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Microstructure of $L1_0$ FePt thin films with anisotropic interfacial energy coefficients and anisotropic atomic mobilities

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ABSTRACT

The microstructure evolutions of FePt-X (segregant) thin films were studied by employing a three-dimensional phase field model. Simulated results show that in the absence of substrate constraint related with elastic energy, the morphology of the FePt-X thin films significantly depends on the film thickness, anisotropic interfacial energy coefficients, and anisotropic atomic mobility. Small in-plane anisotropic interfacial energy coefficients or out-of-plane anisotropic mobility of atom diffusion are beneficial to induce columnar shape FePt grains, using any one of parameters of which can make the FePt grains keep columnar shape when FePt-X thin films thickness is 10 nm. Using segregant with both proper in-plane anisotropic interfacial energy coefficients and out-of-plane anisotropic mobility can make the FePt grains keep columnar shape when the FePt-X thin films thickness reaches to at least 15 nm.

1. Introduction

$L1_0$ FePt thin film, as a candidate for the potential Heat Assisted Magnetic Recording (HAMR) media due to its large magnetic anisotropy ($K_u \approx 7 \times 10^7$ erg/cc), has being extensively studied in many research groups [1–3]. The HAMR media demands that the $L1_0$ FePt thin films must have small grain size, columnar FePt grains, and high coercivity. Especially, the aspect ratio of each columnar FePt grain should be large enough so as to keep the thermal stability of the magnetic moment in the FePt-X thin films [4,5]. Recently, the microstructures of FePt were extensively studied in experiments for preparing the columnar FePt grains by changing various fabrication conditions, e.g., temperature, deposition pressure, the choice of segregants, segregant volume fractions, and thickness of the thin film [6–8]. In order to study the formation mechanisms of microstructure in FePt-X thin films, the phase field model was used to simulate the morphology of FePt-X thin films [9,10]. The simulated results show that the morphology of the FePt-X thin films significantly depends on the interfacial energy, film thickness, and anisotropic atomic mobility. And low interfacial energy can induce small FePt grains, while the high interfacial energy can form big FePt grains when the films thickness is fixed. It also shows that the formation of columnar or the bilayer microstructure of FePt highly depends on the film thickness [10]. However, there are still many challenges lie ahead to fabricate the desired well-separated slim and tall FePt grains from laboratory, the underlying physical mechanisms are still very deficient at present on how to improve the microstructure of the FePt-X thin films media for HAMR [11]. Accordingly, it is extremely essential to investigate the mechanisms about how to form the columnar FePt grains for future HAMR media through theoretical simulation, and thus to guide the experiments. In this work, based on our previous study about the microstructure of FePt-X thin films [10], the influence of film thickness, anisotropic interfacial energy coefficients and anisotropic atomic mobility to morphology of $L1_0$ FePt-X thin films were studied in detail by using the three-dimensional phase

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field model.

2. Phase field method

Phase field method is a powerful tool to simulate the microstructure evolution in various materials [12–15]. In this work, a conserved field composition $c(\boldsymbol{r},t)$ and a nonconserved field order degree $s(\boldsymbol{r},t)$ are chosen as the phase field variables to describe the microstructure change of the FePt-X thin films. $c(\boldsymbol{r},t)$ describes the concentration of FePt. Thus, the concentration of amorphous segregant is 1-$c(\boldsymbol{r},t)$ based on the mass conservation. $s(\boldsymbol{r},t)$ describes the ordered FePt with s = 1 and the disordered FePt with s = 0. The spatial and temporal evolutions of composition and order degree are controlled by the conserved field equation (Cahn–Hilliard equation (1)) and nonconserved field equation (Allen–Cahn equation (2)), respectively as

$$\frac{\partial c\left(\vec{r},t\right)}{\partial t} = M\nabla^2\frac{\delta F}{\delta c\left(\vec{r},t\right)} \tag{1}$$

$$\frac{\partial s\left(\vec{r},t\right)}{\partial t} = -L\frac{\delta F}{\delta s\left(\vec{r},t\right)} \tag{2}$$

where, F is the total free energy of the FePt-X thin films, which is constructed as

$$F = \int\left[f_{chem} + f_{grad} + f_{elas}\right]dV \tag{3}$$

M is the atomic mobility determined by both diffusivities of FePt and segregant, L is the kinetic coefficient related to ordering, V is the system volume of the FePt-X thin films, f_{chem} denotes the chemical free energy density. The expression of f_{chem} can be found in Ref. [9]. f_{grad} is the gradient energy density calculated by $f_{grad} = \kappa_c(\nabla c_{FePt})^2 + \kappa_s|\nabla s|^2$, where κ_c and κ_s are gradient energy coefficients of composition field $c(\boldsymbol{r},t)$ and order degree field $s(\boldsymbol{r},t)$, respectively. f_{elas} is the elastic energy density, which is not considered in the current simulations. M and κ_c are usually assumed that only the diagonal values are non-zero for the tensor matrix. They have the following matrix form for isotropic and anisotropic materials, respectively [16–18],

$$M_{iso} = \begin{pmatrix} M_{11} & 0 & 0 \\ 0 & M_{11} & 0 \\ 0 & 0 & M_{11} \end{pmatrix} \quad M_{anis} = \begin{pmatrix} M_{11} & 0 & 0 \\ 0 & M_{11} & 0 \\ 0 & 0 & M_{33} \end{pmatrix}$$

$$\kappa_{iso} = \begin{pmatrix} \kappa_{11} & 0 & 0 \\ 0 & \kappa_{11} & 0 \\ 0 & 0 & \kappa_{11} \end{pmatrix} \quad \kappa_{anis} = \begin{pmatrix} \kappa_{11} & 0 & 0 \\ 0 & \kappa_{11} & 0 \\ 0 & 0 & \kappa_{33} \end{pmatrix}$$

