Investigation of magnetic properties of thin films using computer simulation

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Abstract. A two-dimensional dendrite is generated within the diffusion limited aggregation (DLA) model in the presence of an external magnetic field. The magnetic interaction between a grown dendrite and diffusing atoms results in the elongation of the dendrite in the direction of the magnetic field. The dependence is studied of the dendrite elongation on the grid occupation. The energy of the magnetic anisotropy is calculated for an elongated dendrite. The FMR spectra are calculated in geometries when the static magnetic field is either perpendicular or parallel to dendrite plane. It is shown that the FMR signals in latter case depend on the static magnetic field orientation with respect to the elongation direction.

1. Introduction
The fabrication of thin magnetic film with pronounced in-plane magnetic anisotropy on the surface of a semiconductor is a current problem in spintronic technologies [1]. Such a film is considered to serve as an injector of spin polarized electrons into the semiconductor. One method to solve this problem is the deposition of films of ferromagnetic metals or their compounds on a semiconductor. There have been many investigations performed to obtain in-plane magnetic anisotropy in thin metal films by ion beam methods (see for example [2–4]). However, the efficiency of spin injection from metal into semiconductor is drastically reduced due to the large difference between their conductivities [5,6]. It is suggested that the problem can be solved by using a ferromagnetic semiconductor as an injector. In silicon spintronics, the ferromagnetic silicide Fe₃Si is promising in this respect [7]. Recently, thin films of magnetic iron silicide Fe₃Si with uniaxial anisotropy were synthesized by high-dose Fe⁺ ion implantation (ion-beam synthesis) into silicon in an external magnetic field [8]. In that work it was suggested that the magnetic anisotropy of the films synthesized is determined by the shape anisotropy of ferromagnetic silicide dendrites created due to the anisotropy of diffusion of implanted atoms. During ion implantation, clusters of a new phase are synthesized within a thin layer near the target surface. Due to radiation damages, the in-plane diffusion of implants in the layer is more intensive than that out of the plane. In a model approximation, ion implantation can be considered as a two-dimensional DLA problem. In [9], a modified multicenter DLA model was developed to take into account the magnetic dipole-dipole interaction between diffusing atoms and created dendrites. The importance of such interactions were emphasized in investigations of DLA problems [10,11], the diffusion limited deposition processes [12], and the transformation of the shape of magnetic precipitate.

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during Ostwald ripening processes [13]. It was shown that this interaction results in the elongation of grown clusters in the direction of the external magnetic field. In the present work, the magnetic anisotropy and the ferromagnetic resonance (FMR) of a model system - a single elongated 2D-dendrite - were numerically investigated.

2. DLA model in the case of ion-beam synthesis

The formation of a new phase during ion-beam synthesis is considered as a two dimensional DLA problem. The computer model is based on a kinetic Monte Carlo simulation on a square lattice. The simulation is performed at a square 400×400 grid. The implanted atom is simulated as a particle generated at some random site of the grid. Then it undergoes random walking until it attaches to the growing dendrite. If the generated particle walks out of the grid, it is discarded and a new particle is introduced into a random point of the grid, etc. The motion of i-th adatom is governed by the probability of a jump between adjacent sites of the grid. To jump from point (x_i; y_i) to point (x_i+1; y_i) the random walking i-th adatom must overcome the energy barrier \( \Delta E_B(x_i, y_i | x_i + 1, y_i) \), whose maximum is located at point \( (x_i + \lambda; y_i) \), where \( 0 \leq \lambda \leq 1 \). Here \( x_i \) and \( y_i \) are dimensionless coordinates in unit of grid spacing \( a \). The probability of the jump is:

\[
P(x_i, y_i | x_i \pm 1, y_i) = \frac{\exp\left\{- \frac{\Delta E_B(x_i, y_i | x_i \pm 1, y_i)}{k_B T}\right\}}{W(x_i, y_i)},
\]

