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Magnetism and Magnetocrystalline Anisotropy in Tetragonally Distorted γ-Fe (001) Surface

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Magnetic thin films exhibit significantly different magnetic properties from their bulks, such as magnetocrystalline anisotropy (MCA), enhanced magnetic moments, and critical behaviors. These differences are caused by the increasing influence of the reduced dimensionality and by the strain induced by the epitaxial constraint at the interface. In the bulk, α-Fe is ferromagnetic (FM) and metastable γ-Fe can exist in various magnetic states of paramagnetic (PM), antiferromagnetic (AFM), FM, and spin-spiral states, depending on the lattice constant and the lattice distortion. It was reported that γ-Fe can be stabilized by epitaxial growth on appropriate substrate such as Cu (001) or Cu (111) at low temperature.

Recently first principles calculations on fcc-based bulk Fe showed its complex magnetic structure [1]. The bulk γ-Fe in AFM state was found to accompany tetragonal distortion and was more stable compared to a high spin (HS) FM state which was stabilized in a cubic symmetry. Even though an AFM state is most stable as expected, the energy difference between AFM and HS FM states was calculated to be quite small (about 20 meV). Hence, it would be a quite interesting question what are the most stable magnetic state at a surface and how far below the surface the magnetism are affected. Thickness dependence of the magnetic anisotropy of a pure γ-Fe film has not been studied in detail yet.

In this work, we have carried out extensive studies the correlation between magnetism and atomic structure of γ-Fe (001) surfaces, using the highly precise full-potential linearized augmented plane-wave (FLAPW) method based on generalized gradient approximation (GGA). In order to take surface and size effects into account, the tetragonally distorted γ-Fe films with different thickness were simulated by single slabs. We used a equilibrium lattice constant (3.49 Å) [1] of bulk tetragonally distorted γ-Fe for AFM state as the in-plane lattice constant. The total energies of Fe thin films composed of 3-, 5-, 7-, 9-, and 11-layers for possible different collinear spin configurations were calculated.

As a result, the magnetic state of FM coupling between two adjacent Fe layers at the surface and AFM coupling between the rest inner layers was found to be most stable, not depending on the film thickness. The MCA energies of the systems were calculated by using a torque method. It was proved that the spin orientations of the systems are perpendicular to the surface regardless of their thickness. The calculated total magnetic moment of a Fe atom at the surface was found to be significantly enhanced to about 2.70μ_B compare d to the tetragonally distorted bulk γ-Fe (1.63 μ_B). Detailed discussion on the origin of ferromagnetism at the surface will be discussed in the conference.

[1] D. Lee and S.C. Hong, J. of Magnetics 12, 68 (2007).