Relationship between magnetic orbital moments and magnetocrystalline anisotropy in transition-metal thin films on MgO(001)

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In 3d transition-metal (TM) thin films, it was theoretically suggested that magnetocrystalline anisotropy (MCA) energy, E_{MCA}, is related to the anisotropy of magnetic orbital moments along the in-plane and the perpendicular plane directions of the thin films [1]. Here, by using first principles calculations and machine learning techniques, the relationship between the orbital moments and the E_{MCA} of TM thin films on MgO(001) is analyzed. Calculations of the orbital moments and the E_{MCA} were carried out using first principles full-potential linearized augmented plane-wave method [2] for single slabs with six atomic-layers of binary Fe-Au, Co-Au, and Fe-Co films on MgO(001). All atomic-layer configurations (2^6=64) for all thin-film systems were considered in the calculations. The E_{MCA} is defined as difference in total energy for magnetizations oriented along the in-plane and perpendicular directions with respect to the film plane. The calculated E_{MCA} strongly depends on the atomic-layer alignments. For Fe-Au (Co-Au) thin films, there is very large variation from 4.8 (6.1) meV/atom-area of the perpendicular MCA to -2.5 (-1.2) meV/atom-area of the in-plane MCA while for Fe-Co thin film, the variation is rather small from 1.4 to -1.5 meV/atom-area. We have successfully regressed the E_{MCA} against the anisotropy of orbital moments in the Fe-Co thin films. For the Au-Fe and Au-Co thin films, however, our analysis shows no relation between them, implying that further analysis, e.g. by including the magnetic dipole moments [3], may be required.

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