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Tailoring magnetocrystalline anisotropy of FePt by external strain

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We propose using strain assisted reduction in anisotropy of FePt to control magnetization reversal in the writing on the magnetic storage devices. Our first-principles calculations show 21% decrease of the magnetocrystalline anisotropy energy (MAE) with application of 1.5% tensile biaxial strain. The reduction of MAE is primarily due to the change of the c/a ratio and to some extent due to the increase in volume. We propose building bilayer (or heterostructure) of FePt and piezoelectric film. This system is expected to allow the control of anisotropy constant by applying electric field to the system. Finally, we discuss the possibility of forming medium using bi-layer of FePt and soft magnetic material with the gradient of anisotropy constant. © 2012 American Institute of Physics. [doi:10.1063/1.3673853]

Thin ferromagnetic films are widely utilized in modern high density magnetic recording technology. FePt nanoparticles having large magnetocrystalline anisotropy and large magnetization can provide further increase of perpendicular recording density. The large coercivity of these materials, however, requires high magnetic field to “write” bit information on them, thus significantly restricting this recording technology in portable or ultrahigh-speed processing devices. Thermally assisted magnetization reversal,¹ and the current induced magnetization switching² have been proposed to solve this problem. Recently, the formation of exchange coupled composites of soft and hard phases was proposed to reduce switching field.^{3,4} The switching field could be further reduced in a graded anisotropy medium where anisotropy constant varies smoothly across the bit.⁵

FePt is well known hard magnetic material with tetragonal ground state $L1_0$ structure and it preserves its bulk magnetic properties at nanoscale. Experimentally prepared 4 nm FePt nanoparticles show large coercivity of 1.8 T and large magnetization.⁶ Ability to tailor coercivity and anisotropy constant of FePt could be beneficial for various applications. The sensitivity of the anisotropy constant of FePt to the modification of lattice parameters has been observed both experimentally^{7,8} and theoretically.⁹ However, the detailed analysis of magnetoelastic properties of FePt is lacking.

We show that magnetocrystalline anisotropy of FePt can be altered significantly by a moderate applied biaxial strain. We propose two potential implementations of this effect: (1) forming gradient anisotropy medium, (2) electrically controllable coercivity of nanoparticle films by forming FePt/piezoelectric bilayers (or heterostructures). These devices could be used as magnetic recording medium and in sensor applications.

Figure 1 shows the schematic view of the FePt cell in the ground state $L1_0$ structure. We perform first principles

calculation of MAE as function of applied biaxial strain. We use the projector augmented wave (PAW) method,¹⁰ implementation of PAW in VASP code¹¹ within a local density approximation of the density functional theory. We use k -point sampling of $20 \times 20 \times 20$ with Monkhorst-Pack integration scheme.¹²

We use force theorem approach, i.e., MAE is calculated in pseudopotential manner as the difference between the sums of single particle eigenvalues for the magnetization perpendicular (001) and parallel (100) to the easy axis. We perform calculations in the wide range of the strain values for both tensile and compressive strain. Moderate biaxial strain is usual for tetragonal lattices near interfaces with misfit in lattice parameters. When in-plane tensile biaxial strain is applied, the lattice parameter, a , in the plane increases, while lattice parameter along perpendicular direction, c , decreases. The experimental lattice parameters for FePt nanoparticles are $a = 0.387$ nm, $c = 0.373$ nm ($c/a = 0.96$) and the Poisson's ratio is 0.33. Because Poisson's ratio is less than 0.5 the

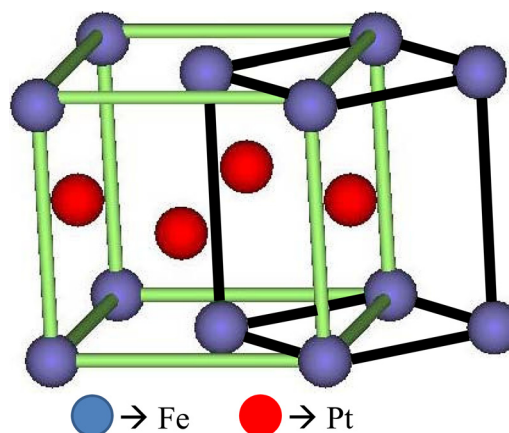


FIG. 1. (Color online) Tetragonal $L1_0$ structure - alternating Fe and Pt atomic planes with square lattice along (001) direction.