\[
W(x_i, y_i) = \exp\left\{- \frac{\Delta E_B(x_i, y_i | x_i + 1, y_i)}{k_B T}\right\} + \exp\left\{- \frac{\Delta E_B(x_i, y_i | x_i, y_i - 1)}{k_B T}\right\} + \exp\left\{- \frac{\Delta E_B(x_i, y_i | x_i - 1, y_i)}{k_B T}\right\} + \exp\left\{- \frac{\Delta E_B(x_i, y_i | x_i, y_i + 1)}{k_B T}\right\},
\]

where \( W(x_i; y_i) \) is a normalizing coefficient, \( T \) is the temperature, and \( k_B \) the Boltzman constant. Usually, in two-dimensional DLA models statistically isotropic random walking is assumed, that is the energy barriers around point \( (x_i; y_i) \) are supposed to be equal, or \( \Delta E_B(x_i, y_i | x_i \pm 1, y_i \pm 1) = \Delta E_B^0(x_i; y_i) \), providing probability \( P_0(x_i; y_i) = 1/4 \) for all four available jump directions in a square grid.

In the case of Fe ion implantation, the growing silicide aggregate is assumed to be ferromagnetic (in the experiments reported in [8], the presence of a ferromagnetic phase in implanted layer was confirmed by Mossbauer measurements). The interaction of the adatom’s magnetic moment with the magnetic field \( \vec{B}_{dd} \) created by the ferromagnetic dendrite changes the energy barrier:

\[
\Delta E_B(x_i, y_i | x_i \pm 1, y_i) = \Delta E_B^0(x_i, y_i) \pm \frac{\partial E_{dd}}{\partial x},
\]

where

\[
E_{dd} = -\vec{\mu}_i \cdot \vec{B}_{dd} = \vec{\mu}_i \cdot \frac{\mu_0}{4\pi a^3} \sum_k \left( \vec{\mu}_k \cdot \frac{3r_{ik}^2 (\vec{r}_{ik} \times \vec{r}_{jk})}{r_{jk}^5} \right)
\]

is the energy of dipole-dipole interaction between magnetic moment \( \vec{\mu}_i \) of i-th adatom and the moment of k-th dendrite atom.

If the model of isotropic random walking without magnetic interaction is taken into account, then the jump probability (1) becomes:
The DLA model described is used below to generate ferromagnetic dendrites on a two dimensional square grid.

3. Results

3.1 Dendrite simulation

The examples of simulated isolated dendrites created after the addition of 20000 particles on the 400x400 grid in the presence of an external magnetic field $\mathbf{B}_e$ and without it are presented in figure 1 and figure 2, correspondingly. The simulation assumes that field $\mathbf{B}_e$ is sufficient to saturate the ferromagnetic dendrite magnetization. The magnetic moments of both the moving adatom and the dendrite are supposed to be parallel to $\mathbf{B}_e$. It is evident that the dendrite created in a magnetic field is elongated by $\varepsilon = \langle R_x \rangle / \langle R_y \rangle$, where $\langle R_x \rangle$ and $\langle R_y \rangle$ are the average sizes of the dendrite along the external field direction (OX axis) and in the perpendicular one (OY axis). The $\langle R_x \rangle$ and $\langle R_y \rangle$ were calculated relatively to the center of mass of the dendrite. The elongation $\varepsilon$ as function of the grid occupation is presented in figure 3. The function exhibits a maximum and then decreases. Such a dependence is due to boundary effects.

$$P(x_i, y_i | x_i + 1, y_i) = \exp \left( -\frac{\partial E_{dd}(x_i, y_i)}{\partial x} \frac{1}{2k_B T} \right) \right) \right) / \left( \frac{\partial E_{dd}(x_i, y_i)}{\partial y} \frac{1}{2k_B T} \right)$$

(3)

The DLA model described is used below to generate ferromagnetic dendrites on a two dimensional square grid.

