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UDC: Theoretical Condensed Matter Physics

DETERMINATION OF ENERGY OF THICK SPINEL FERRITE FILMS USING HEISENBERG HAMILTONIAN WITH SECOND ORDER PERTURBATION

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Abstract
The energy of thick spinel ferrite films have been calculated by means of classical Heisenberg Hamiltonian. In all cases, maximum energy in ferrite thick films is larger than that of ferromagnetic thick films with 2nd order perturbation. The energy required to rotate from easy direction to hard direction is very small near N=90. Also energy of ferrite thick films with 2nd order perturbation is lager than that of oriented ferrite films. The first energy maximum and minimum can be observed at θ=34.4^0 and 103.2^0, respectively. Especially the effect of stress induced anisotropy on energy was investigated, and the film can be easily oriented in some certain directions by applying certain stresses.

Keywords: *Heisenberg Hamiltonian, spins, ferrites.*

1. Introduction:

Thin and thick films of ferrites are potentially useful in microwave[1,2] and magnetic memory devices[3-6] because of their soft magnetic properties and higher resistivity. Because all the spinel ferrites are oxides, their resistivity is higher. As these spinel ferrites belong to soft magnetic materials, their coercivtiy and anisotropy are lower. Since easy axes of spinel ferrites direct along one of the cubic edges or the body diagonal of cubic cell, spinel ferrites are not magnetically uniaxial. The classical energy of oriented[7] and non-oriented thin spinel ferrites has been found earlier.

The cubic spinel cell was divided into eight spin layers, and a film with (001) cell orientation was considered for these simulations. All the energy terms such as spin exchange interaction, spin dipole interaction, magnetic field energy and stress induced anisotropy have been taken into account. The stress induced anisotropy is also considerable because of the soft magnetic properties of ferrites[8, 9]. The spin structure of cubic ferrites has been discussed widely in some previous reports[10-12]. The energy of ferrite thin films with few terms only has been found in some early reports[13-15]. Spinel ferrite unit formula can be given as AFe_2O_4, where A can be Ni, Zn or Fe.

2. Model:

The Heisenberg Hamiltonian of any thin film with some layers can be given as

$$H= - J\sum_{m,n}\vec{S}_m.\vec{S}_n + \omega\sum_{m\neq n}\left(\frac{\vec{S}_m.\vec{S}_n}{r_{mn}^{\ 3}} - \frac{3(\vec{S}_m.\vec{r}_{mn})(\vec{r}_{mn}.\vec{S}_n)}{r_{mn}^{\ 5}}\right) - \sum_m D_{\lambda_m}^{\ (2)}(S_m^{\ z})^2 - \sum_m D_{\lambda_m}^{\ (4)}(S_m^{\ z})^4$$
$$- \sum_m \vec{H}..\vec{S}_m - \sum_m K_s Sin2\theta_m \qquad \textbf{(1)}$$

Here J is spin exchange interaction, ω is the strength of long range dipole interaction, θ is azimuthal angle of spin , $D_m^{(2)}$ and $D_m^{(4)}$ are second and fourth order anisotropy constants, H_{in} and H_{out} are in plane and out of plane applied magnetic fields, K_s is stress induced anisotropy constant, n and m are spin plane indices and N is total number of layers in film. When the stress applies normal to the film plane, the angle between mth spin and the stress is θ_m.

The spinel cubic cell can be divided into 8 spin layers with alternative A and Fe spins layers [10]. The spins in one layer and adjacent layers point in one direction and opposite directions, respectively.

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The spins of A and Fe will be taken as 1 and p, respectively. A cubic unit cell with length a will be considered. Due to the super exchange interaction between spins, the spins are parallel or antiparallel to each other within the cell. Therefore the results proven for oriented case in one of our early report[7] will be used for following equations. But the angle θ will vary from θ_m to θ_{m+1} at the interface between two cells.

Following equations will be proven for a thin film with thickness Na.

Spin exchange interaction energy=$E_{exchange}$= $N(-10J+72Jp-22Jp^2)+8Jp\sum_{m=1}^{N-1}\cos(\theta_{m+1}-\theta_m)$

Dipole interaction energy=E_{dipole}

$$E_{dipole} = -48.415\omega\sum_{m=1}^{N}(1+3\cos 2\theta_m) + 20.41\omega p\sum_{m=1}^{N-1}[\cos(\theta_{m+1}-\theta_m)+3\cos(\theta_{m+1}+\theta_m)]$$

The first and second term in each above equation represent the variation of energy within the cell[7] and the interface of the cell, respectively.

