Magnetic properties of Fe/Pd(001) bilayer affected by quantum-well states in Pd layer

Kousuke Mochihara[1], Hiroyuki Kageshima[2], and Tetsuya Sato[1]

1Department of Applied Physics and Physico-Informatics, Keio University, 3-14-1 Hiyoshi, Kohoku-ku, Yokohama 223-0061, Japan

2Interdisciplinary Graduate School of Science and Engineering, Shimane University, 1060 Nishikawatsu-cho, Matsue 690-8504, Japan

It is known that at interface between 3d transition metal and (Pd, Pt), strong magnetic anisotropy is generated. We found experimentally that the magnetic anisotropy and magnetic moment of Fe/Pd depend on the thickness of Pd layer [1]. In order to clarify the magnetization change, we performed first-principles calculation using the PHASE/ 0 program.

We used the pseudopotential method and LDAPW92 to the exchange and correlation interactions. A slab of vacuum (two monolayers) /Fe (three monolayers) /Pd (N monolayers) /vacuum (three monolayers), 59 × 59 × 1 k-points, and 36Ry of cut-off energy were used.

We calculated lattice constant which obtains the lowest energy. Using the obtained lattice constant, we calculated Pd layer thickness dependency of the magnetic moment of Fe / Pd slab. As a result, magnetic moment of Fe/Pd changed in oscillatory manner with Pd 6 MLs period, which was in agreement with the experiment. It is known that quantum well states formed in Pd layer changes the electronic state near the Fermi energy in a 6 MLs period [2]. The change of the electronic state based on the Pd quantum well states is considered to be the cause of the change of magnetic moment of Fe/Pd.

We also calculated the energy difference between when the magnetic moment was directed in the out-of-plane direction and when it was directed in the in-plane direction. The energy difference changed depending on Pd layer thickness. In order to investigate the mechanism, electronic band dispersions were calculated. As a result the electronic state near Fermi energy changes depending on the thickness of Pd layer. The magnetic anisotropy is considered to have changed because they depend on electronic states near the Fermi energy.

References

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