Development and control of spin texture by band engineering using quantum-well state

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We have studied a magnetism induced by quantum-well states using density functional theoretical calculation. This year, we focused on a mechanism by which the magnetism of Pd(100) ultrathin film, which shows ferromagnetism induced by quantum-well states, can be controlled by tailoring the Pd/stacking layer interface electronic states (i.e., scattering phase shift of the quantum-well states) [1].

For the experimental observation of the control of magnetism in metals using an external field, thin films with a few monolayers are generally used because of the screening effect. Although previous research showed the effect of the change in the Fermi energy and polarization of the orbital character of the electrons by applying the electronic field, the standpoint of tuning the quantum size effect which was occurred by nano-scaling of the materials was not well discussed. Our present study was focused on quantum-well induced ferromagnetism, which appeared after forming the ultrathin film. Using DFT calculation with PHASE/0 code [2], we clearly show the possibility of paramagnetic to ferromagnetic switching by modifying the interface electronic states of the quantum-wells. Our present discovery opens up a new way to control magnetism by tuning the size effect.

Generally, the quantum-well states, which is the origin of the ferromagnetism in Pd(100) ultrathin films, are described in a one-dimensional quantum-well model containing the phase shift, which is the effect of the electron scattering at the interfaces of wells. First, we expand the function of the phase shift from the real space to momentum space dependency. This theory means that controlling the shape of quantum-well band dispersion will be artificially achieved by modifying the interface electronic states. For the appearance of ferromagnetism, making a flat band at the Fermi energy is important, and we clearly show that stacking of the fcc *d*-electron transition metal layer on Pd quantum-wells makes a flat band, from the DFT calculation based on this theory. We expect that the control of magnetism predicted in our present theory will be experimentally observable in a system of a stacking layer/Pd ultrathin film on a piezo substrate. This can modify the layer spacing (i.e., tune the hybridizing of the wave functions at the interfaces of the wells), and the nonmagnetic to ferromagnetic switching using the multilayer nano film system should be easily achieved.

References

[1] Shunsuke Sakuragi, Hiroyuki Kageshima, and Tetsuya Sato : submitted to Phys. Rev. B.

[2] https://azuma.nims.go.jp/software/phase