Project Title:

Numerical study on new functionality of spin-heat cross effect

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Motivated by recent experimental discovery of a huge Peltier cooling effect on CuNi/Au junctions with the maximum cooling power of 1mW reported by Fukushima *et al.*, we have been studying thermopower on metallic junctions. For a quantitative analysis on Peltier cooling effect on metallic junctions, the thermoelectric parameters for bulk as well as interfaces are estimated by first principles calculations based on the framework of density functional theory with a tight-binding muffin-tin orbitals basis. The Landauer-Büttiker formalism is used to study quantum transport coefficients, and the energy dependence of quantum scattering is determined based on the well-known Mott's law.

As a test case, first, we have studied the thermopower of bulk CuNi (constantan) alloy, and found it in good agreement with the corresponding experimental data. Here, the resistivity is estimated by numerically calculating resistance for different energy levels around the Fermi energy E_F (Fig. 1), which is essentially linear to the thickness of CuNi, as expected from Ohm's law. The resistivity is thus given by the slope of the total resistance as a function of the thickness, which is estimated about 30.46 μΩcm (at Fermi level), consistent with the experiments. The Seebeck coefficient (S) being determined by Mott's law, the thermopower (=–S/T) at room temperature (T) is estimated about 171.75 nV/K^2.

Encouarged by the success of the bulk calculations, next, we have studied the transport properties for CuNi/Au junction. We took gold as one lead and CuNi as another lead, with 10 layers of CuNi and 10 layers of gold in scattering region. For electronic structure calculation, we use virtual crystal approximation to treat an alloy of CuNi in the lead, and coherent potential approximation in the scattering regiom. We have studied two case with and without lattice relaxation due to the latice mismatch of CuNi and gold. We found that the estimated interface thermopower for both cases is around 100 nV/K^2, which is significantly large compared to the bulk value.Therfore, we conclude that the interface contribution to the thermal transport in metallic junctions is much more important than one might have expected, and it needs to be considered for any quantitative comparisons with theoretical calculations and experimental observations.

In further step, we will continue to study the NiFe and CoFe alloys system. We have to extend my account for next usage.

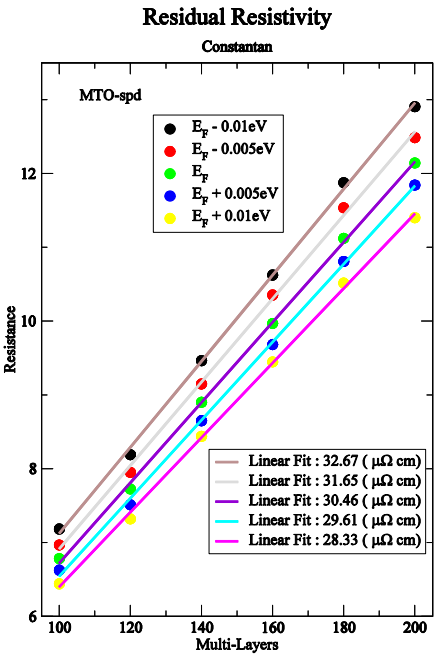

Fig.1. Resistance for CuNi as a function of thickness of CuNi for different energy levels close to Fermi energy E_F indicated in the figure.