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Micromagnetic and Macrospin Simulations for the "Perpendicular Polarizer-Planar Free Layer" Spin Torque Oscillator

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The possibility of inducing large angle steady state oscillations of the magnetization in a magnetic thin film element by the transfer of spin angular momentum has been widely discussed by theoreticians and experimentalists. In terms of applications, of particular interest are structures containing an out of plane magnetized polarizer. This provides the possibility to excite steady state out-of-plane (OP) magnetization oscillations in an in-plane magnetized free layer at the threshold current and in zero external field [1]. Experimentally, the observation of such OP precessions requires an in-plane magnetized analyzer to monitor the magnetisation motion of the in-plane magnetized free layer. Such double spin valve structures have recently been studied [2] confirming the excitation of OP precessions. In order to compare the experimental results to theory we have performed macrospin and micromagnetic simulations using two different approaches for including the spintorque term in the Gilbert equation of magnetisation motion. In the first case we have used the model introduced by Slonzcewski [3] to describe the dynamics of the free layer by only taking the perpendicular polarizer into consideration. While in a macrospin approximation, the out-of-plane oscillation frequency increases monotonously with increasing current density J, micromagnetic simulations reveal that due to finite sizeeffects two frequency branches exist: a first branch at small J, with increasing frequency for increasing J, and a second branch at larger J, with decreasing frequency. Such behaviour was also observed experimentally [2] and can be explained by the formation of a non-homogenous magnetisation configuration that tends to minimize the out of plane demagnetisation field. While these simulations provide the main features arising from a perpendicular polarizer, an important question remains on the affect of the analyser on the behaviour of the out-of-plane precessional mode. We therefore have used a more general description for the spin torque term which is written as the vector product between the spin accumulation and the magnetization, where the spin accumulation is calculated within the Valet-Fert model [4]. This approach takes into account implicitly any number of magnetic layers in the structure with arbitrary magnetization orientation. It allows us to describe in a self-consistent way the effects of the spin polarized current for the double spin valve structure. An important result of our numerical simulations is that the presence of the analyzer does not modify significantly the character of the out-of-plane precession, neither in terms of the current-field state diagram nor in its frequency dependence. However, besides the OP precessions, we show that an additional excitation mode of in-plane oscillations exists that has also been observed in the experiment.

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First Principles Calculations of Mn_2As

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There has been increasing interest in the use of half-metallic ferromagnets (HMFs) as spin injectors into semiconductors and someHeusler alloys have been predicted to be HMFs. In particular Co_2MnSi is one of them with a highest Curie temperature (985 K). Recently it is shown [1] that the magnetic moment of Co_2MnSi thin film on GaAs is quite reduced, which was attributed to the formation of the antiferromagnetic (AFM) Mn_2As phase. Hilton *et al.* [2] studied the interfacial reactions of Mn/GaAs thin films and it was observed that Mn atoms diffuse at 300 °C into GaAs and form epitaxial two alloy phases of Mn_2As and MnGa.

Mn_2As has a tetragonal Cu_2Sb crystal structure. In the crystal lattice of Mn_2As there are two kinds of cation sites Mn (I) and Mn (II) which are surrounded tetrahedrally and octahedrally by arsenic atoms, respectively.

We employed spin polarized, full potential linearised augmented plane wave (FLAPW) method in generalized gradient approximation (GGA) adopted for the exchange-correlation functional. We used the magnetic unit cell with a=3.78 Å and c=12.56 Å for our calculations. We considered different spin orderings i.e. ferromagnetic (FM), ferrimagnetic (FIM), antiferromagnetic(AFM)-1, and AFM-2. The calculated total energy for these configurations shows that AFM-2 is the ground state of Mn_2As which is consistent with the experimental observations [3]. The total energy difference between AFM and FIM is so small that AFM-FIM transition may occur at low temperature. The calculated magnetic moments are 1.89 and 3.44 μ_B per Mn atom for Mn (I) and Mn (II) respectively. Yuzuri and Yamada [3] found the experimental magnetic moment 3.7 and 3.5 μ_B for Mn (I) and Mn (II) respectively. Our calculated magnetic moment of Mn (II) is very close to the experimental value whereas for Mn (I) there is a disagreement. We will discuss the magnetism with single particle energy spectra.

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