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Strain control magnetocrystalline anisotropy of Ta/FeCo/MgO heterostructures

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Using ab initio electronic structure calculations, we have investigated the effect of epitaxial strain on magnetocrystalline anisotropy (MCA) of Ta/FeCo/MgO heterostructure. At small expansive strains on the FeCo layer, the system exhibits perpendicular MCA (PMA). Strain not only has a profound effect on the value of MCA but also induces a switching of magnetic easy axis. Analysis of the energy- and k-resolved distribution of orbital characters of the minority-spin band reveals that a significant contribution to PMA at zero strain arises from the spin-orbit coupling between occupied $d_{x^2−z^2}$ and unoccupied $d_y$ states, derived from Fe at the FeCo/MgO interface. The strain effect is attributed to strain-induced shifts of spin-orbit coupled d-states. Our work demonstrates that strain engineering can open a viable pathway towards tailoring magnetic properties for spintronic applications. © 2015 AIP Publishing LLC. [http://dx.doi.org/10.1063/1.4916115]

I. INTRODUCTION

Magnetic tunnel junctions (MTJ) with strong perpendicular magnetocrystalline anisotropy (PMA) have attracted much attention for applications in high density and nonvolatile random access memory (RAM), in which magnetization reversal is induced by spin-polarized current via the spin transfer torque (STT-RAM)1 or by electric field via the magnetoelectric effect (MeRAM).2–4 A MTJ consists of ferromagnetic (FM) thin films sandwiched between a MgO barrier and heavy metal electrodes. As there are usually large lattice mismatches, the component layers experience significant strain. Owing to the spin-orbit coupling (SOC), spin degree of freedom is coupled to lattice distortion. Consequently, the strain can significantly modify the magnetocrystalline anisotropy (MCA) and other magnetic behavior of the system. It has been shown that epitaxial strain has strong effect on magnetic correlation length5 and PMA of magnetic oxides.6 Moreover, recent experiments showed that epitaxial strain in thin films of magnetic oxides and semiconductors grown of different substrates can induce a rotation of magnetic easy axis.7–9 The dependence of MCA on pressure and structural distortion has been studied on thin film and bulk FeCo alloys.10,11 Therefore, it is desirable to understand the effect of strain on MCA of MTJ before the system can be implemented in further spintronic applications.

In this paper, we report the results of ab initio electronic structure calculations on the effect of epitaxial strain on the MCA of Ta/FeCo/MgO heterostructure. We show that MCA is strongly decreases with expansive strain on the FM layer. Furthermore, a switching of magnetic easy axis from perpendicular to in-plane direction is obtained at a critical value of strain. The mechanism of strain effect is explained by analyzing the energy- and k-resolved distribution of the orbital character and strain-induced shifts of spin-orbit coupled d-states. Our work demonstrates that strain engineering can open a way to develop MTJ with desired properties for spintronic applications.

II. COMPUTATIONAL METHOD AND MODEL

First-principles density functional calculations were performed within the framework of the plane wave projector augmented wave formalism,12 as implemented in the Vienna ab initio simulation package (VASP) code.13–15 The generalized gradient approximation (GGA) in PerdewWang (PW91) parameterization16 has been employed to treat the exchange-correlation interaction. To simulate epitaxial growth of the Ta/FeCo/MgO junction, we employed the slab supercell approach along [001] consisting of three monolayers (MLs) of bcc Ta, three MLs of B2-type FeCo, seven MLs of rocksalt MgO, and a 15 Å-thick vacuum region separating the periodic slabs [Fig. 1(a)]. The FeCo/MgO interface is designed by placing the O atoms atop the Fe atoms [Fig. 1(b)]. Lattice constants of MgO and FeCo have experimental values of 4.2120 and 2.8504 Å, respectively. Due to this lattice mismatch, the FeCo is under large expansive strain, $\eta_{FeCo}$, of 4% assuming that the MgO substrate is unstrained. On the other hand, recent experiments showed that the ultrathin (~2 nm) MgO film is significantly compressed to match that of the FM film.17 Consequently, in order to investigate the effect of strain on MCA of the system we have varied $\eta_{FeCo}$ from zero to 4%. At each strain, the magnetic, electronic degrees of freedom and atomic z positions are fully optimized until forces acting on the ions become less than $5 \times 10^{-3}$ eV/Å and the change in the total energy between two ionic relaxation steps is smaller than $10^{-6}$ eV. The plane-wave cutoff energy is 500 eV and the Monkhorst-Pack...
The atomic interlayer distances, spin moment, and orbital-moment difference of Fe1 (at FM/MgO interface), the Fe1 exhibit very large and positive orbital contribution the MCA of the whole system. In fact, the Bruno relation to be valid, this would indicate the FM/MgO interface has negative contribution the MCA of the whole system. In fact, experiments also showed that the FeCo/Ta interface favors in-plane MCA.