In this simulation, the real interfacial energy coefficients are κ_c timing κ_{iso} or κ_{anis}.

The coupled equations (1) and (2) were numerically solved by using the finite different method under the periodic boundary conditions. The 128 × 128 discrete grid points were used in the x and y directions, which correspond to real size 50 × 50 nm^2, and the grid points in z direction vary by choosing different FePt-X thin films thicknesses. The grid spacing in real space is about 0.39 nm. The time step for integration is 10^{-4}. The evolution time of system is 100,000 steps. The initial structure of FePt-X thin films with a small conserved composition fluctuation and a small order degree fluctuation are set by using a computer generated random number. The used calculating parameters are: ordering temperature is 973 K, the atomic ratio is $Fe_{55}Pt_{45}$, the interfacial energy γ_s between FePt and segregant X is 1.82 J/m^2 for isotropic case, the composition of FePt is set as 0.4 according to the TEM image in the experimental work [1]. Then, the influences of the film thickness, anisotropic interfacial energy coefficients, and anisotropic atomic mobility on the microstructure of the FePt-X thin films in three-dimensions have been studied.

3. Results and discussion

The anisotropic interfacial energy plays an important role in determining the microstructure of material [19, 20]. And there are few related reports in study of FePt-X thin films. To this end, we first studied the effect of anisotropic interfacial energy on the structure feature of FePt-X thin films. Fig. 1 shows the microstructure of the FePt-X thin films with different values of anisotropic interfacial energy. The film thickness keeps the same as 10 nm for all simulations. The dimensionless atom mobilities in the x, y, and z directions are set as $M_x = M_y = M_z = 1.0$, and the dimensionless interfacial energy coefficient κ_z is set as 1.0. The interfacial energy coefficients $\kappa_x = \kappa_y$ in the x and y directions decrease from 1.0 to 0.2 for four simulation cases. The amorphous segregant, the ordered FePt, and the disordered FePt are represented by a blue, yellow, and red color in the figures, respectively. Fig. 1(a) shows the bilayer microstructure due to the thicker FePt-X thin films and isotropic M and κ, and it also shows the large FePt grains size in the FePt-X thin films. The number of isolated FePt grains is relatively small when κ is isotropic. When $\kappa_x = \kappa_y$ decreases to 0.6, the FePt grains size decreases and more FePt grains become isolated, and the columnar FePt grains appears as shown in Fig. 1(b). The increase of the columnar FePt grains is more obvious when $\kappa_x = \kappa_y$ decreases to 0.4 as shown in Fig. 1(c). And when $\kappa_x = \kappa_y$ decreases to 0.2, the FePt grains almost completely become columnar shape and smaller further. This is because the evolution of the system tends to decrease the interfacial energy, thus less interfaces is favorable in order to decrease the system energy, which means that the smaller interfacial energy will give more interfaces. This is also consistent with our previous study that the small interfacial energy between FePt and X can result in small FePt grains [10].

Fig. 2 shows the variations of microstructure of the FePt-X thin films with different film thicknesses, where $M_x = M_y = M_z = 1.0$, $\kappa_x = \kappa_y = 0.2$, and $\kappa_z = 1.0$. The film thickness varies from 8 to 15 nm.

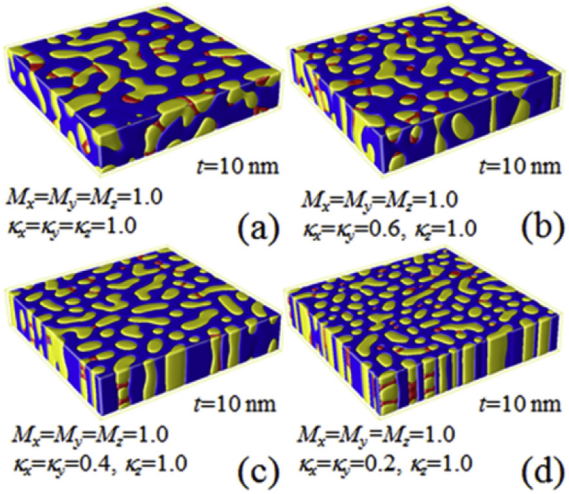

Fig. 1. The microstructures of the FePt-X thin films when the film thickness is 10 nm and with $M_x = M_y = M_z = 1.0$, $\kappa_z = 1.0$, and $\kappa_x = \kappa_y$ are set as: (a) 1.0; (b) 0.6; (c) 0.4; (d) 0.2.