of energy versus angle and stress induced anisotropy constant is given in figure 1 for $\frac{D_1^{(2)}}{\omega} = 10$, $\frac{D_2^{(2)}}{\omega} = 5$ and $\frac{D_3^{(2)}}{\omega} = 10$. Here other parameters are fixed at $\frac{J}{\omega} = \frac{D_1^{(4)}}{\omega} = \frac{D_2^{(4)}}{\omega} = \frac{D_3^{(4)}}{\omega} = \frac{H_{in}}{\omega} = \frac{N_d}{\mu_0 \omega} = \frac{H_{out}}{\omega} = 10$ for this simulation. The energy maximums can be observed at $\frac{K_s}{\omega} = 4, 27, 50, 75, 94$. The major maximum observed at about $\frac{K_s}{\omega} = 75$. Energy in these graphs is in the order of 10^6 . The peaks along the axis of angle are closely packed in the fourth order perturbed case compared to the second and third order perturbed cases [7, 11, 12]. The shape of the graph is also entirely different from the graphs obtained using the second and third order perturbed Heisenberg Hamiltonian [7, 11, 12]. The peaks are periodically distributed. The total magnetic energy decreases when compared to sc structured ferromagnetic thin films with the same number of spin layers [13]. But it was found (1049) significantly higher in the two spin layer for the same structure [14].

Figure 2 shows the graph of energy versus angle for $\frac{K_s}{\omega} = 75$ after fixing the other parameters at the values given above. In this graph, energy minimum can be observed at 0.754 and 3.896 radians. The energy maximums can be found at 2.356 and 5.435 radians. The angle between consecutive magnetic easy and hard directions is approximately 90 degrees.

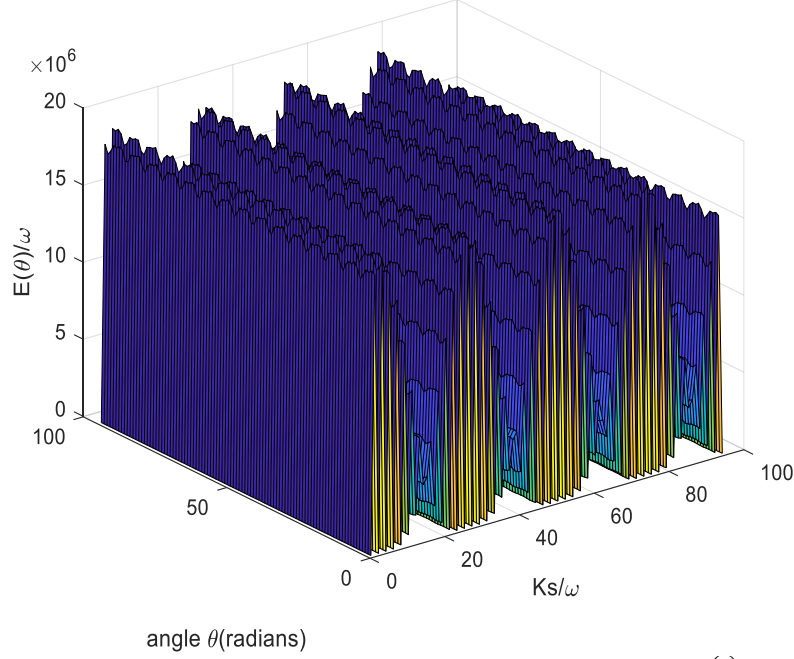


Figure 1: 3D plot of energy versus angle and stress induced anisotropy for $\frac{D_1^{(2)}}{\omega} = 10$, $\frac{D_2^{(2)}}{\omega} = 5$ and $\frac{D_3^{(2)}}{\omega} = 10$.

