Specular to Diffusive Scattering in Fe/MgO/Fe Magnetic Tunnel Junctions

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Nanoelectronic device properties are usually influenced rather strongly by impurities and atomistic disorder. Examples are electron scattering by dopants in semiconductor nano-wires, spin scattering by disorder in magnetic tunnel junctions, and spin polarized current in dilute magnetic semiconductors. Theoretically, any calculated transport quantity must be averaged over the ensemble of possible impurity configurations. There has been no theoretical formalism and computational tool that can effectively carried out disorder averaging for nonequilibrium quantum transport problems. In this poster presentation, we report our recently developed formalism and numerical implementation of the non-equilibrium vertex correction (NVC) theory which is a first principles solution of the *nonequilibrium* impurity average problem for quantum transport. We apply this theory to investigate effects due to oxygen vacancy to spin polarized quantum transport in magnetic tunneling junction (MTJ) Fe/MgO/Fe.

To treat nonequilibrium quantum transport properties of nanoelectronic devices having atomistic substitutional disorder under external bias potential, our first principle formalism is based on carrying out density functional theory (DFT) within the Keldysh non-equilibrium Green's function (NEGF) framework, where the configurational average over random disorder is handled by a nonequilibrium vertex correction (NVC) theory at the density matrix level [1,3]. We use Coherent Potential Approximation to reconstruct translational invariance in the disordered Hamiltonian and one-particle Green's function; and use NVC to perform disorder average for the nonequilibrium density matrix that is determined by NEGF. The NEGF-DFT-NVC formalism is implemented within a tight-binding linearized Muffin tin orbital(TB-LMTO) electronic package. By using the NEGF-DFT-NVC theory, disorder effect to nonlinear and non-equilibrium quantum transport can be calculated from atomic first principles in a self-consistent and efficient manner.

The NEGF-DFT-NVC theory has been applied to investigate the significant physics of diffusive impurity scattering in the realistic nano-devices[1,2,3].   In this poster, as an application, we show new results of the barrier defect scattering in MTJ Fe/MgO/Fe. The

oxygen vacancy has been the major defect but is entirely neglected in all the previous first principle calculations. Our results show a dramatic effect of oxygen vacancy scattering in the MgO barrier. The vacancies next to the interfaces can effectively scatter electrons of d states in the minority spin channel of Fe into the s states with Δ-1 symmetry which can tunnel through MgO by suffering the lowest decay rate. This leads to a huge increase of anti-parallel conductance and reduces the TMR significantly. Furthermore, the vacancy diffusive scattering inside the MgO barrier significantly increase the decay of s-state with $\Delta-1$ symmetry, which enhances the device resistance dramatically. By including oxygen vacancies in the MgO barrier, our calculated results are found to be in excellent agreement with the experimental data of G.X. Miao *et al* (PRL,2008).

Reference:

1, Youqi Ke, Ke Xia and Hong Guo, Phys. Rev. Lett. 100, 166805 (2008).

*2, Youqi Ke, Ferdows Zahid, V. Timoshevskii, Ke Xia, D. Gall, and Hong Guo, Phys. Rev. B **79**, 155406 (2009)*

3, Theoretical issues related to multiple impurity scattering in solid state devices (a book chapter to be published by Springer-Verlag).