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FIRST PRINCIPLES MODELLING OF SPIN-DEPENDENT ELECTRON TRANSPORT IN NANOSCALE DEVICES

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Recently there has been a large effort to develop new electronic devices that use the electron spin to store or process information. The basic physical phenomenon that is utilized is that some materials display a difference in the resistance for transport of majority and minority spin electrons. Thus, there is a great technological interest to find new materials which have strong spin-dependent transport properties.

The spin-dependent transport properties of materials can be accurately modelled using first principles quantum transport methods. Based on such calculations, Butler *et. al.* [1] suggested that an MgO crystal sandwiched between Fe electrodes should display a giant magneto-resistance, i.e. the resistance of junctions with parallel alignment of the electrode spins was found to be orders of magnitude smaller than the resistance of junctions with anti-parallel alignment. Subsequently, there has been a number of experiments that try to realize such materials, however, so far the measured magneto-resistances have been much smaller than predicted by theoretical studies[2].

We have used the Atomistix ToolKit (ATK)[3,4] to model the spin-dependent transport across MgO layers coupled with Fe electrodes, and investigated how the interface structure and defects in the MgO layers affect the spin transport. The results of the calculations will be discussed, and compared with experimental studies.

References:

[1] W. H. Butler, X.-G. Zhang, T. C. Schulthess, and J. M. . Maclaren, *Spin-dependent tunnelling conductance of Fe/MgO/Fe sandwiches*, Phys. Rev. B **63**, 054416 (2001).
[2] S. S. P. Parkin, C. Kaiser, A. Panchulla, P. M. Rice, B. Hughes, M. Samant, and S.H. Yang, *Giant tunnelling magnetoresistance at room temperature with MgO(100) tunnel barriers*, Nature Materials **3**, 862 (2004).
[3] M. Brandbyge, J.-L. Mozos, P. Ordejon, J. Taylor, and K. Stokbro, *Density functional method for nonequilibrium electron transport*, Phys. Rev. B. **65**, 165401 (2002).
[4] Atomistix Tool Kit (ATK). www.atomistix.com

Figures:

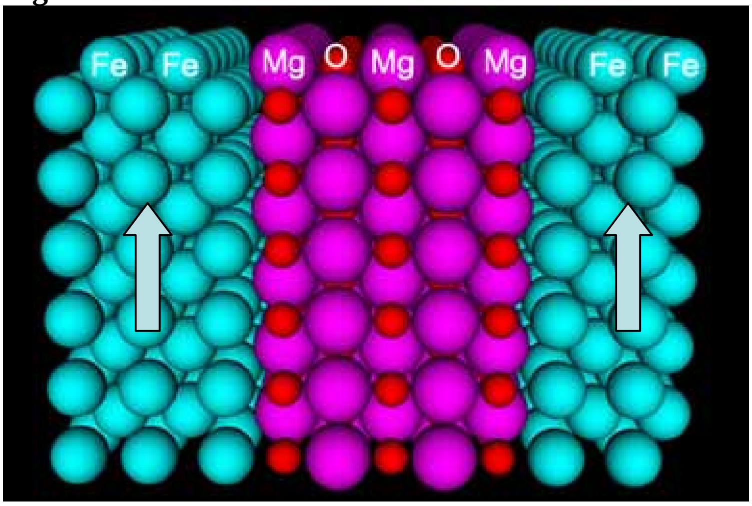

Figure 1: The geometry of an ideal Fe-MgO-Fe interface

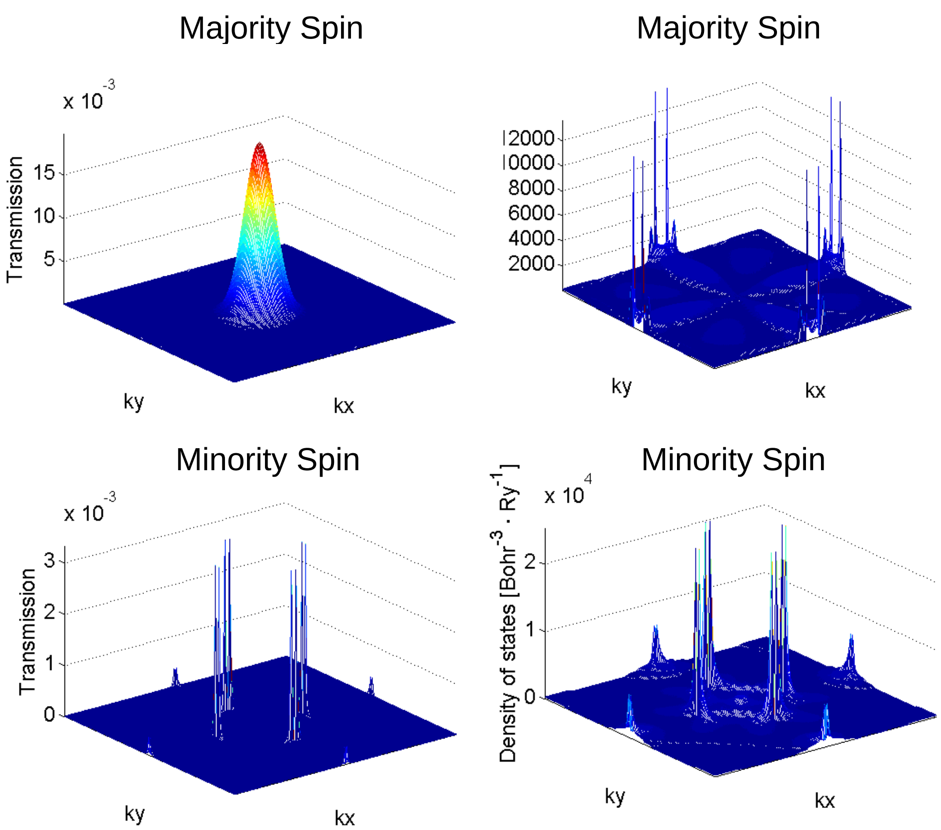

Figure 2: The dependence of the transmission coefficient and DOS on the spin and the k-vector of the electron. Note the large difference in the transmission between majority and minority electrons.