First-principles calculations of Fe/Cu(001) magnetic thin films

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The ground state of Fe bulk is ferromagnetic with the bcc structure, and nonmagnetic fcc structure is not stable below about 1200 K. Surprisingly, fcc or face-centered tetragonal (fct) Fe films have been grown onto Cu(001) even below room temperature. In this system, peculiar structural and magnetic properties of Fe have been reported[1, 2]. For 1-4 monolayers (ML) of Fe, the crystal structure is fct type and the magnetic structure is ferromagnetic. In the thickness between 5 and 10 ML, the crystal structure is fcc type but the magnetic structure is antiferromagnetic or spin density wave at inner layers but ferromagnetic at the top two layers. For the purpose of understanding electronic and magnetic structures of fct Fe/Cu(001) films, first-principles calculations have been performed. The structural optimisation is considered to calculate a realistic structure of this system. From our calculations, the amount of the magnetic moment in Fe films within 4ML is close to that of bulk fct Fe. On the other hand, the enhanced magnetic moment is obtained at the interlayer and surface. In this talk, more details will be presented.

References:

[1] H. Abe *et al.*, Phys. Rev. B **77**, 054409 (2008)

[2] D. Pescia *et al.*, Phys. Rev. Lett. **58**, 2126 (1987)