Total energy

$$\begin{aligned} E= {} & N(-10J+72Jp-22Jp^2)+8Jp\sum_{m=1}^{N-1}\cos(\theta_{m+1}-\theta_m) \\ & -48.415\omega\sum_{m=1}^{N}(1+3\cos 2\theta_m) + 20.41\omega p\sum_{m=1}^{N-1}[\cos(\theta_{m+1}-\theta_m)+3\cos(\theta_{m+1}+\theta_m)] \\ & -\sum_{m=1}^{N}[D_m^{(2)}\cos^2\theta_m + D_m^{(4)}\cos^4\theta_m] \\ & -4(1-p)\sum_{m=1}^{N}[H_{in}\sin\theta_m + H_{out}\cos\theta_m + K_s\sin 2\theta_m] \end{aligned} \qquad \textbf{(2)}$$

The anisotropy energy term and the last term given in above equations have been explained in our previous report for oriented spinel ferrite[7]. The angle can be given as $\theta_m=\theta+\varepsilon_m$ with perturbation ε_m.

The total energy can be given as $E(\theta)=E_0+E(\varepsilon)+E(\varepsilon^2)$

Here the energy is given only up to the second order perturbation of ε. Here E_0, $E(\varepsilon)$ and $E(\varepsilon^2)$ are the terms independent of ε, terms with ε and terms with ε^2, respectively [18], after expanding sin and cosine terms.

$$\begin{aligned} E_0= {} & -10JN+72pNJ-22Jp^2N+8Jp(N-1)-48.415\omega N-145.245\omega N\cos(2\theta) \\ & +20.41\omega p[(N-1)+3(N-1)\cos(2\theta)] \\ & -\cos^2\theta\sum_{m=1}^{N}D_m^{(2)} - \cos^4\theta\sum_{m=1}^{N}D_m^{(4)} - 4(1-p)N(H_{in}\sin\theta + H_{out}\cos\theta + K_s\sin 2\theta) \end{aligned} \qquad \textbf{(3)}$$

After using constraint $\sum_{m=1}^{N}\varepsilon_m = 0$, first and last three terms of equation of E(ε) become zero. Here $\vec{\varepsilon}$ is a matrix with single column (or row) similar to an Eigen vector.

Then, $E(\varepsilon)=\vec{\alpha}.\vec{\varepsilon}$ **(4)**

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

$$B_\lambda(\theta) = -122.46\omega p + D_\lambda^{(2)} + 2D_\lambda^{(4)}\cos^2\theta$$

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

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where the elements of matrix C can be given as following,
$C_{m,\,m+1}$=8Jp+20.4ωp-61.2pωcos(2θ)
For m=1 and N,

C_{mm}= -8Jp-20.4ωp-61.2pωcos(2θ)+581ωcos(2θ) $-2(\sin^2\theta-\cos^2\theta)\ D_m^{(2)}$

$$+4\cos^2\theta(\cos^2\theta-3\sin^2\theta)\ D_m^{(4)}+4(1-p)[H_{in}\sin\theta+H_{out}\cos\theta+4K_s\sin(2\theta)] \quad \textbf{(5)}$$

For m=2, 3, ----, N-1

C_{mm}= -16Jp-40.8ωp-122.4pωcos(2θ)+581ωcos(2θ) $-2(\sin^2\theta-\cos^2\theta)\ D_m^{(2)}$

$$+4\cos^2\theta(\cos^2\theta-3\sin^2\theta)\ D_m^{(4)}+4(1-p)[H_{in}\sin\theta+H_{out}\cos\theta+4K_s\sin(2\theta)]$$

Otherwise, C_{mn}=0
Finally the total energy can be given as

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

Here C^+ is the pseudo-inverse given by

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

For a thick film with N=10000, the second term in equation number 7 can be neglected. Then C^+ is the normal inverse of matrix C.

3. Results and Discussion:

If anisotropy constants $D_m^{(2)}$ and $D_m^{(4)}$ do not vary within the film, then $C_{11}=C_{NN}$ and $C_{22}=C_{33}$= ------ $=C_{N-1,\,N-1.}$ When H_{in}, H_{out} and K_s are very large, $C_{22}>>C_{12}$.
If $C_{m,m+1}$ is zero, then the matrix C will be diagonal. Then the elements of inverse matrix (C^+) is given by $C^{+}{}_{mm}=\frac{1}{C_{mm}}$. To avoid tedious calculations, the solution will be found under assumption $C_{m,m+1}$=0.

