Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Theoretical analysis of magnetic structures in the fcc-Fe/Cu(001) system[1] YASUTOMI TATETSU, The University of Tokyo, SHINJI TSUNEYUKI, The University of Tokyo, Institute for Solid State Physics, YOSHIHIRO GOHDA, The University of Tokyo, Tokyo Institute of Technology — Magnetic thin films have been studied due to its peculiar magnetic behaviors compared to their bulk systems. Fe/Cu magnetic thin films have been studied for the past decades, because of their uncertain magnetic structures. As is well known, the ground state of Fe has the bcc structure, but the fcc-Fe, which is stable above 1184 K, can epitaxially grow on a Cu(001) substrate even below room temperature, since the lattice parameters of Cu (3.62Å) and fcc Fe (3.58Å) are quite close to each other. Many kinds of studies for the systems have been reported, but its ground state is controversial. We applied first-principles calculations to the fcc-Fe/Cu(001) system using a computational code OpenMX for understanding of its electronic and magnetic structures. Our structural model is a slab model consisting of seven Cu layers and several Fe layers capped by a 10-Å vacuum layer. According to our collinear-spin calculations, an antiferromagnetic structure is stable in the 4 to 7-ML systems and a ferromagnetic coupling at the top two layers can be obtained, which is in good agreement with experimental results. We also calculated the non-collinear spin configuration, which considers the spin-orbit interaction.

[1]This work was supported by the Elements Strategy Initiative Center for Magnetic Materials under the outsourcing project of MEXT and was done by using K computer.

Yasutomi Tatetsu
The University of Tokyo

Date submitted: 14 Nov 2014 Electronic form version 1.4