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Reversal of spin polarization in Fe/GaAs (001) driven by resonant surface states: First-principles calculations A.N. CHANTIS, Theoretical Division, Los Alamos National Laboratory, K.D. BELASHCHENKO, Nebraska Center for Materials and Nanoscience, University of Nebraska-Lincoln, D.L. SMITH, Theoretical Division, Los Alamos National Laboratory, E.Y. TSYMBAL, Nebraska Center for Materials and Nanoscience, University of Nebraska-Lincoln, M. VAN SCHILFGAARDE, Arizona State Univesrity, R.C. ALBERS, Theoretical Division, Los Alamos National Laboratory — A minority-spin resonant state at the Fe/GaAs(001) interface is predicted to reverse the spin polarization with voltage bias of electrons transmitted across this interface. Using a Green's function approach within the local spin density approximation we calculate spin-dependent current in a Fe/GaAs/Cu tunnel junction as a function of applied bias voltage. We find a change in sign of the spin polarization of tunneling electrons with bias voltage due to the interface minority-spin resonance. This result explains recent experimental data on spin injection in Fe/GaAs contacts [1,2] and on tunneling magnetoresistance in Fe/GaAs/Fe magnetic tunnel junctions [3].
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