RB14

A Theoretical Study on MgO-Based Magnetic Tunnel Junctions with Half-Metallic Heusler-Alloy Electrodes

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Remarkable progress in tunneling magnetoresistance (TMR) has been achieved by the development of magnetic tunnel junctions (MTJ) with crystalline MgO barrier [1-4]. So far transition metals and their alloys, such as Fe, Co, CoFe, and CoFeB, have been usually exploited as electrodes of MgO-based MTJ and the experimentally observed TMR ratio exceeds 500% at low temperatures [3, 4]. On the other hand, a similar value of TMR ratio has been observed for the MTJ composed of a Heuslar alloy, Co2MnSi, with amorphous aluminum oxide barrier [5]. It can be understood as theconsequence of high spin polarization of the Heusler alloy despite the presence of B2-type atomic disorder [6] and proves the usefulness of half-metallic electrodes evidently to improve the TMR ratio. In the present work, we study the tunneling conductance theoretically for the MgO-based MTJ with half-metallic Heusler-alloy electrodes in order to assess the feasibility of the Heusler alloys as electrodes of the MTJ. The tunneling transmittance via the MgO barrier are calculated as functions of in-plane wave-vector and incident electron energy on the basis of the electronic structure of the MTJ obtained in the framework of the density functional theory [7]. For $Co_2MnSi/MgO/Co_2MnSi$ (001) MTJ, the electronic states having $\Delta 1$ symmetry predominantly contribute to the tunneling transmittancein the parallel magnetization configuration as predicted previously for Fe/MgO/Fe (001) MTJ [8, 9]. For $Co_2CrAl/MgO/Co_2CrAl$ (001) MTJs, on the other hand, the tunneling transmittance is smaller by several orders of magnitude than that of the $Co_2MnSi/MgO/Co_2MnSi$ (001) MTJ, and shows so called *hot-spot*-like dependence on the in-plane wave-vectors even in the parallel magnetization configuration. The characteristic feature obtained for the MgO-based MTJ with Heusler-alloy electrodes can be explained by the electronic structure of each Heusler alloy, i.e. the relative position of the $\Delta 1$ band to the Fermi energy. It is concluded that Heusler alloys withmore than 28 valence electrons, such as Co_2MnSi, Co_2FeAl, and Co_2FeSi, are promising as electrodes of the MgO-based MTJ. In particular, the half-metallic Heusler alloys could bring in high TMR ratio even for low-resistance MTJ with thinner MgO barrier.

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RB15

Calculation of Magnetostatic Fields in Magnetic Cells Relevant to High Density Magnetic Random Access Memory

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Conventional magnetic random access memory (MRAM) using a single free layer has some notable problems of a small write margin between half select and full select and thermal stability [1]. In order to solve these problems, Savchenko *et al.* invented toggle MRAM using an exchange-coupled (usually antiferromagnetic) trilayer as the free layer structure where two magnetic free layers are separated by a very thin nonmagnetic layer [2]. Recently, Worledge was able to derive the total energy in an analytical form for the trilayer structure [3]. One novel feature is the inclusion of the magnetostatic energy in the total energy. In doing so, four simple assumptions were used and two of themwith particular relevance to this work were (1) each magnetic layer was in the single domain state and (2)for an identical magnetic layer thickness, the demagnetization field of a layer is equal to the stray field from the other layer. Although the latter assumption appears reasonable for a very thin space layer (~1 nm or smaller),this has a serious implication, zero shape anisotropy even for the geometry of high aspect ratios as far as the magnetization is aligned antiparallel. This results in the fact that the switching field and magnetic energy (which are closely related to the thermal stability) are nearly independent of the aspectratio of the magnetic thin film, although these parameters are expected to be very sensitive to the aspect ratio [4]. In this paper, we calculate the demagnetization field and the stray field in exchange-coupled trilayers relevant to high density MRAM in order to verify the assumption.

The calculations were carried out using a commercial program package (multiphysics finite element analysis COMSOL). The trilayer thin films with an elliptical geometry consisted of two free layers and a spacer layer between them. The long (x axis) and short (y axis) axes were fixed at 212 nm and 106 nm, respectively. The thickness (z axis) of the two free layers was varied while the total thickness was fixed at 6 nm (3, 3), (3.27, 2.73), (3.5, 2.5), (3.69, 2.31), (3.81, 2.19) where the numbers in the parentheses are in nm. The thickness of the spacer layer was fixed at 1 nm. The saturation magnetization was 1,500,000 A/m. Preliminary calculations were performed in a 2D geometry (212 nm (x axis) and 3 nm (z axis)) where the mesh generation was much easier resulting in more accurate results.

The demagnetization field isuniform over the entire thin film and this can be expected from the ellipsoidal geometry. Also its magnitude is nearly identical to the theoretical estimation using the equations reported by Osborn [5]. In the centralregion, the magnitude of the stray field is nearly identical to the demagnetization field, in agreement with the assumption made by Worledge. However, the effective stray field, averaged over the entire volume, is much smaller than the demagnetizing field. This is mainly due to a large nonuniformity of the stray field at the edge. The present results clearly indicate the need of the modification of the Worledge model.

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