Machine learning approaches for determination of the atomic-layer alignments with large perpendicular magnetic anisotropy in transition-metal thin films on MgO(001)

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Magnetic tunnel junctions with large perpendicular magnetocrystalline anisotropy (MCA) are strongly desired for spintronic devices. A key way to control large perpendicular MCA may be by tuning atomic-layer alignments of multilayer thin films [1]. Here, by utilizing the machine-learning technique, we investigated magnetic spin moments and magnetocrystalline anisotropy energy for prototypical multilayers of transition metal thin films (Au-Fe, Au-Co, and Fe-Co) on MgO(001) and revealed the underlying trends, i.e. key factor in the atomic-layer alignments, for designing thin films with large perpendicular MCA. Calculations were carried out by using full-potential linearized augmented plane-wave method. A model of six atomic-layer slab, consisted of Fe, Co and Au layers, on MgO(001) were employed, where all atomic-layer configurations (2^6=64) for all thin-film systems were considered. Within a linear regression with respect to cluster correlation functions [2], we applied exhaustive search method [3] for analyzing magnetic moments and magnetocrystalline anisotropy in terms of atomic-layer alignments. We find that the magnetic moments are mainly represented by the point cluster functions. Thus, the magnetic moments depend on the transition-metal composition, and a small deviation from the composition dependence arises from the nearest-neighbor pair cluster function. In contrast, the MCA energy strongly depends on the atomic-layer alignments. The exhaustive search method, however, leads to a set of key atomic-layer alignments for large perpendicular MCA. For Au-Fe and Au-Co systems, the roles of point correlation function at the interface layer and the pair correlation function between the surface and subsurface layers for the perpendicular MCA cannot be neglected, while for the Fe-Co system, the perpendicular MCA is mainly attributed to the point correlation functions at the interface and surface layers.

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