Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Bound states in electronic transport through Fe/MgO tunnel junctions IVAN RUNGGER, NADJIB BAADJI, STEFANO SANVITO, School of Physics and CRANN, Trinity College, Dublin 2, Ireland — Using the ab initio code Smeagol we calculate the electronic transport properties of Fe/MgO/Fe(100) tunnel junctions for applied bias up to 2 Volt. The correct bias-dependent occupation of the interface states (IS) in the Fe/MgO junction is crucial to obtain a physically meaningful potential drop. The coupling of the IS to the Fe electrodes varies strongly for different k-points, and bound states are found along the high symmetry lines and at those k-points where there are no open channels in the Fe leads. A general method for setting the occupation of both weakly-coupled and bound states, based on the notion of a local Fermi energy and a finite relaxation time, is presented. For parallel alignment of the Fe leads the current through the IS is quenched above 20 mV, whereas for the anti-parallel alignment the current flows mainly through IS up to about 0.4 V. In this bias range the TMR shows a pronounced bias dependence, at higher voltages it decays smoothly. If the transmission through the IS is suppressed, for example by adding a finite imaginary part to the energy, the TMR decays monotonically with bias even at low voltage. Finally we show that oxygen vacancies inside the MgO barrier quench the TMR if they are within the first few layers from the interface, and that a similar reduction is achieved by partially oxidizing the Fe interface layer.

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Date submitted: 27 Nov 2007 Electronic form version 1.4