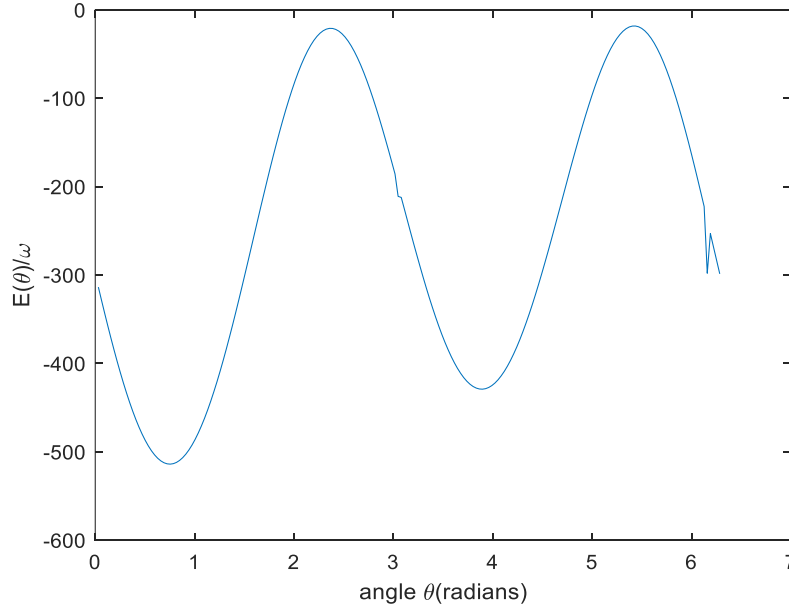


Figure 2: 2D graph of energy versus angle for $\frac{K_s}{\omega} = 75$.

Figure 3 represents the 3D plot of energy versus angle and stress induced anisotropy constant for $\frac{D_1^{(2)}}{\omega} = 10$, $\frac{D_2^{(2)}}{\omega} = 10$ and $\frac{D_3^{(2)}}{\omega} = 5$. Here other parameters are fixed at $\frac{J}{\omega} = \frac{D_1^{(4)}}{\omega} = \frac{D_2^{(4)}}{\omega} = \frac{D_3^{(4)}}{\omega} = \frac{H_{in}}{\omega} = \frac{N_d}{\mu_0 \omega} = \frac{H_{out}}{\omega} = 10$ for this simulation. In this graph, the energy maximums can be observed at $\frac{K_s}{\omega} = 2, 23, 48, 71$ and 94 . The major maximum was observed at about $\frac{K_s}{\omega} = 71$. Energy in these graphs is in the order of 10^{22} . According to figures 1 and 3, when the second order anisotropy constant in the top spin layer is less than those of the bottom and middle spin layers, the total magnetic energy increases. The values of stress induced anisotropy at the maxima of 3D plots are approximately the same, when the values of the second order magnetic anisotropy constant of the middle and top spin layers are interchanged. The minimum value of the energy is zero in both 3D plots. In these graphs, the total magnetic was observed in the range of 10^6 to 10^{22} . However, in the case of sc structures, the total magnetic energy was obtained in the range of 10^{12} to 10^{17} [13]. The change in energy is significantly higher in the graph plotting energy versus angle and stress induced anisotropy constant for fcc structure with three spin layers when compared to sc structured ferromagnetic thin films with the same number of spin layers [13].

Figure 4 shows the graph of energy versus angle for $\frac{K_s}{\omega} = 71$ after fixing the other parameters at the values given above. In this graph, magnetic easy directions can be observed at 0.754 and 3.896 radians. The energy maximums can be found at 2.356 and 5.404 radians. The angle between consecutive magnetic easy and hard directions is approximately 90 degrees. The maximum and minimum energy values in this graph are approximately the same when compared to figure 2. However, a spike did not appear in the graph plotted in figure 2, while it is evident in the current graph.

