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Ferromagnet/Semiconductor junctions (with M. Zwierzycki, K. Xia, G.E.W. Bauer, and I. Turek)

The huge scientific and technological impact of spin-transport in metallic materials has stimulated attempts to study it in semiconductors. The difficulties encountered can be explained in terms of a resistor model in which the small spin-dependent resistivity of typical ferromagnetic metals is completely dominated by the large spin-independent resistivity of the semiconductor [1]. This model neglects the spin-dependent interface resistance caused by band mismatch of the two materials, known to be important in GMR [2]. We calculate the spin-dependence of the interface resistance between ferromagnetic metals (such as Fe) and compound semiconductors (such as InAs) from first-principles whereby specular and diffuse scattering are treated on an equal footing. We focus here on the special case of Fe/InAs which forms an ohmic contact and so should work at low bias voltages. Depending on the concentration of carriers in InAs, we predict ratios of the spin-dependent interface resistance between 10 and 100 for clean interfaces (Fig.1). The absolute value of the resistance is such that spin-injection into InAs should be observable a distance d from the interface when $\rho_{InAs}d_{InAs} < 4 \times 10^4 \Omega m^2$, the minority-spin interface resistance calculated from the transmission matrices following Schep[3]. We discuss the effect of interface disorder modelled in large lateral supercells and present results for non-Ohmic contacts.

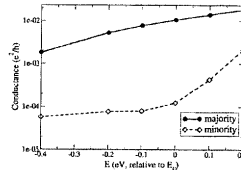


Fig. 1 Spin-dependent conductance for Fe/InAs as a function of the Fermi level in doped InAs. The zero of energy corresponds to a Fermi energy 0.57 eV above the InAs conduction band minimum.

CaB₆ (with H.J. Tromp, P. van Gelderen, G. Brocks, and P.A. Bobbert)

Ferromagnetism was recently observed at temperatures as high as 900 K in La-doped CaB₆ but also in Ca deficient CaB₆ [4] and very recently in CaB₂C₂ [5]. On the basis of local density approximation calculations, CaB₆ has been assumed to be a semimetal. Here we describe how parameter-free quasiparticle calculations of the single-particle excitation spectrum indicate that CaB₆ is not a semimetal but a semiconductor with a band gap of 0.8 eV [5]. If confirmed, this would make it a uniquely interesting material to study from the point of view of spin injection from doped CaB₆ into undoped CaB₆ with zero band mismatch. Magnetism in La_xCa_{1-x}B₆ is found to occur just on the metallic side of a Mott transition in the La-induced impurity band.

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The spin-valve transistor shows very large magnetocurrent ratio exceeding 200%, but the transfer ratio of the transistor, that is, the ratio of the collector to the emitter current, which is important for application, has been only of the order of 10^{-5} [1, 2]. To enhance the transfer ratio by reducing the diffuse scattering in the base, we prepared the transistor using for the base an Fe/Au/Fe (001) epitaxial film that was grown on an nGaAs (001) substrate [3].

The characteristics of the transistor under the external magnetic field were examined by changing the emitter voltage up to 3 V. The transfer ratio increased monotonically with increasing the voltage and that in several samples reached 10^{-3} at 3 V, preserving the magnetocurrent ratio well above 100%. In the voltage dependence of the ratio, we could not observe the transport anomaly, corresponding to the band gap in Au, which exists along <001> direction from about 1.8 eV above E_F . We found a tendency among samples that the samples with the thicker tunnel barrier show the larger transfer ratio. These results as well as the existence of the L valley contribution to the collector current may be ascribed to the broad angular distribution of the injected current, which is caused by the roughness in the tunnel junction. In other words, angular distribution of the current is much wider than the critical angle of reflection at the base/collector interface, and most injected electrons cannot get into the collector. Therefore, the transfer ratio could be further increased not only by increasing the electron transmittance at Fe/GaAs interface, but also by improving the flatness of the tunnel junction.

The dependence of magnetocurrent ratio on the emitter voltage, *i.e.*, on the hot electron energy was analyzed by using a phenomenological model [2] and the enhanced scattering of down-spin electrons in the base was deduced at energies around 1.5 eV above the Fermi level, corresponding to the vacant DOS peak of down-spin bands in Fe. The enhancement is, however, weak, indicating the large contribution of inelastic scattering at these energies.

Recent results on the temperature dependence of magnetocurrent and the prospects of the device for T bits magnetic recording heads will also be discussed.

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