Phase-field study of microstructure formation of FePt-C nanogranular film for heat-assisted magnetic recording media

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Heat-Assisted Magnetic Recording (HAMR) utilizing FePt nanogranular films holds promise for high-density data storage. Achieving target densities requires precise control of film microstructure – small, high-aspect-ratio, and uniform grains. This study employs a phase-field (PF) method to model FePt-C film evolution during sputtering. The model, validated against experimental TEM data, accurately reproduces observed island-like structures. Crucially, simulations demonstrate that elastic strain relaxation, stemming from lattice mismatch with the MgO substrate, drives island formation. This insight provides a foundation for optimizing HAMR film deposition processes and material selection.

Film deposition, Heat-assisted magnetic recording media, Microstructure, Phase-field simulation

I. Introduction

The escalating demands of the digital age are driving unprecedented growth in demand for capacity and power consumption of data center [1]-[2]. Since improving recording density of Hard Disk Drives (HDD) can be a solution for both problems, active research is underway. Heat-Assisted Magnetic Recording (HAMR), utilizing $L1_0$-ordered FePt as a magnetic medium, is a one of the candidates for the solution of these problems, offering potential for high recording density and improved power efficiency per capacity [2]. Currently, development is progressing toward a recording density of 4TB/in^2. Achieving a target density of 4 TB/in^2 requires FePt-X nanogranular films to meet multiple conditions: small grain size (<4.3 nm), high aspect ratio (>1.6), and good size uniformity (<10-15%) [2]. Current research focuses on optimizing sputtering processes and exploring novel materials for substrates and segregants to achieve these microstructural requirements. For the efficient process optimization and material exploration, it is necessary to have a precise understanding of the mechanisms of microstructural formation. While experimental investigations have yielded significant insights into the underlying mechanisms for the microstructural formation, some limitations still remain. For example, the difficulty in *in situ* observation of microstructural evolution hinders the ability of keeping track of the shape change of individual FePt grains. The impossibility of independent control of physical property of substrate/segregant makes the elucidation of the influence of each property on microstructural formation difficult. To overcome these challenges, this study employs a phase-field (PF) method [3] to model the temporal evolution of FePt-C nanogranular films during deposition. This approach allows for investigation of the interplay between material properties, deposition parameters, and resulting microstructures. The model is validated against experimental data and subsequently utilized to elucidate the key mechanisms controlling the formation of island-like FePt grains.

II. Method

This study utilizes a PF method to simulate microstructure evolution of FePt-C nanogranular film during sputtering process. The model tracks the evolution of local volume fractions (f_p) for each phase – vacuum, $L1_0$-FePt, C, and MgO – governed by following time-dependent equation incorporating diffusion and sputtering-driven atomic supply.

$$\frac{\partial f_p}{\partial t} = \nabla \cdot \left(\sum_{q=1}^{4} M_{pq} \nabla \left(\frac{\delta G_{\mathrm{sys}}}{\delta f_q} \right) \right) + B s_p \frac{\partial f_1}{\partial z} \tag{1}$$

Here, M_{pq} is the diffusion mobility, G_{sys} is the Gibbs energy of the system, B denotes the sputtering rate, and s_p is the sputtering concentration of phase p. The total Gibbs energy of the system (G_{sys}) comprises chemical, gradient, and elastic energy ($G_{\mathrm{sys}}=G_{\mathrm{chem}}+G_{\mathrm{grad}}+G_{\mathrm{elas}}$), formulated to accurately represent surface, interfacial and elastic strain energies. The elastic strain energy is calculated using phase-field micro-elasticity theory:

$$E_{\mathrm{str}} = \frac{1}{2} \int_{\mathbf{r}} C_{ijkl} (\varepsilon_{ij} - \varepsilon_{ij}^0)(\varepsilon_{kl} - \varepsilon_{kl}^0) d\mathbf{r} \tag{2}$$

Here, C_{ijkl} is the elastic constant, ε is the total strain, and ε_0 is the eigenstrain. Crucially, the model incorporates elastic strain energy calculated via a micro-mechanics approach, accounting for lattice mismatch between FePt and the MgO substrate through the inclusion of eigenstrain. Model parameters are sourced from existing literature where available, while those lacking published values were carefully calibrated to reproduce experimentally observed microstructural features. This integrated approach allows for a detailed investigation of the interplay between thermodynamic driving forces, kinetic limitations, and resulting nanogranular morphologies during film deposition.