Then $\alpha_1=----=\alpha_n=[-122.46\omega p+D_\lambda^{(2)}+2D_\lambda^{(4)}\cos^2\theta]\sin(2\theta)$

$$\alpha.C^{+}.\alpha=2C^{+}{}_{11}\alpha_1^{\ 2}++\alpha_1^{\ 2}(N-2)C^{+}{}_{22}=\frac{2\alpha_1^{\ 2}}{C_{11}}+\frac{\alpha_1^{\ 2}(N-2)}{C_{22}}$$

For Nickel ferrite with p=2.5,
E_0= 52.5JN-20J-48.415ωN-145.245ωNcos(2θ)+51.025ω(N-1)[1+3cos(2θ)]

$$-N[\cos^2\theta D_m^{(2)}+\cos^4\theta D_m^{(4)}-6(H_{in}\sin\theta+H_{out}\cos\theta+K_s\sin 2\theta)]$$

$C_{11}=C_{NN}$= -20J-51ω+428ωcos(2θ) $+2\cos 2\theta\ D_m^{(2)}+4\cos^2\theta(\cos^2\theta-3\sin^2\theta)\ D_m^{(4)}$

$$-6[H_{in}\sin\theta+H_{out}\cos\theta+4K_s\sin(2\theta)]$$

$C_{22}=C_{33}$=------=$C_{N-1,N-1}$= -40J-102ω+275ωcos(2θ) $+2(\cos 2\theta)\ D_m^{(2)}$

$$+4\cos^2\theta(\cos^2\theta-3\sin^2\theta)\ D_m^{(4)}-6[H_{in}\sin\theta+H_{out}\cos\theta+4K_s\sin(2\theta)]$$

$$\alpha_1=[-306.15\omega+D_\lambda^{(2)}+2D_\lambda^{(4)}\cos^2\theta]\sin(2\theta)$$

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When $\theta=0^0$ and $\theta=90^0$, $\alpha.C^{+}.\alpha$ is zero and, the second order perturbation is zero at in plane and perpendicular orientations. Then the total energy can be found using equation 6. Here θ is the angle between one particular spin and an imaginary line drawn perpendicular to the substrate. So when $\theta=0^0$, all the spins in the lattice are perpendicular to the plane of the substrate. When $\theta=90^0$, all the spins are parallel to the substrate.

When $\frac{J}{\omega}=\frac{D_m^{(2)}}{\omega}=\frac{H_{in}}{\omega}=\frac{H_{out}}{\omega}=\frac{K_s}{\omega}=10, and\ \frac{D_m^{(4)}}{\omega}=5$, the 3-D plot of $\frac{E(\theta)}{\omega}$ versus θ and N is given in figure 1. Near N=90, the energy required to rotate from easy direction to hard direction is very small according to graph implying that anisotropy energy is small at this N. Also this anisotropy energy gradually increases and decreases with N. Same kind of energy variation were observed for ferromagnetic thick films with second order perturbations[17]. But maximum energy in ferrite thick films is larger than that of ferromagnetic thick films with 2nd order perturbation. Also energy is lager than that of oriented ferrite films[7]. Although the equation is valid for large values of N only, the graph has been drawn for even small values of N too in order to study the variation of energy at small values of N too.

