NT-P053

The effects of structural defects on the magnetism of Fe/Cu(111) thin film system

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The unique magnetic behaviors of Fe/Cu(111) thin film system have attracted enormous research activities over decades. Since the portion of perpendicular and in-plane magnetization components and the transition between them are very important to the device performance, accurate controls of magnetic behaviors are necessary. The magnetization directions of the thin film are decided as the result of the competition between in-plane and perpendicular components. In previous experimental and theoretical studies, the magnetic properties of Fe/Cu(111) film were demonstrated to strongly depend on the structural imperfections such as surface roughness, step formation and the twinning boundary formation. Since the anomalous magnetic behaviors of Fe/Cu(111) are due to the complex and simultaneous interplay of quantum mechanical and magneto-static factors, it is extremely difficult to accurately investigate each factor, experimentally. Therefore, we focused on the effects of structural imperfections on the Fe/Cu(111) magnetism using the *ab initio* calculations. The dominant contribution of the intrinsic spin-orbit coupling of Fe atom to the enhanced magnetic moment of Fe on Cu(111) was demonstrated with electron density of states data and the changes in the spin-moment. In addition, the spin-reorientation of growing Fe films on Cu(111), which is generally observed in the epitaxial film growth, could be successfully explained with the electron total energy difference of ferromagnetic and paramagnetic systems.