The increase in in-plane lattice due to expansive strain leads to decreases in the interlayer distances by about 0.10 to 0.18 Å. A dramatic change occurs at the FM/Ta interface, where the Ta1-Fe2 distance is reduced by about 0.40 Å. This would lead to an enhancement in Ta1-Fe2 hybridization, which is evident from a strong reduction (~1 μB) in spin moment of Fe2 and a concomitant magnetization of the otherwise nonmagnetic Ta1 ion. With increasing expansive strain, the absolute values of Δms for Fe1, Fe2 and Ta1 are strongly decreased, correlating well with the decrease in MCA. Interestingly, the magnetization of the system is switched from perpendicular at ηFeCo = 2% to in-plane orientation at ηFeCo = 4%. Such a strain-induced variation and magnetic switching have also been predicted in a similar model of the Ta/FeCo/MgO heterostructure by He and Chen, in which the FeCo layer is not of B2-type, but in L6 structure with Fe and Co present on the same atomic plane.

To elucidate the mechanism of the strain effect, we calculated the energy- and k-resolved distribution of the orbital character of d-states. For ηFeCo = 0, the distributions of Fe1 dxy and dxz-dyz characters of minority-spin bands are shown in Fig. 2. Within the second-order perturbation of the total energy due to the SOC, the MCA is determined by the matrix elements of the orbital angular momentum operators Lx and Lz between occupied and unoccupied d-states and by the energy difference between these states. As the majority spin states of Fe are well below the Fermi energy, the MCA contribution from the SOC between states of opposite spin can be neglected. The MCA can in turn be expressed as

\[
MCA \propto \xi^2 \sum \frac{\langle \Psi_o^L | \hat{L}_z | \Psi_o^I \rangle^2 - \langle \Psi_o^L | \hat{L}_z | \Psi_o^I \rangle^2}{E_B - E_o},
\]

where mspin and morb are the orbital moments when magnetization is oriented along the [001] and [100] directions, respectively.

### III. RESULTS AND DISCUSSION

The atomic interlayer distances, spin moment, and orbital-moment difference of Fe1 (at FM/MgO interface), Fe2 and Ta1 (at FM/Ta interface), and MCA of the system under various strains are shown in Table I. At ηFeCo = 0, the distances between Ta ions are significantly larger than those between Fe and Co. This is due to a considerable compressive strain on the Ta layer, as lattice constant of bcc Ta is much larger than that of Fe or Co. At the FM/MgO interface, the Fe1 exhibit very large and positive orbital moment difference Δms = 4.7 × 10^-2 μB, which is more than one order of magnitude larger than that for Fe monolayer.

On the other hand, at the FM/Ta interface the Fe2 possesses large negative Δms. Assuming the Bruno relation to be valid, this would indicate the FM/Ta interface has negative contribution the MCA of the whole system. In fact, experiments also showed that the FeCo/Ta interface favors in-plane MCA.

### TABLE I. Calculated interlayer distances (d½), spin moment (ms), orbital moment differences (Δms), and MCA at zero field. Here, Δms = mspin - morb, where mspin and morb are the orbital moments when magnetization is oriented along the [001] and [100] directions, respectively.

