磁気トンネル接合 Fe/MgO/Fe および $Fe/MgAl_2O_4/Fe$ における ゼーベック係数の第一原理計算

First-principles calculation of Seebeck coefficients for Fe/MgO/Fe and $Fe/MgAl_2O_4/Fe$ magnetic tunneling junctions

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Recent progress of spin caloritronics enables us to manipulate heat and spin currents. One of the emerging interesting phenomena in spin caloritronics is the analogue of the classical Seebeck effect, such as the magneto-Seebeck effect in magnetic tunneling junctions (MTJs) [1], which is caused by spin-dependent charge current combined with heat current in parallel and anti-parallel magnetization configurations. Similar to the tunnel magnetoresistance (TMR) ratio, the tunnel magneto-Seebeck (TMS) ratio was proposed [1]. However, understanding of the TMS ratio from the property of the material has been less developed than that of the TMR ratio, although it has been measured and calculated in previous studies.

In the present work, we calculated the Seebeck coefficients and the TMS ratios of Fe(5ML)/MgO(5ML)/ Fe(5ML) and $Fe(5ML)/MgAl_2O_4(9ML)/Fe(5ML)$ MTJs using the first-principles density functional method. The electronic transport coefficients of the MTJs were calculated from the Landauer formula. Figure 1 shows the temperature dependences of the Seebeck coefficients of the MTJs in parallel and anti-parallel magnetization configurations from 10 to 300 K. We obtained the positive Seebeck coefficients for the $Fe/MgAl_2O_4/Fe$ MTJ around 300K, while we obtained negative ones for the Fe/MgO/Fe MTJ, which was explained by considering the energy dependence of the electronic conductance relative to the Fermi energy. For the Fe/MgO/Fe MTJ in parallel and anti-parallel configurations, large electronic conductance was obtained above the Fermi energy, which results in the negative Seebeck coefficients in almost all the temperatures, while for the $Fe/MgAl_2O_4/Fe$ MTJ, large electronic conductance was obtained below the Fermi energy, which results in the positive ones. These results may help to understand the origin of the TMS effects.

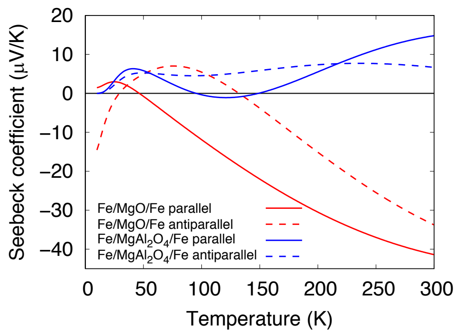

Fig. 1: Temperature dependences of the Seebeck coefficients of Fe/MgO/Fe and $Fe/MgAl_2O_4/Fe$ MTJs

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