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Texture formation in FePt thin films via thermal stress management

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The transformation variant of the fcc to fct transformation in FePt thin films was tailored by controlling the stresses in the thin films, thereby allowing selection of in- or out-of-plane c-axis orientation. FePt thin films were deposited at ambient temperature on several substrates with differing coefficients of thermal expansion relative to the FePt, which generated thermal stresses during the ordering heat treatment. X-ray diffraction analysis revealed preferential out-of-plane c-axis orientation for FePt films deposited on substrates with a similar coefficients of thermal expansion, and random orientation for FePt films deposited on substrates with a very low coefficient of thermal expansion, which is consistent with theoretical analysis when considering residual stresses. © 2005 American Institute of Physics. [DOI: 10.1063/1.1924889]

There is continued strong interest in Fe–Pt alloys near the 1:1 atomic stoichiometry because of the excellent magnetic properties, especially the high magnetocrystalline anisotropy, of the ordered L10 compound. Particularly, thin film FePt with the L10 structure is a potential material for magnetic recording media, especially perpendicular media development. The development of out-of-plane c-axis orientation during the fcc-to-L10 transformation provides its own challenges, as thin films deposited at room temperature form the disordered fcc structure. Deposition onto heated substrates leads to the development of the ordered L10 structure, and epitaxial growth on selected (heated) substrates or buffer layers has led to the development of out-of-plane c-axis orientation. However, deposition onto heated substrates provides its own challenges, and there is continued interest in controlling the c-axis orientation during the fcc-to-L10 phase transformation.

The transformation from the fcc disordered structure to the tetragonal L10 structure can occur along any of the three fcc (100) variants. As a result, one must control the transformation variant in order to control the c-axis orientation during the fcc-to-L10 transformation. The fcc-to-L10 transformation involves a distortion of the fcc unit cell. The a lattice parameter expands approximately 2%, while the c lattice parameter contracts approximately 2.5%. This distortion creates significant stresses in the material, on the order of several gigapascals. The stress and strain involved in the transformation provides the opportunity to control the transformation variant through externally applied stresses. For example, applying an in-plane tensile stress would force in-plane unit cell expansions (i.e., favor (100) in-plane a-axis transformation variants), which would relieve the externally applied stress, and result in c-axis texture perpendicular to the film.

In this paper, we explore controlling the transformation variants by applying stresses during heat treatment to form the L10 structure. The stresses are applied by using differences in thermal expansion coefficients between the FePt thin films and the substrate.

Stresses that arise due to differences in thermal expansion coefficients can be calculated from the equation

$$\sigma = \Delta \alpha \Delta T E/(1 - \mu),$$

where $\Delta \alpha$ is the difference in thermal expansion coefficient between the substrate and FePt film, $\Delta T$ is the change in temperature between room temperature and the heat treatment temperature, $E$ is the elastic modulus of the FePt film ($\sim 180$ GPa), and $\mu$ is Poisson’s ratio (0.33). A negative value of $\sigma$ means that the film is in compression, while a positive value means it is in tension. If the film is in compression, the c-axis contraction associated with the L10 transformation will prefer the in-plane variant (or the one that projects to in plane) to alleviate the thermal stresses caused by the differences in the coefficients of thermal expansion. As a result, the c axis will preferentially lie in plane. If the FePt film is in tension, out-of-plane variants will preferably contract, again to alleviate the thermal stresses, and in this case the c axis will preferentially be perpendicular to the film plane. The condition to generate a tensile stress in the FePt film is $\alpha_{\text{sub}} > \alpha_{\text{FePt}}$.

Table I shows the coefficients of thermal expansion for the substrates used in this study and FePt. Figure 1(a) shows the calculated thermal stresses that arise from thermal expansion mismatches between the film and substrate. As observed, significant thermal stresses, on the order of 1–2 GPa, can occur. This is the same order expected to arise from strain induced during the transformation to the L10 structure, based on Hooke’s law.

FePt thin films were deposited by dc magnetron sputtering onto Si, Al2O3, and MgO substrates at room temperature. The sputtering target was a composite with Pt plugs imbedded in Fe. The Fe:Pt ratio was close to 1:1, based on magnetic measurements and x-ray analysis. The film thickness

<table>
<thead>
<tr>
<th>Material</th>
<th>Coefficient of thermal expansion (CTE) × 10⁻⁶ K⁻¹</th>
</tr>
</thead>
<tbody>
<tr>
<td>(001) Si</td>
<td>2.5</td>
</tr>
<tr>
<td>Al2O3</td>
<td>8.2</td>
</tr>
<tr>
<td>(100) MgO</td>
<td>10</td>
</tr>
<tr>
<td>FePt</td>
<td>10.5</td>
</tr>
</tbody>
</table>

TABLE I. Coefficients of thermal expansion for the substrates used in this study, and estimated for FePt.
was \(\sim 30\) nm for each deposition. The Si and MgO substrates were single crystalline with an [001] orientation. The \(\text{Al}_2\text{O}_3\) substrate was polycrystalline. The FePt thin films were characterized by x-ray diffraction using a Rigaku using \(\theta-\theta\) diffractometry. X-ray data were analyzed using the Rietveld technique. The analysis also included a preferred orientation fitting parameter, which we also use to evaluate texture in the FePt films. Additionally, integrated intensities were determined by fitting individual peaks using a Gaussian function and calculating the area. These intensities were compared with calculated intensities using standard peak intensity procedures\(^{10}\) in order to analyze the degree of texture. The optimum annealing treatment that produced high coercivity was found to be \(600^\circ\text{C}\) for 10 min. The annealing was done by rapid thermal annealing using an IR heat source.