<table>
<thead>
<tr>
<th>Strain (%)</th>
<th>Ta3-Ta2</th>
<th>Ta2-Ta1</th>
<th>Ta1-Fe2</th>
<th>Fe2-Co</th>
<th>Co-Fe1</th>
<th>Fe1-MgO</th>
<th>d½ (Å)</th>
<th>m½(μB)</th>
<th>Δms (10^-2 μB)</th>
<th>MCA (erg/cm²)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>2.199</td>
<td>2.323</td>
<td>1.825</td>
<td>1.391</td>
<td>1.357</td>
<td>2.210</td>
<td>2.693</td>
<td>2.291</td>
<td>-0.001</td>
<td>1.43</td>
</tr>
<tr>
<td>2</td>
<td>2.091</td>
<td>2.267</td>
<td>1.543</td>
<td>1.439</td>
<td>1.239</td>
<td>2.137</td>
<td>2.550</td>
<td>1.569</td>
<td>-0.237</td>
<td>0.4</td>
</tr>
<tr>
<td>4</td>
<td>2.032</td>
<td>2.122</td>
<td>1.430</td>
<td>1.471</td>
<td>1.277</td>
<td>2.117</td>
<td>2.591</td>
<td>1.334</td>
<td>-0.277</td>
<td>0.3</td>
</tr>
</tbody>
</table>

FIG. 1. (a) Schematic model of the Ta/FeCo/MgO heterostructure. (b) Atomic configuration at the FeCo/MgO interface, where the O atoms are placed atop Fe atoms.

FIG. 2. Energy- and k-resolved distribution of orbital characters of minority-spin bands for Fe1 dxy (green) and dxz-dyz (red).
FIG. 3. Projected density of states (PDOS) of minority Fe1 $d_{xy}$ and $d_{x^2-y^2}$ under 0%, 2%, and 4% strain.

where $\Psi^\parallel_{\uparrow}$ and $\Psi^\parallel_{\downarrow}$ denote the occupied and unoccupied minority spin bands.

As the $d_{xy}$ and $d_{x^2-y^2}$ are coupled through $\hat{L}_z$, the small separation of these states around $\frac{1}{2} (\Gamma - M)$ induces a dominant contribution to perpendicular MCA. This explains the large PMA of the heterostructure under small strain on the FM layer.

At $\eta_{FeCo} = 0$, the dominance of $d_{xy}$ and $d_{x^2-y^2}$ orbital characters near the Fermi level is evident from the projected density of states (PDOS) shown in Fig. 3. With increasing $\eta_{FeCo}$, the $d_{x^2-y^2}$ state shift up, but its PDOS feature right below the Fermi level is just slightly changed. On the other hand, the $d_{xy}$ PDOS is dramatically changed. In particular, the $d_{xy}$ state strongly shifts down and becomes almost fully occupied at 2% and 4%. The shift of this state from above to below level causes the $\langle x^2 - y^2 | \hat{L}_z | xy \rangle$ to vanish, leading to the reduction in MCA of the system.

IV. CONCLUSION

In summary, we have presented ab initio electronic structure calculations of the effect of epitaxial strain on the MCA of the Ta/FeCo/MgO epitaxial heterostructure. At zero strain on the FM layer, the system has a large PMA. The $\langle x^2 - y^2 | \hat{L}_z | xy \rangle$ coupling of Fe at the FeCo/MgO interface provides a dominant contribution to PMA. With increasing expansive strain, the MCA is strongly decreased. The switching of magnetic easy axis from perpendicular to in-plane orientation occurs at a critical strain between 2% and 4%. It is shown that the strain-induced shift of Fe1 $d_{xy}$ from above to below the Fermi level is the underlying origin of the reduction in MCA of the system. Our work demonstrates that strain engineering can open a unique avenue to tailor magnetic properties for spintronic applications.

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