Perpendicular magnetic anisotropy obtained by inserting an ultrathin LiF layer at an Fe/MgO interface: a first-principles calculations

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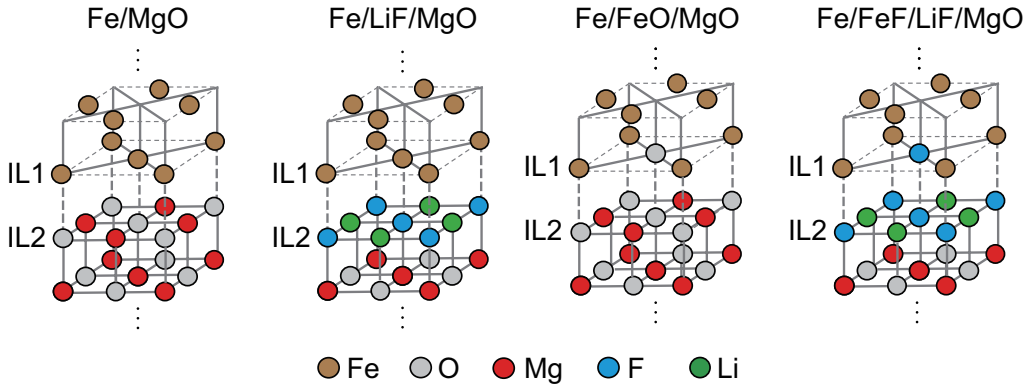
Perpendicular magnetic anisotropy (PMA) is a key property of magnetoresistive random access memory (MRAM). To increase areal density of MRAM it is important to find a way to enhance the PMA. Recently a strong enhancement of the PMA by inserting an ultrathin LiF layer at an Fe/MgO interface ware reported [1, 2]. It is important to understand the origin of the observed enhancement of the PMA.

Here, we investigate the magetocrystalline anisotropy energy (MAE) of the Fe/LiF/MgO system by using the first-principles calculations. The calculated MAE of the Fe/LiF/MgO and the Fe/FeF/LiF/MgO structures are almost the same as the MAE of the Fe/MgO structure, while the MAE of the Fe/FeO/MgO structure is less than a half of the MAE of the Fe/MgO structure. This can be explained by the difference in MAE induced by the Fe-F and Fe-O in-plane couplings. We find that the in-plane Fe-F coupling gives a positive contribution to the MAE while the in-plane Fe-O coupling gives a negative contribution. The results show that the major origin of the enhancement of the PMA obtained by inserting an ultrathin LiF layer at an Fe/MgO interface is the suppression of the mixing of Fe and O atoms at the interface.



Model	A	B	C	D
IL1	Fe	Fe	FeO	FeF
IL2	MgO	LiF	MgO	LiF
MAE (meV/unit cell)	1.015	0.992	0.405	0.979

The Schematic illustrations of crystal structures and the calculated results of the MAE for the Fe/MgO, Fe/LiF/MgO, Fe/FeO/MgO, and Fe/FeF/LiF/MgO.

[1] T. Nozaki et al., NPG Asia Mater. 4 (2022) 5. [2] S. Sakamoto et al., Phys. Rev. B 106 (2022) 174410.