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Citation: Journal of Applied Physics 117, 17B518 (2015); doi: 10.1063/1.4916115
View online: http://dx.doi.org/10.1063/1.4916115
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Strain control magnetocrystalline anisotropy of Ta/FeCo/MgO heterostructures

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(Presented 6 November 2014; received 22 September 2014; accepted 15 November 2014; published online 25 March 2015)

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 \( d_{x^2-y^2} \) and unoccupied \( d_{z^2} \) 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 rock-salt MgO, and a 1 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, \( \eta_{\text{FeCo}} \) 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 \( \eta_{\text{FeCo}} \) 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

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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 Δm_o 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 η_FeCo = 2% to in-plane orientation at η_FeCo = 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,23 in which the FeCo layer is not of B2-type, but in L60 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 η_FeCo = 0, the distributions of Fe1 d_{xy} and d_{x^2-y^2} 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 \( L_x \) and \( L_z \) 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:

\[
MCA \propto \xi^2 \sum_{\alpha,\beta} \frac{|\langle \Psi_{\alpha} | \tilde{L}_z | \Psi_{\beta} \rangle|^2 - |\langle \Psi_{\alpha} | \tilde{L}_x | \Psi_{\beta} \rangle|^2}{E_{\alpha} - E_{\beta}},
\]

where \( \xi \) is the overlap integral between the initial and final states, \( |\langle \Psi_{\alpha} | \tilde{L}_z | \Psi_{\beta} \rangle|^2 \) is the probability of creating a magnetic moment by a Zeeman field, and \( E_{\alpha} - E_{\beta} \) is the energy difference between the two states.

### Table I. Calculated interlayer distances (\( d_i \)), spin moment (\( m_i \)), orbital moment differences (\( \Delta m_o \)), and MCA at zero field.

<table>
<thead>
<tr>
<th>Strain (%)</th>
<th>Ta3-Ta2 (Å)</th>
<th>Ta2-Ta1</th>
<th>Ta1-Fe2</th>
<th>Fe2-Co</th>
<th>Co-Fe1</th>
<th>Fcl-MgO</th>
<th>Fe1 (μB)</th>
<th>Fe2</th>
<th>Ta1</th>
<th>Fe1 (10^2 μB)</th>
<th>Ta1</th>
<th>MCA (erg/cm^2)</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>4.7</td>
<td>-1.8</td>
<td>1.1</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>
<td>-0.8</td>
<td>0.1</td>
</tr>
<tr>
<td>4</td>
<td>2.032</td>
<td>2.122</td>
<td>1.430</td>
<td>1.471</td>
<td>1.175</td>
<td>2.117</td>
<td>2.591</td>
<td>1.334</td>
<td>-0.277</td>
<td>0.3</td>
<td>0.1</td>
<td>0.2</td>
</tr>
</tbody>
</table>
where $\Psi_\uparrow$ and $\Psi_\downarrow$ 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 also 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 $\langle \gamma^2 - \gamma^2 | \hat{L}_z | \gamma \rangle$ 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 $\langle \gamma^2 - \gamma^2 | \hat{L}_z | \gamma \rangle$ 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.

ACKNOWLEDGMENTS

This research was supported by NSF Grant No. ERC-Translational Applications of Nanoscale Multiferroic Systems (TANMS)-1160504.

1C. Chappert, A. Fert, and F. N. Van Dau, Nat. Mater. 6, 813 (2007).