The as-deposited FePt films were in the disordered fcc structure for all substrates. The FePt structure showed random crystallographic orientation, as indicated by the presence of all the diffraction peaks. After annealing, all films transformed to the \(L1_0\) structure, as indicated by the presence of the (100) and (110) superlattice reflections and the splitting of the (002) into (200) and (002) variants in the x-ray diffraction patterns (Fig. 2). Comparing calculated and experimental peak intensities revealed that the long-range order parameter was close to one.

Comparing the relative peak intensities of the x-ray diffraction peaks also reveals the presence of preferred crystallographic orientation. For FePt deposited on Si, all peak intensities closely matched calculated values. Furthermore, full-pattern fitting by Rietveld analysis showed excellent agreement with the ideal \(L1_0\) structure, and revealed random crystallographic orientation (Fig. 2). For comparison, the x-ray diffraction pattern of the FePt deposited on polycrystalline \(\text{Al}_2\text{O}_3\) and [001] MgO shows different intensity distributions (Fig. 3). The intensity of the (001) peak is dramatically enhanced compared to the (110) peak. Calculated intensities reveal that \(I_{(001)}/I_{(110)} \sim 1\), while the experimental intensity ratio is greater than two for FePt on both substrates (Table II). Similarly, \(I_{(002)}/I_{(200)}\) is enhanced over the expected ratio of 0.5 to approximately 1.0. These are clear indications of out-of-plane texture, and the orientation parameter \((R^*\) determined from the Rietveld analysis also indicated texture. These \(R^*\) values were calculated relative to the (001) plane; values less than unity indicate that the (001) peak intensities were greater than expected, and had to be scaled down to improve the fit. Similar fits relative to the (100) plane resulted in values greater than unity for the MgO and \(\text{Al}_2\text{O}_3\) substrates, and unity for the Si substrate. Analysis relative to the (111) plane resulted in values close to unity for FePt films deposited on all substrates.

Figure 1(a) suggests that the Si substrate should induce an in-plane [001] texture, as contraction of the structure in plane would relieve the compressive stresses that arise due to thermal expansion mismatch. Furthermore, \(\text{Al}_2\text{O}_3\) and [100] MgO, with coefficients of thermal expansion (CTEs) close to that of FePt, would produce minimal thermal stresses and thus not influence transformation variants during ordering, resulting in random \(c\)-axis orientation. However, the analysis of the x-ray diffraction results indicate that no preferred orientation exists for the FePt on Si, while both \(\text{Al}_2\text{O}_3\) and [100] MgO induce perpendicular [001] \(L1_0\) orientation, suggesting that tensile stresses exist in the film. Residual tensile stresses on the order of 1.2–1.5 GPa have been observed in thin films produced by dc magnetron sputtering.\(^{11}\) If these residual stresses are accounted for, the total stress in the film (thermal plus residual) changes significantly from Fig. 1(a);
this is shown in Fig. 1(b). The thermal stresses due to differences in CTE for the Si substrate would approximately counteract the residual tensile stresses. As a result, the FePt would transform on any $\{100\}$ variant, resulting in an isotropic $c$-axis orientation, which we observed. Conversely, the net stress in the FePt on Al$_2$O$_3$ and $[001]$ MgO would induce transformations such that the $c$-axis contraction occurs along out-of-plane $\{100\}$ variants, resulting in perpendicular $c$-axis orientation. Our x-ray diffraction results are consistent with this analysis. The strong influence of stress on inducing in- or out-of-plane $c$-axis development may explain the transition from in-plane to out-of-plane $c$-axis orientation as a function of film thickness, as the residual stress is a function of film thickness.

FePt thin films were deposited by dc magnetron sputtering at ambient temperatures, resulting in the formation of the disordered fcc structure. Heat treatment at 600 °C for 10 min resulted in the formation of the ordered $L1_0$ structure. Perpendicular $c$-axis texture was induced and was dependent on the substrate. The texture developed as a result of in-plane tensile stresses that induced in-plane $\{100\}$ variants to expand and out-of-plane variants to contract to form the $c$ axis of the tetragonal $L1_0$ structure. The stresses arose from residual tensile stresses and thermal stresses due to the difference in thermal expansion between the FePt film and substrate. The degree of texture was observed to be dependent on the differences in thermal expansion coefficients between the substrate and FePt.

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