III. Results and Discussion

A. Comparison with experimental observation

Figure 1 presents a comparison of simulated microstructures (Fig. 1a-c) and a TEM micrograph (Fig. 1d) of a 4.5 nm thick FePt-35 vol.% C film. For the simulated results, a 3D view (Fig. 1a), a cross-section along the (010) plane (Fig. 1b), and a projection along the [001] direction (Fig. 1c) are shown. In both experimental and computational results, well-separated island-like structure of FePt grains are formed. In addition, many FePt grains have rounded square shapes, and some have irregular shapes due to the coalescence of multiple FePt grains. Notably, the simulated microstructure exhibits in-plane anisotropy, with the FePt grains arranged along the [100] or [010] directions. Previous studies have demonstrated that the in-plane anisotropy of thin film microstructures is influenced by elastic anisotropy and surface energy anisotropy [4]-[5]. Given that the PF model employed in this study assumes isotropic surface and interfacial energies, the observed anisotropy is likely attributable to the elastic anisotropy of MgO and FePt.

Collectively, the simulation reproduces the key features observed in the experiment, indicating that the microstructural evolution during sputtering have been correctly modeled by proposed PF model.

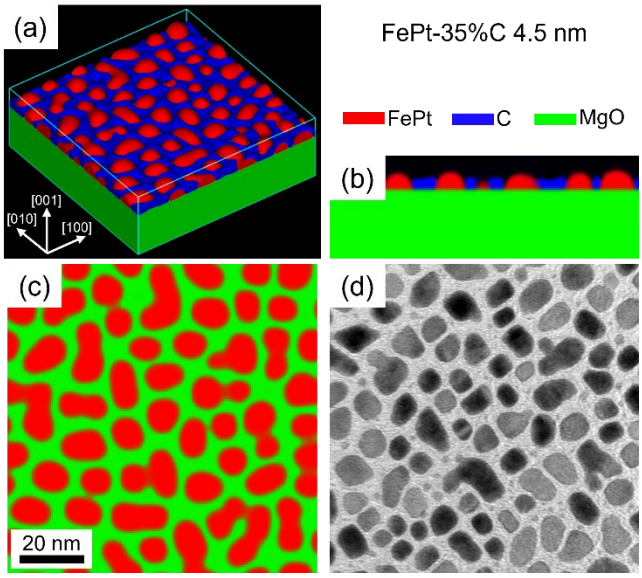

Fig. 1. The simulated (a-c) and experimentally observed (d) microstructure of FePt-35%C film with the thickness of 4.5 nm. For the simulated results, a 3D view (a), a cross-section along the (010) plane (b), and a projection along the [001] direction (c) are shown. Note that the C is not displayed in the projection view (c) for better visibility.

B. Influence of elastic energy relaxation

A key advantage of computational modeling lies in its ability to isolate and verify factors governing microstructural formation by changing parameters or conditions. Here, we investigate the influence of elastic strain energy—arising from lattice mismatch between the substrate and FePt—by performing simulations excluding its contribution.

The resulting microstructure, presented in Fig. 2, reveals the formation of a network-like structure where adjacent FePt grains connect—a morphology distinct from that observed when elastic strain energy is considered (Fig. 1). These results demonstrate that elastic strain energy is crucial for the formation of the uniform, fine, island-like microstructure. Given that phase-field simulations calculate microstructural evolution by minimizing the Gibbs energy of the system, the formation of island-like structure is considered to be driven by the relaxation of elastic strain energy.

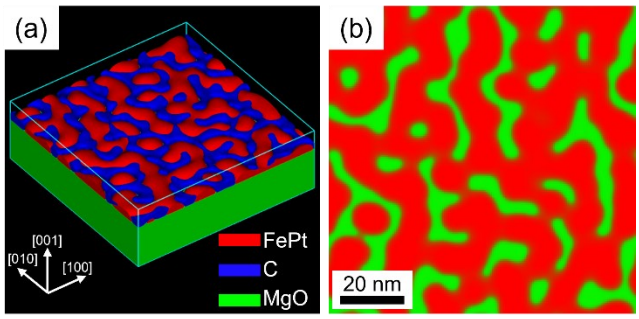

Fig. 2. A 3D view (a) and a projection along the [001] direction (b) of the microstructure of FePt-35%C film with the thickness of 4.5 nm simulated without considering elastic strain energy. Note that the C is not displayed in the projection view (b) for better visibility.

IV. Conclusion

This study modeled microstructural formation of FePt-C nanogranular films on MgO substrates during sputtering using the phase-field method. The main findings are as follows:

- The model, incorporating strain energy between the MgO substrate and the film, successfully reproduced island-like structures in the FePt-C nanogranular film.
- Relaxation of elastic strain energy plays a key role in the formation of island-like microstructure.

Based on these findings, our numerical experiment provides critical insight for the mechanisms behind the microstructural formation of FePt magnetic recording films and will be useful for future studies on process optimization and material exploration of substrate and segregant.

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