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volume will increase with applied tensile biaxial strain. Thus, there are two different constituents to the change in MAE: (1) volume change, (2) change in c/a ratio.

Figure 2 shows MAE of FePt as a function of biaxial strain. As one can see MAE decreases when tensile strain is applied. MAE is equal to 2.98 eV/f.u. at the equilibrium lattice parameter (in good agreement with previous calculation and experimental results), but can be reduced by about 21% when 1.5% in-plane tensile strain is applied. Inset in Fig. 2 shows c/a and volume as functions of applied strain. There is 2% volume change and 4% change in c/a at 2% biaxial strain, the two possible mechanisms of MAE variation.

In order to separate the contribution due to the volume change we analyze MAE as a function of the cell volume at the fixed c/a ratio. The increase in volume by 1.5% results in reduction of MAE by about 4%. This is very small compared with 21% MAE reduction due to 1.5% tensile strain.

Next we fix the volume at the value of unstrained cell (see the zero point on the inset in Fig. 2) and vary the c/a ratio. The change in c/a , i.e. the elongation of FePt unit cell is expected to give considerable change to the orientation and length of Fe–Pt bonds which results in anisotropy variation. The distance between Fe and Pt layer changes as well. MAE as a function of c/a ratio is shown in Fig. 3. This dependence is nearly linear at both tensile and compressive strains. In the considered range of c/a ratio our results are consistent with earlier reports.⁹ It is interesting to note that the effect of the volume increase is very minor compared with the change in c/a ratio.

To better understand the nature of the MAE change under external stress we consider the electronic band structure of FePt. Figure 4 shows the energy band structure and the k -point resolved contribution to MAE defined as

$$\text{MAE}(k\text{-resolved}) = \sum_{i=1}^{N_{\text{bands}}} \left(\epsilon_i^{(001)} n_i - \epsilon_i^{(100)} n_i \right) \quad (1)$$

along the symmetry lines for lattice constants corresponding to the unstrained cell (a) and 2% tensile strain (b). Here $\epsilon_i^{(001),(100)}$ is the eigenvalue of i^{th} band, while n_i is its occupation number. Fig. 4 shows that bands in the minority spin channel are shifted

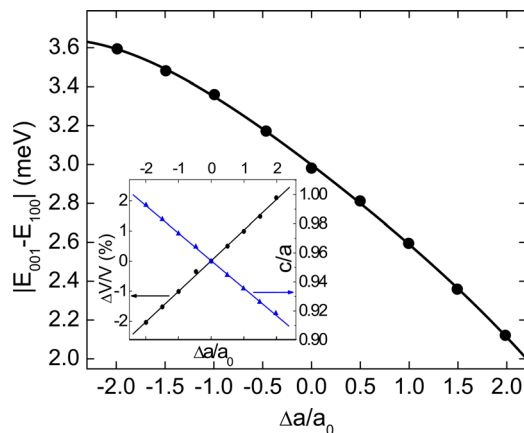


FIG. 2. (Color online) MAE as a function of in-plane biaxial strain. MAE reduces with positive value of $\Delta a/a_0$ (tensile strain). Inset: $\Delta V/V_0$ and c/a as a function of an in-plane biaxial strain.

