Perpendicular magnetocrystalline anisotropy of 5*d* TM/Co_xFe_{1-x}/MgO (TM=Hf, Ta, and W; x=0, 0.5, 1): A first principles study

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One of key requirements for STT-RAM is high thermal stability [1]. Ta-capped CoFeB/MgO is widely employed in a typical magnetic tunnel junction (MTJ), but it has been reported that its perpendicular magnetocrystalline anisotropy (PMCA) degrades during the annealing process at temperatures higher than 300 ºC [2, 3]. Therefore, to achieve a thermal stability simultaneously with keeping PMCA, it is demanded to replace the Ta-capping layer with other films [4-7]. In this work, we propose possible candidates with strong PMCA, performing a first principles study on magnetism and MCA of Hf/Co_xFe_{1-x}/MgO and W/Co_xFe_{1-x}/MgO (x=0, 0.5, 1) and comparing them with those of Ta/Co_xFe_{1-x}/MgO. We demonstrate that the magnitude of MCA energy of Fe/MgO strongly depends on capping layers, as shown in Fig. 1(a). And Fig. 1(b) shows that MCA sensitively depend on the composition, x: the W-capping has PMCA of 2.02 and 0.29 meV/cell for Fe/MgO and Co/MgO, respectively, while in-plane MCA for CoFe/MgO. Interestingly, the MCA behavior of W/Co_xFe_{1-x}/MgO is quite similar to that of Ta/Co_xFe_{1-x}/MgO. On the other hand, Hf/Co_xFe_{1-x}/MgO exhibits PMCA without respect to x. The largest MCA energy is 2.34 meV/cell for CoFe/MgO, where the Hf is interfaced with Fe. Further explanation for origin of MCA for different capping and FM thin films will be elucidated.

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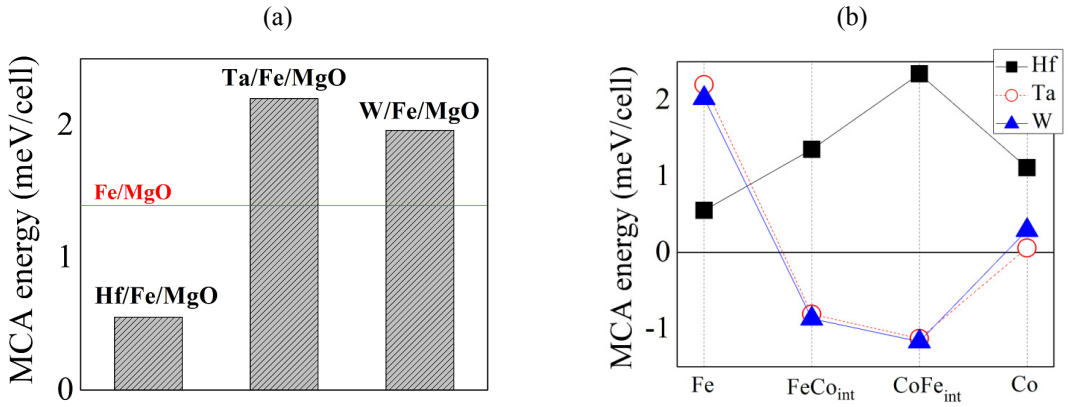

Fig 1. (a) MCA energies of Hf, Ta, and W capping layers on Fe/MgO; Red-dashed line indicates Fe/MgO; (b) MCA energies of Hf/Co_xFe_{1-x}/MgO, Ta/Co_xFe_{1-x}/MgO and W/ Co_xFe_{1-x} /MgO [x=0; 0.5; 1;]. Co_{int} and Fe_{int} imply Co and Fe interfaced with Hf, Ta or W, respectively.

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