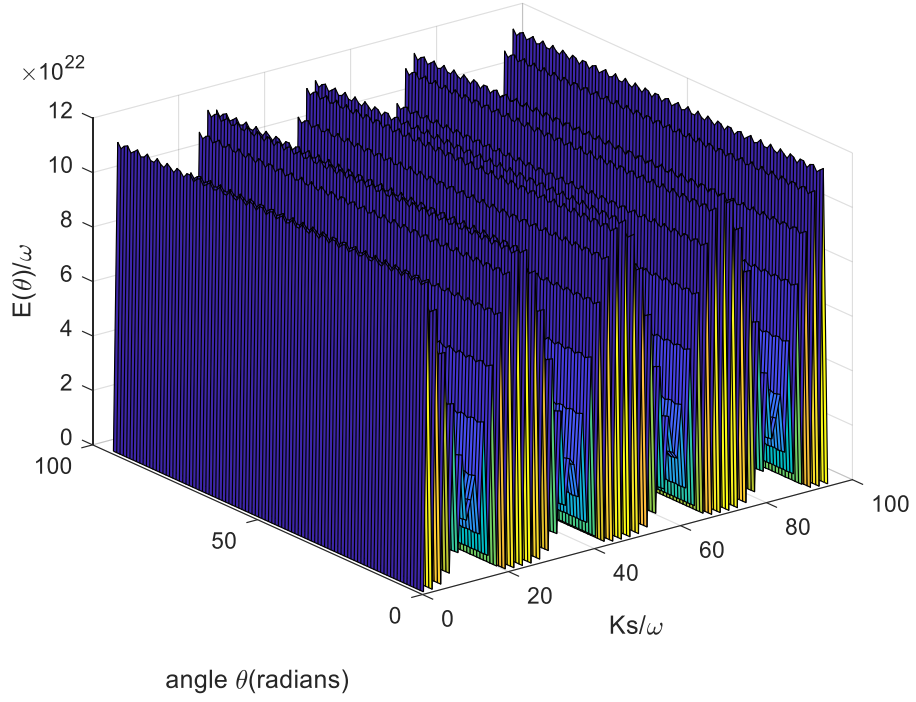


Figure 3: 3D plot of energy versus angle and stress induced anisotropy for $\frac{D_1^{(2)}}{\omega} = 10$, $\frac{D_2^{(2)}}{\omega} = 10$ and $\frac{D_3^{(2)}}{\omega} = 5$.

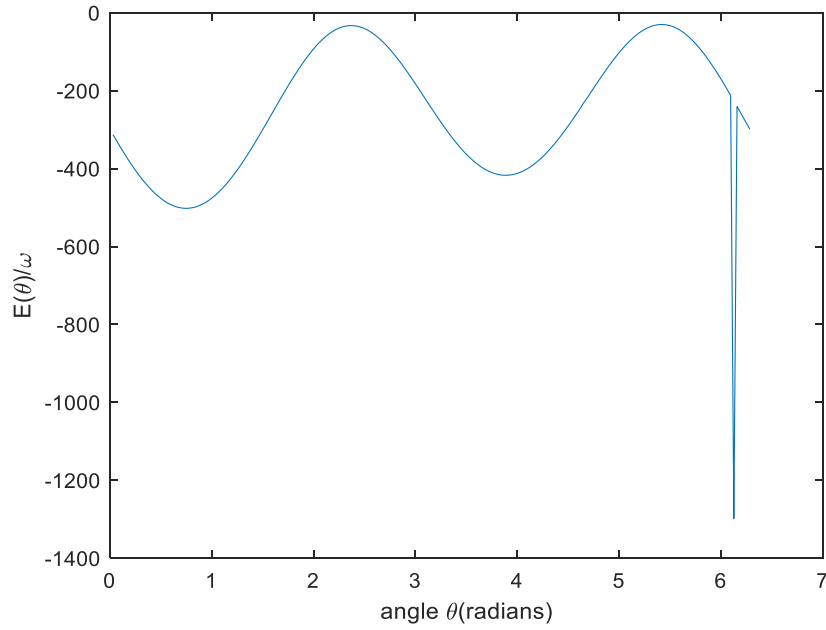


Figure 4: 2D graph of energy versus angle for $\frac{K_s}{\omega} = 71$.

4. CONCLUSION

All the graphs showing the total magnetic energy versus angle and the stress-induced anisotropy constant were plotted using the fourth-order perturbed Heisenberg Hamiltonian equation with all seven magnetic energy parameters for face centered cubic structured ferromagnetic thin films with three spin layers. The total magnetic energy of fcc structured ferromagnetic thin films with three spin layers was observed to be in the order of 10^6 to 10^{22} . This range is significantly higher compared to simple cubic structured ferromagnetic thin films with the same number of spin layers, where the total magnetic energy was obtained in the range of 10^{12} to 10^{17} . This indicates that the fcc structure exhibits higher energy values, suggesting potential differences in stability or magnetic behavior. When the second order anisotropy constant in the top spin layer is less than those of the bottom and middle spin layers, the total magnetic energy increases. This suggests that the distribution of anisotropy constants among the spin layers can have a significant impact on the overall magnetic properties of the thin film. The values of stress induced anisotropy at the maxima of the 3D plots are approximately the same when the values of the second order magnetic anisotropy constant of the middle and top spin layers are interchanged. The graphs of energy versus angle show that the magnetic easy directions are located at approximately 0.754 and 3.896 radians, with energy maximums at 2.356 and 5.404 radians. This suggests that the magnetic moments preferentially align along specific directions, which is important for understanding the magnetic behavior and stability of the thin film. The peaks along the axis of angle are closely packed in the fourth-order perturbed case compared to the second and third-order perturbed cases, indicating a more complex energy landscape with higher-order interactions. Additionally, the shape of the energy-angle graph is entirely different from the graphs obtained using lower order perturbed Heisenberg Hamiltonians, highlighting the importance of considering higher order interactions for an accurate description of the magnetic properties.

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