The magnetic anisotropy of the Co films on ZnO with Zn- and O-terminated interfaces

RIEC, Tohoku Univ.[1], CSRN, Tohoku Univ.[2], WLRCS, Tohoku Univ.[3]

◦(M1)Riku Okado[1], Masahito Tsujikawa[1,2], Masafumi Shirai[1,2,3]

E-mail: riku.okado.s1@dc.tohoku.ac.jp

The control of the magnetic anisotropy is important subject for developing spintronics devices such as magnetic tunnel junctions. Recently, the magnetic properties of the Co film on ZnO with the Zn- and O-polar surfaces were investigated experimentally [1]. It was found that the magnetic anisotropy energy (MAE) strongly depends on the built-in electric field caused by the polarity of the surface of ZnO substrate. In this work, we investigated the effect of terminal atoms of ZnO on the MAE at the ZnO/Co interface by using first-principles density-functional calculations.

We consider ZnO/Co/Pt films, whose in-plane lattice constant is set to that of bulk ZnO (3.25 Å). The Co layers and the Pt layers were set to have fcc structure, and the ZnO layers were set to have Wurtzite structure. We found that the Co atom at the Zn (or O)-terminated ZnO/Co interface favors the hollow site (or the on-top site) of the Zn (or O) atom. By subtracting the MAE at the Co/Pt interface, we obtained the MAE at the ZnO/Co interface, i.e. -0.95 and 0.87 mJ/m^2 for the Zn- and O-terminated interfaces, respectively. As shown in Fig.1, the MAE of the Co atoms at the interface changes its sign depending on the termination. This result implies that the bonding scheme of the Co atom is crucial for determining the sign of the interfacial MAE.

In the Zn-terminated interface, a broad peak structure originated from Co 3d($3z^2 - r^2$) orbital exists just at the Fermi level in the minority-spin density of states, and it contributes to the in-plane MAE. In the O-terminated interface, on the other hand, the minority-spin Co 3d($3z^2 - r^2$) state is located above the Fermi level due to the charge transfer from the Co 3d to the O 2p orbitals. As a result, the minority-spin Co 3d(xz) and 3d(yz) states near the Fermi level are responsible for the perpendicular MAE in the O-terminated interface.

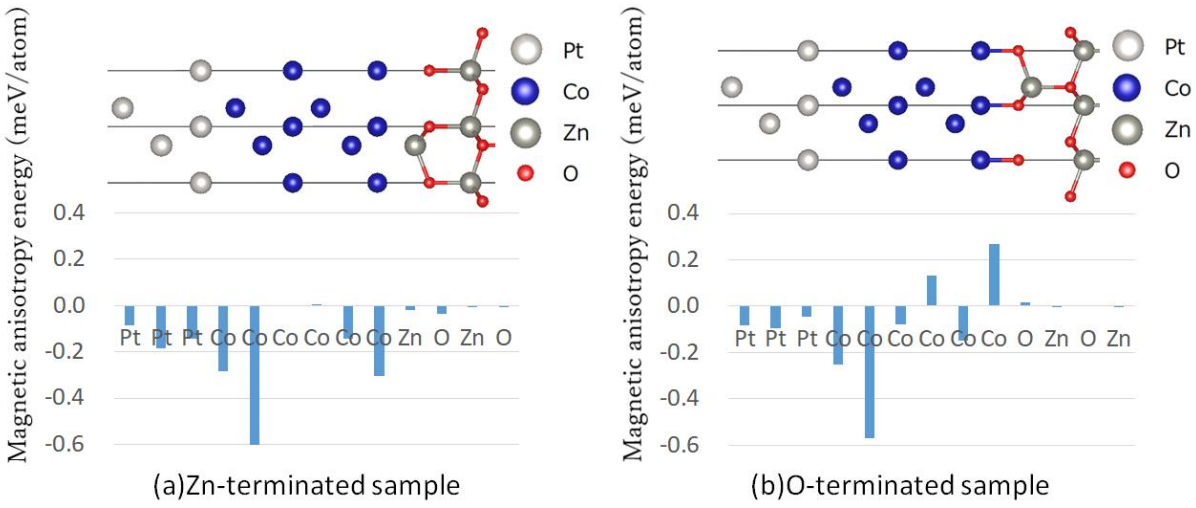

Figure 1. The magnetic anisotropy energy (MAE) arising from each atom in ZnO/Co/Pt films with (a) Zn- and (b) O-terminated interfaces

[1] D. Chiba, N. Shibata, and A. Tsukazaki, Sci. Rep., **6**, 38005 (2016).