3.2 In-plane magnetic anisotropy

The ferromagnetic dendrite elongation results in a magnetic in-plane anisotropy. The energy of the anisotropy $E_{anis}$ can be numerically calculated as the sum of the dipole-dipole energies of all atoms of the dendrite. This energy depends on the angle $\varphi$ between the direction of elongation (OX axis) and the magnetic moments of the dendrite atoms. An example of the dependence is presented in figure 4. The elongation for the given dendrite is $\varepsilon = 1.55$. Other dendrites within this simulation have elongations in the range [1.4 - 1.65] and exhibit an angular dependence of $E_{anis}$ similar to that in figure 4:

$$E = K \cdot \sin^2 \varphi + \text{const},$$

(4)
where $K$ is the anisotropy constant $K = \alpha \frac{\mu_0 h^2}{4\pi a^3} \rho_{Fe}$. The coefficient $\alpha$ strongly depends on the dendrite elongation and for the given dendrite $(\varepsilon = 1.55)$ is equal to 1.4, $\rho_{Fe}$ is the density of Fe atoms in the dendrite. If $\rho_{Fe}$ corresponds to the silicide Fe$_3$Si then $K$ is in the order of $10^2 - 10^3 J/m^3$.

![Figure 3. Relative elongation $\varepsilon$ versus grid occupation.](image)

![Figure 4. The dependence of $E_{\text{anis}}$ on angle $\varphi$ between dendrite magnetization and X axis.](image)

3.3. Ferromagnetic resonance (FMR)

The FMR signal $P(H_0)$ is calculated as the sum of the resonance absorption $P_i(H_0)$ of $i$-th magnetic moment $\mu_i$ involved in the dendrite.

$$P(H_0) = \frac{1}{N} \sum_{i} P_i(H_0)$$ (5)

According to Kittel theory resonance absorption function $P_i(H_0)$ is obtained from the solution of Bloch equation for magnetic moment $\mu_i$ [14]. The magnetic moment $\mu_i$ experiences the static magnetic field $H_0$, microwave magnetic field $\vec{h}_i$ and dipole magnetic field $H_d$ created by all other magnetic moments of the dendrite.

Below two geometries of the magnetic fields arrangement are considered: case A (figure 5) and case B (figure 6). In both cases resonance absorption function $P_i(H_0)$ is described by formula:

$$P_i(H_0) = \frac{2\pi \omega_0 \omega h^2 \gamma (\cos^2(\varphi) + \sin^2(\varphi) \cos^2(\theta))}{T\left[\omega^2 - \omega_0^2 + \frac{1}{T^2}\right]^2 + \frac{4\omega_0^2}{T^2}};$$ (6)

$$\omega_{0i} = \gamma \sqrt{(H_0 + H_d)^2 + H_{d,\perp}^2},$$ (7)

where $\vec{h}_i$ and $\omega$ are the amplitude and frequency of microwave field, $T$ is the relaxation time. The fields $H_{d,\parallel}$, $H_{d,\perp}$ and the angles $\varphi$ and $\theta$ are shown in the figures below.

Case A: $H_0$ is perpendicular to the dendrite plane (OZ axis), the microwave field $\vec{h}_i$ lies in the dendrite plane (parallel to the OX axis).
The components of the dipole field $H_d$ strongly depend on the $H_0$ value. Without external magnetic field, the dipole field $H_d$ lies in the plane of the dendrite, or it has only x- and y-components. When $H_0$ increases, the magnetic moments rotate out of the plane and have an angle $\theta$ with respect to $H_0$. Consequently, in (7) the components of the dipole field are $H_{d\parallel} = H_{\text{ax}}(0)$, $H_{d\perp} = \sqrt{H_{d\text{ax}}^2 + H_{d\text{ay}}^2}$. At the critical value $H_0 = H_r$ all magnetic moments become perpendicular to the dendrite plane ($\theta = 0$) and $H_d$ has only a z-component, or $H_{d\parallel} = H_{\text{ax}}(0)$, $H_{d\perp} = 0$. The value of $H_r$ is determined by grid spacing $a$ and dendrite size:

$$H_r = \frac{\frac{3}{8} a^3 \sum_{i=0}^{N-1} \sum_{j=0}^{N-1} \left( r_{ij}^3 \right)^2}{8 \pi a^3 N}$$

where $N$ is the number of particles within the dendrite. The results of the computer calculation of the resonance absorption $P(H_0)$ in this case are presented in figure 7 as a function of the grid occupation.