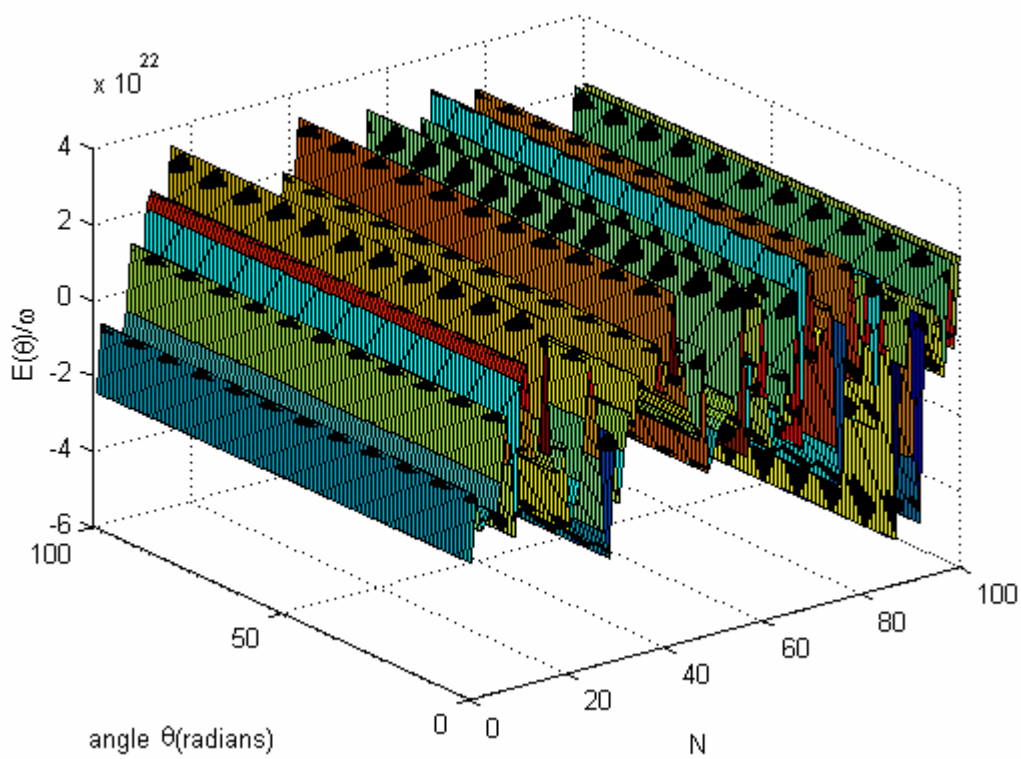

Figure 1: 3-D plot of $\frac{E(\theta)}{\omega}$ versus θ and N for Nickel ferrite

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When N=10000, the graph between $\frac{E(\theta)}{\omega}$ and θ is given in figure 2. The energy required to rotate from easy to hard direction vary with the angle. The first energy maximum and minimum can be observed at $\theta=34.4^0$ and 103.2^0, respectively. The angle between easy and hard directions is not 90^0. Maximum energy in this case is larger compared with that of ferromagnetic thick films with 2nd order perturbation.

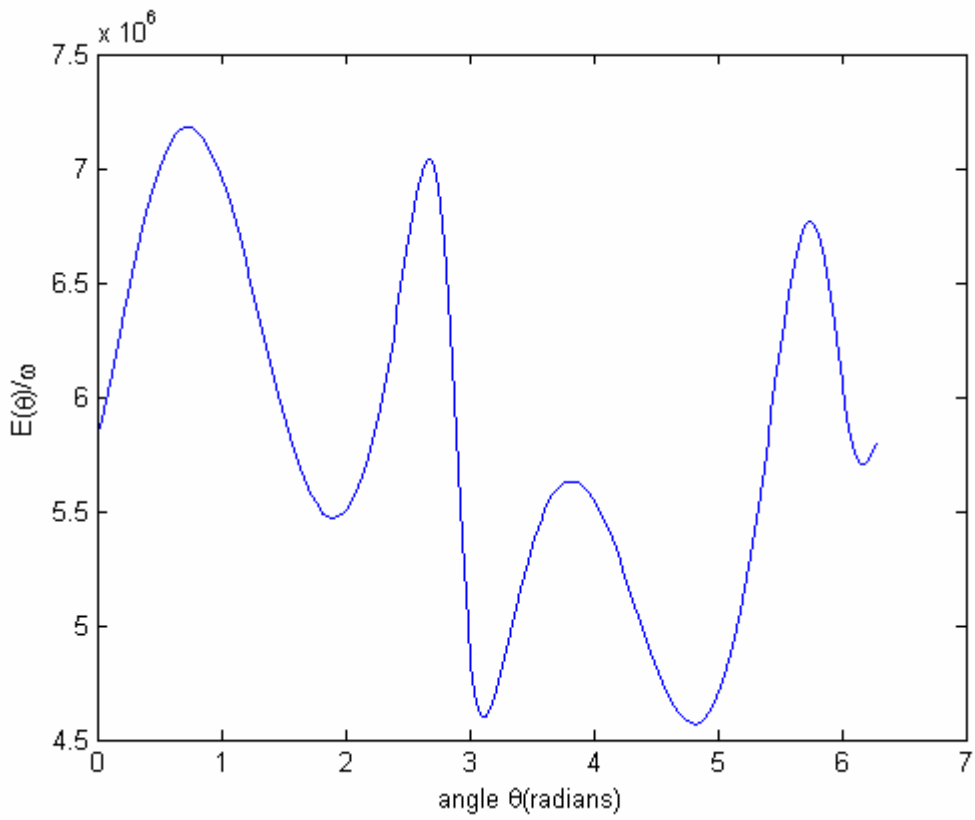

Figure 2: Graph between $\frac{E(\theta)}{\omega}$ and θ for N=10000

When N=10000 and $\frac{K_s}{\omega}$ is a variable, the 3-D plot of $\frac{E(\theta)}{\omega}$ versus θ and $\frac{K_s}{\omega}$ is given in figure 3. The energy is minimized at some angles for certain values of stress induced anisotropy indicating that the film can be easily oriented in that direction by applying this stress. The maximum energy is larger than that of thin ferrites with second order perturbation [16]. Energy is larger than that of oriented ferrite films[7].

