Atomic-layer alignment dependence of spin-orbit included magnetism in thin films

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Significant progress has been made from first principles calculations for investigating the spin-orbit (SO) induced magnetism, e.g., magnetocrystalline anisotropy (MCA), Dzyaloshinskii-Moriya interaction (DMI), and spin-orbit torque (SOT) in thin films, which play important roles in modern spintronics. However, it may remain an issue treating the atomic-configurational dependence of such SO induced magnetism since the relevant energy is very small, typically less than 1 meV/atom, so that the SO induced properties are very sensitive to the detail of atomic-configurations in films, defects, substrates, and surface/interface structures.[1] In order to investigate underlying trends of atomic-configurations in properties, previously, we have developed a data-science technique based on the cluster expansion method in combination with first-principles calculations (full-potential linearized augmented plane-wave method), and applied this method to the MCA of transition-metal multilayer thin-films. Here, we extend this method to derive the energy contribution of atomic-layer alignments, i.e. the short-range order effect to the SO induced magnetism. We first present the short-range order effect to the MCA in the Co-Fe and Au-Fe multilayer thin films on MgO(001), where although the MCA complicatedly behaves to the atomic-layer alignments the double atomic-layer stacking of Fe on MgO is found to be promising for an interfacial perpendicular magnetization, and then the electric-field induced change of the MCA will be discussed. We have furthermore developed the method to investigate for the other SO induced magnetism, like DMI and SOT, which will be discussed.