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Magnetic properties of $Mn_2As(001)$ surface: A first-principles study

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One of the manganese-arsenic compounds, Mn_2As, attracted an attention as a spacer in MnGa-based magnetic multilayer [1]. In the Mn_2As with a tetragonal Cu_2Sb structure of space group P4/nmm, there are two different symmetry types of Mn atoms: the Mn(I) atoms positioned at (0.0, 0.0, 0.0) and (1/2, 1/2, 0.0) are surrounded tetrahedrally by As atoms and the Mn(II) atoms at (0.0, 1/2, z) and (1/2, 0.0, -z) with the parameter z=0.33 are surrounded octahedrally by As atoms. The experimentally measured magnetic moments of Mn(I) and Mn(II) atoms by neutron diffraction were 3.7 and 3.5 μ_B, respectively [2]. A theoretical calculation [3] for the ground state (the antiferromagnetic 2 phase) bulk Mn_2As gave much smaller magnetic moment (1.87 μ_B) for the Mn(I) atom comparing with the experiment, while that of the Mn(II) atom (3.43 μ_B) was comparable to the experimental value. It is usual that the surface electronic structures and magnetic properties are different significantly with those of the bulk due to the symmetry breaking at the surface. Creating Mn-terminated (001) surfaces for Mn_2As, there are two different terminating surfaces with Mn(II) atoms, i.e. the Mn(II)1-term and Mn(II)2-term in which the surface Mn atoms lose four next nearest neighbour As atoms and two nearest neighbour As atoms, respectively.

In this study, the magnetic properties of Mn-terminated (001) surfaces of Mn_2As were investigated by use of the full-potential linearized augmented plane wave (FLAPW) method [4] embodied in QMD-FLAPW code within the generalized gradient approximation (GGA) [5]. We considered three different types of the Mn-terminated surfaces, i.e., Mn(I)-term, Mn(II)1-term, and Mn(II)2-term, in the calculation. The calculated results showed that the magnetic moment of surface Mn(II) atom in the Mn(II)1-term was greatly increased to 4.46 μ_B which is close to the value of free Mn atom, and those of the surface Mn(I) atom in the Mn(I)-term and the surface Mn(II) atom in the Mn(II)2-term were also enhanced to 3.38 and 3.77 μ_B compared with the bulk value. The magnetic moment of the center layer Mn(I) atom was about 1.97 μ_B and thoseof the Mn(II) atoms in the deep inner were about 3.23 μ_B, regardless of the terminations, which are consistent with the results of bulk system [3]. The calculational results are discussed in relation with the band narrowing effect at surface and the hybridizations between the Mn-d and As-p states using the calculated spin polarized layer projected density of states (LDOS).

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Design optimization of the bit and word lines in magnetic random access memory in the Stoner-Wohlfarth model

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In conventional magnetic random access memory (MRAM) where the magnetization switching is based on the asteroid curve, the main issues to be addressed as the density increases are a narrow write window and a high switching field. The cross-talk effect can be another important issue. There are four half-selected cells lying immediately adjacent to the full-selected cell andthese half-selected cells experience stray fields from the adjacent bit line and word line currents. The magnitude of these stray fields is typically less than 10% of the corresponding bit line or word line field [1]. Obviously, the stray field problem becomes more significant as the density increases. In this work, the simple Stoner-Wohlfarth model was used to optimize the bit and word lines.

The total energy under the simple model consists of the Zeeman energy and the intrinsic anisotropy energy. Magnetic fields are applied in two different directions in order to simulate the magnetic fields from the bit line and word line currents. Then the total energy can be expressed as follows;

$$E = K_u \sin^2\theta - H_b M_S \cos\theta - H_w M_S \cos(\alpha - \theta)$$

In this equation, α is the angle between the word line and bit line fields. Normally, $\alpha = 90^\circ$(namely the word line and bit lines are crossed at right angle); this is no longer true in this work, however. By finding a minimum in the energy, the way in which the bit line switching field varies with α and the word line field can be calculated and some of these results are shown in Fig. 1. The results can be of great value in the optimization of the switching field and the write margin. The total energy equation can also be used to predict the thermal stability of half-selected cells.

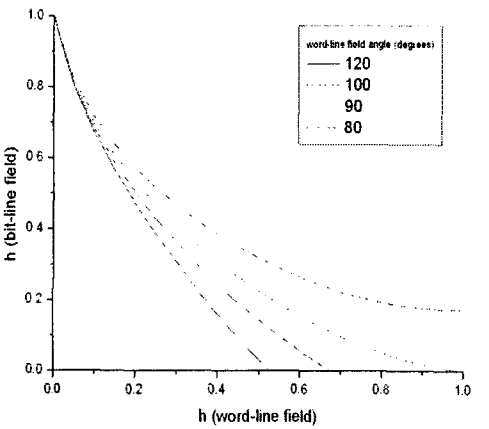

Fig. 1. The asteroid curves in the first quadrant as a function of the angle between the word line and bit line fields.

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