Optik 127 (2016) 8951–8955

Contents lists available at ScienceDirect

Optik

journal homepage: www.elsevier.de/ijleo

Electric field induced transitional magnetic coupling in (Ga, Cr)N/GaN magnetic tunnel junctions

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ARTICLE INFO

Article history:
Received 26 April 2016
Accepted 21 June 2016

PACS:
73.61.Ey
75.50.Pp
75.30.Ev

Keywords:
First-principles calculations
Magnetic tunnel junction
Antiferromagnetic
Electric field

ABSTRACT

Diluted magnetic semiconductor (DMS) composed in magnetic tunnel junctions (MTJs) are predicted to have potential applications in spintronics. However, the crucial issue is how to control the magnetic order of DMSs. In our semiconductor MTJs (SMTJs) model, formed of (Ga,Cr)N/GaN/(Ga,Cr)N multilayers, we found that the electrons can transfer from one (Ga,Cr)N electrode to another upon the external electric field, hence the magnetic interaction between two doped Cr ions in each (Ga,Cr)N DMS electrode can be changed from ferromagnetic to antiferromagnetic. The phenomenon proposes a possible way for the application of SMTJs.

1. Introduction

Since the discovery of electric-field effect on magnetism, first demonstrated in ferromagnetic semiconductors [1,2], extensive studies are extended on many other materials [3,4]. Much attention has been paid on magnetic tunnel junctions (MTJs), the electrical switching of magnetization was realized for changing the magnetic anisotropy by using electric-field pulses [5,6]. Conventional MTJs are composed of metal and insulator. In recent years, another MTJs have been become hot spots, which are formed from diluted magnetic semiconductor (DMS) and pure semiconductor (SMTJs). In contrast to metal electrodes, high quality DMSs have many special properties and can be prepared easily or integrated with different devices. Many DMSs have been applied for SMTJs, such as GaAs [7], SbTe [8], GaN [9], and ZnO [10], however, the SMTJs have some difficulty in actual applications because of the unstable magnetism of DMSs. Various theoretical models have been investigated, for instance, the reliable ferromagnetism in transition metal (TM) doped GaN systems has been widely observed [11–13]. For the practical application of SMTJs, the extremely important issue is how to control the magnetism in the DMS multilayers effectively. As we know, the electronic properties of materials can be obviously changed by external electric field [14–16], which suggests a possible way to control the magnetic coupling of DMS electrodes in the SMTJs.

In this paper, we applied an external electric field to investigate (Ga,Cr)N based SMTJs by density functional theory. Without the electric field, the magnetic coupling between the uper and lower DMS electrodes is ferromagnetic. However, while increasing the intensity of electric field, the magnetic coupling switched from ferromagnetic to antiferromagnetic. It is

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http://dx.doi.org/10.1016/j.ijleo.2016.06.080
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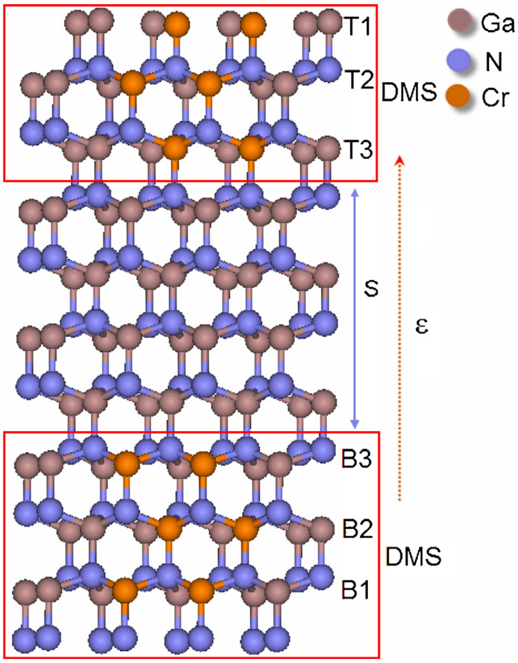

Fig. 1. The structure of (Ga,Cr)N/GaN/(Ga,Cr)N junction based on 10 layers of GaN along the [001] direction of $4 \times 2 \times 5$ GaN supercell. The external electric field across the SMTJs is from bottom to top electrode.

found that the transferation of electrons between the two DMS electrodes plays an crucial role on such magnetic switching. Our results give an effective way to control the magnetic properties in DMSs and also broaden the functionality of SMTJs consequently.

2. Calculation details

In present model, the SMTJ is simulated as shown in Fig. 1, a $4 \times 2 \times 5$ GaN supercell is constructed along [001] direction as a vacuum layer (10 Å). We denote these layers as top and bottom layers, marked as T_n and B_n ($n = 1$–3), respectively. Two nearest neighbor Cr^{3+} ions are doped in both T_n and B_n GaN layer, which is referred to as the (T_n, B_n) model. Therefore the artificial dipole sheet has been made separately by the vacuum GaN layers. The concentration of Cr atoms is 5.0%. As our previous paper, the nearest neighbor Cr atom has the strongest ferromagnetic interaction and the d orbit of Cr^{3+} ions presents as high-spin ions with electron configurations$(e\uparrow)^2(t_2\uparrow)^2$. Our calculations were performed within first-principles DFT using the projected augmented wave (PAW) method [17] was used within the Vienna ab initio simulation package (VASP) [18]. Electron exchange and correlation effects were described within the generalized gradient approximation (GGA) in the Perdew-Burke-Ernzerh of (PBE) parameterization [19]. In all calculations, an energy cut off of 450 eV for the plane-wave expansion of the wavefunctions was used. The electronic calculations were performed using a dense mesh with $5 \times 5 \times 1$ k-points and the planar dipole layer method [20] is employed which has been used in several studies sucessfully [21,22]. The electric field is applied along the [001] direction.

3. Results and discussion

For the present SMTJs,we mainly investigated the nearest distance between the uper and lower layers, which is marked (T_3, B_3) model. As predicted in our previous theoretical work [23], the interaction between the two Cr^{3+} ions in each (Ga,Cr)N-based electrodes (the magnetic moment is about $4.45\mu_B$ per Cr atom) and the coupling between the two (Ga,Cr)N electrodes are both ferromagnetic (FM). We expected to transfer electrons from one (Ga,Cr)N electrode to another electrode and the magnetism of each (Ga,Cr)N electrode might be changed, then an external electric field was employed across the (Ga,Cr)N/GaN/(Ga,Cr)N junction from the bottom (B_3) to the top (T_3) layers. As shown in Fig. 2, the magnetic interaction between two Cr atoms in the (Ga,Cr)N electrode is intrinsically FM in the present (T_3, B_3) model. We also calculated the (T_2, B_2) and (T_1, B_1) models, the results are similar to the (T_3, B_3) model, but the FM coupling became much more weaker. Wang et al. had studied the magnetic coupling in the (Ga, Mn)N system and they considered the surface effect played an important role in the magnetic properties of Mn-doped GaN DMS [24]. Although a detailed investigation of Cr-doped GaN DMS is beyond the scope of present work, the same conclusion should apply to the (Ga,Cr)N system. From Fig. 2, it is clear that as the electric field intensity (estimated as ε) increases, the FM interaction in the SMTJs becomes more and more weaker.