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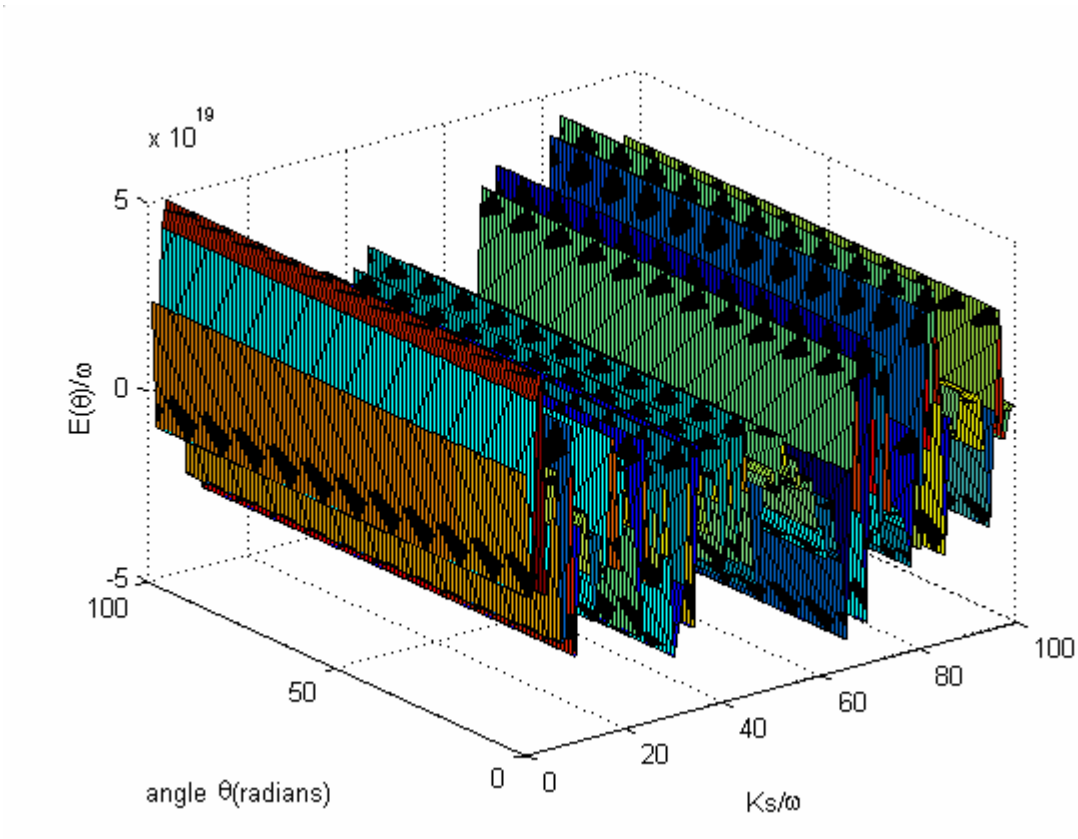

Figure 3: 3-D plot of $\frac{E(\theta)}{\omega}$ versus θ and $\frac{K_s}{\omega}$ for N=10000

4. Conclusion:

The maximum energy of ferrite thick films are larger compared with that of ferromagnetic thick films with 2nd order perturbation. The energy required to rotate from easy direction to hard direction is very small for thicknesses corresponding to N=90. Also energy of ferrite thick films with 2nd order perturbation is lager than that of oriented ferrite films. Two of consecutive energy maximum and minimum can be observed at $\theta=34.4^0$ and 103.2^0, respectively. The film can be easily oriented in some certain directions by applying certain stresses. Although this simulation was performed for $\frac{J}{\omega}=\frac{D_m^{(2)}}{\omega}=\frac{H_{in}}{\omega}=\frac{H_{out}}{\omega}=\frac{K_s}{\omega}=10, and \frac{D_m^{(4)}}{\omega}=5$ only, this simulation can be carried out for any other values of $\frac{J}{\omega},\frac{D_m^{(2)}}{\omega},\frac{H_{in}}{\omega},\frac{H_{out}}{\omega},\frac{K_s}{\omega}, and \frac{D_m^{(4)}}{\omega}$ as well as for other spinel ferrites.

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