**Figure 7.** The FMR signal in A geometry at different degree of grid occupation 10, 30, 50 and 100 %.

**Figure 8.** The FMR signal in B geometry at different degree of grid occupation 10, 30, 50 and 100 %.

Case B: $H_0$ lies in the dendrite plane, the microwave field $\vec{h}$ is perpendicular to the dendrite plane (|| OZ axis). If $H_0$ is perpendicular to the OX axis (the direction of elongation of the dendrite), the...
absorption signal is described by formula (6) with \( \cos(\theta) = 0 \) and 
\[ \omega_0 = \gamma \sqrt{\left( H_0 + H_{\text{dist}} \right)^2 + H_{\text{dist}}^2}. \]

The absorption signals are presented in figure 8.

If \( H_0 \) is parallel to the OX axis, then for grid occupation greater than 10% one has similar absorption spectra, but for low grid occupation (\( \leq 5\% \)) the absorptions for the case \( H_0 \parallel OX \) axis and \( H_0 \perp OX \) axis are substantially different, as presented in figure 9.

4. Discussion

The resonance absorption spectra presented in figure 7 and figure 8 reveal the main feature of the FMR - strong dependence of the position of the resonance absorption line on the sample shape due to the influence of a demagnetization field. In ferromagnetic spherical samples, resonance absorption occurs at \( H_{\text{res}} = H_{0\text{res}} \) (\( H_{0\text{res}} = 3300 \) Oe at \( \nu = 9.33 \) GHz). For thin continuous ferromagnetic films when a static magnetic field \( H_0 \) is perpendicular to the film plane, the resonance signal is shifted to \( H_{\text{res}} = H_{0\text{res}} + 4\pi M \), where \( M \) is the ferromagnet magnetization (so called “high field” signal) [14]. When \( H_0 \) lies in the film plane, the resonance takes place at \( H_{\text{res}} \) lower than \( H_{0\text{res}} \). It was shown in [15] that a similar orientational dependence of the resonance signal is pertains to a thin granular film consisting of spherical particles. The resonance spectra of the isolated dendrites simulated in the present work also exhibit a shift of the resonance line position at different orientation of \( H_0 \) with respect to the dendrite plane. The case of 100% grid occupation is well described by Kittel formulas and corresponds to a continuous ferromagnetic film. When occupation is lower than 50%, one has low density clusters and the resonance signals become broader and assymetric. In this case the simple Kittel formulae for resonance absorption cannot be used and only numerical calculation of the absorption signal is possible. For a very low degree of grid occupation (less then 5%) a noticeable dependence of the absorption line on the static magnetic field orientation relatively to the direction of dendrite elongation is seen. Dendrites with the highest degree of elongation are typical for such a low grid occupation (see figure 3). If \( H_0 \) is perpendicular to the long dendrite axis, satellite signals on the high field side are observed in addition to the main absorption signal at \( H_0 = 3300 \) Oe. If \( H_0 \) is parallel to the long dendrite axis, then the additional signals appear on the low field side. Therefore, monitoring the FMR absorption can be used as a method for studying the induced uniaxial anisotropy of a film consisting of dendrites grown in the presence of an external magnetic field. When the grid occupation increases, the dendrite elongation decreases, which is connected with the boundary conditions. The dendrite becomes much more “symmetric”. In the case of an isolated dendrite, the boundary conditions are determined by the grid edges. For multicenter DLA problems, the reduction in the dendrite elongation is caused by the influence of other dendrites.

Conclusions

Two-dimensional isolated dendrites are generated within the DLA model in the presence of an external magnetic field. It is shown that the magnetic interaction between the grown dendrite and a diffusing atom leads to elongation of the dendrite in the direction of the magnetic field. The dependence is demonstrated of the dendrite elongation on the grid occupation. The energy of the in-plane magnetic anisotropy is numerically estimated for an elongated dendrite. The FMR spectra are calculated for the cases when the static magnetic field is perpendicular or parallel to dendrite plane. It is shown that the
FMR signals in the latter case depend on the static magnetic field orientation with respect to the direction of dendrite elongation.

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