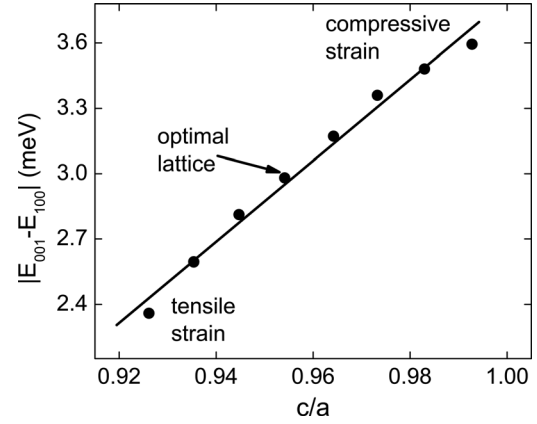


FIG. 3. MAE as function of the ratio of lattice parameters c/a at fixed cell volume corresponding to experimental data. MAE reduces by about 20% at 3% c/a reduction.

lower relative to the Fermi level in case of the tensile strain (due to the increased exchange splitting). As a result of this shift two bands move below the Fermi level and reduce their contribution to MAE.

This sensitivity of MAE to the external strain can be used for electric control of anisotropy in heterostructures of two ferromagnetic materials, i.e., FePt and a piezoelectric film. The piezoelectric materials in these systems provide a biaxial strain that can be modified by an applied external electric field. This strain, transferred to FePt layer, should change MAE of FePt layer. Observation of the coercivity change in

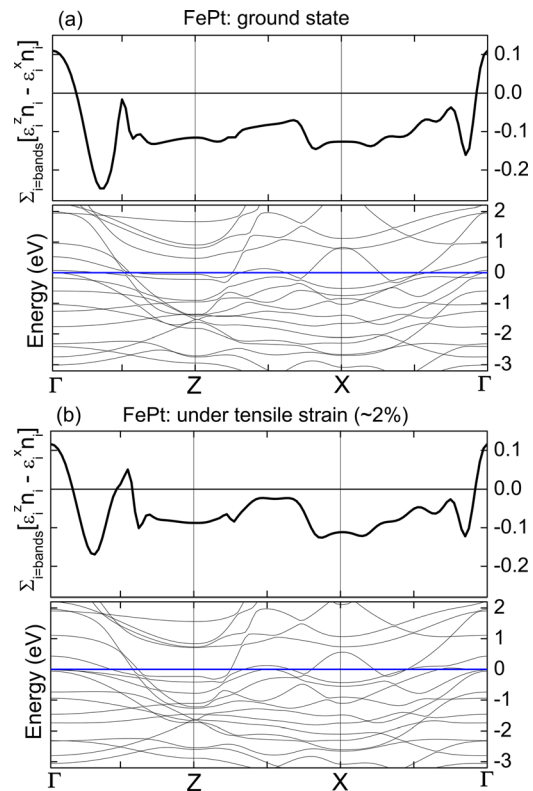


FIG. 4. (Color online) (a) Band structure of FePt for the unstrained cell (lower panel) and corresponding contributions to MAE (top panel). (b) Band structure of FePt under ~2% tensile strain (lower panel) and corresponding contributions to MAE (top panel).

Fe films deposited on top of BaTiO₃ ferroelectric was recently reported.¹³ Traditional ferroelectrics such as BaTiO₃ or PZT can provide about 0.1% strain. The new “relaxor” ferroelectrics such as lead magnesium niobate compounds could provide up to 2% strain with applied voltage, about 10 times that in conventional ferroelectrics.¹⁴

Recently a recording gradient medium was proposed by Suess.⁵ Strain gradient in FePt can be used to make a structure with gradual change in the local anisotropy constant. Strain gradient can be obtained in trilayer where FePt is sandwiched by two materials with sufficiently different lattice parameters. For example, FePt can be made unstrained (or possibly strained compressively) to keep/increase its anisotropy constant at one interface while at the other interface FePt layer would have tensile strain. One of the interfaces can be made of the magnetically soft material to further provide a gradient of anisotropy constant. The non-uniform profile of anisotropy constant across such column should reduce considerably the coercivity preserving the thermal stability.

In summary, we have shown that application of the 1.5% biaxial strain reduces MAE of FePt by about 21% which is primarily due to the reduction of the c/a ratio. The reduction of MAE can be used in magnetization reversal in the writing on the magnetic storage devices. The required strain can be obtained by placing layer of FePt on piezoelectric film and by applying electric field to the system. Another possible appli-

cation of the strain controlled MAE is the gradient medium composed of FePt and soft magnetic material.

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