Properties of VAs/GaAs interface from first principles study

R. Q. Wu, G. W. Peng, L. Liu and Y. P. Feng
Department of Physics, National University of Singapore, 2 Science Drive 3 117542, Singapore
E-mail: Phyfyp@nus.edu.sg

Abstract. Density functional theory calculations with local spin density approximation (LSDA) have been performed to study the properties of VAs/GaAs interface. It was found that the half-metallicity of Cr layers close to the interface remains unchanged for an abrupt interface. The valence band minimum (VBM) of the minority spin lies well below the Fermi level of the majority spin (1.0 eV). The Schottky barrier height (SBH) to GaAs (n-type) is calculated to be 1.09 eV, which is acceptable regarding the band gap of GaAs. The conservation of half-metallicity at the interface indicates that such a heterostructure is a promising candidate for high efficiency spin current injection at high temperature.

1. Introduction
Efficient electrical injection of highly polarized spin current into conventional semiconductors at room temperature becomes critical in the field of spintronics. Many efforts have been made but there is still a long way to a realistic application. Ferromagnetic transitional metals and semiconductors heterostructures were thought a straightforward approach for polarized spin current injection based on the fact that the substantial conductivity difference between the majority spin and the minority spin can induce spin polarized current under bias. This concept was initially tested by Hammar et al. [1] but only a few percent polarization of the current was obtained at very low temperature. Similar effort in this approach did not show significant improvement [2, 3, 4]. Temperature is one of the reasons responsible for the poor efficient spin current injection as at room temperature, the magnetic electrodes may partially loose its ferromagnetism and thus the polarization decreases. The interface structure, disordering, mixing or discontinuity can also deteriorate the polarization by severe spin-flipping. The most fundamental reason is the giant conductivity mismatch between the ferromagnetic electrode and the semiconductor, as proposed by Schmidt et al. [5]. Yet, according to their prediction, an efficient spin current injection requires a 100% polarized spins at Fermi level in the magnetic electrode.

Half metallic (HM) compounds thus attracted much interest as they have a band structure with only one occupied set of spin density of states at the Fermi level, and thus shuld be capable of 100% polarized spin current injection in principle. Half-metallic Heusler compounds [6] and other ferromagnets [7] have been proposed and studied for this purpose. Unfortunately, according to the available experimental results on the Co$_2$MnGe-GaAs heterostructure by Dong et al. [8], the injected spin current polarization decreases with increasing temperature and the value at room temperature is much lower than the expected value of 100%. The unexpected
experimentally observed poor efficiency probably can be explained by the magnetic properties at the interface from studies by Picozzi et al. [9, 10]. In the Co$_2$MnGe layers at the interface, the half-metallicity is partially lost so that 100% polarization does not exist. The second possible reason can be the band alignment at the interface. The majority Fermi level falls into the gap of GaAs. Thus a bias should be applied for the majority spin injection. Yet, Co$_2$MnGe is a narrow gap semiconductor ($E_g=0.2$ eV) with the minority spin valence band maximum (VBM) being very close to the majority Fermi level (0.03eV below the Fermi level). As a result the majority spin can be excited to the conduction bands of the minority spin and injected to GaAs along with the majority spin. This suggests that interface between the HM ferromagnet and the semiconductor plays an essential role in the spin current injection and it is necessary to evaluate the half-metallic ferromagnet in combination with the semiconductor on which it is epitaxially grown. The half-metallicity and the band alignment should be carefully examined for designing a high efficient spin current injector.

With less than 1% lattice constant mismatched to GaAs, zinc-blende VAs favors a ferromagnetic rather than antiferromagnetic ordering [11] with a half-metallic electronic structure. From the mean field approximation calculation by Sanyal et al. [11] and the spin fluctuation theory calculation by Kübler [12], ZB-VAs possesses a Curie temperature much higher than room temperature. The minority band gap is estimated over 2.0 eV by DFT-GGA calculation [13]. The high Curie temperature and the wide minority band gap make it a promising magnetic electrode candidate for high polarization spin injection. Also, its zinc-blende structure and lattice constant make it probable to form geometrically coherent interface with zinc-blende GaAs substrate to minimize spin-flipping caused by interface disorder and discontinuity.

However, other important issues remain unresolved. For example, whether the VAs layers can maintain half-metallicity and the wide minority energy gap remain under strain are not clear. The relative positions of the majority Fermi level and the minority VBM of GaAs have not been studied which is important for technological considerations (for instant, a majority Schottky barrier height (SBH) to $n$-type GaAs larger than the band gap of GaAs is obviously not acceptable for GaAs IC). Thereby in this report, we perform spin density functional theory calculation to study the magnetic properties and the band alignment at the VAs/GaAs interface.

2. Computational Details
Our calculation is based on the spin polarized density functional theory (DFT) as implemented in the plane wave code VASP [14, 15]. The local spin density approximation (LSDA) is used for the exchange-correlation functional. The Vanderbilt ultrasoft pseudopotentials [16] are used to represent the electron-ion interactions. For Gallium, 3$d$ electrons are treated as valence state to ensure the transferribility. Two six-layer slabs, one for ZB-VAs (001) and the other for GaAs (001) were stacked along $c$ direction to form the interface. The in-plane lattice parameter $a$ was set to that of the GaAs and the $c$ was optimized to minimize the total energy. The atomic coordinates in GaAs layers were fixed while those in CrAs were fully relaxed. A kinetic energy cutoff of 520 eV was used. A $6\times6\times1$ K-mesh according to the Monkhorst-Pack scheme [17] was adopted to sample the Irreducible Brillouin Zone (IBZ). All these parameters were carefully checked to ensure a good convergence.

3. Results and Discussion
The lattice constant of ZB-GaAs is 5.60 Å and VAs 5.55 Å. So the lattice constant mismatch is less than 1%. The LDA gap of GaAs is 0.56 eV with valence band maximum and conduction band minimum (CBM) of 1.27 and 1.83 eV respectively. The lattice constant of VAs agrees well with those of previous similar calculations [11].
Figure 1. Band structures of the majority spin (a) and the minority spin (b) along with concerned energies, $E_f$ of the majority spin, CBM and VBM of the minority spin. Unit: eV.

Figure 2. The spin density of states projected on the third (a), the second (b) and the first (c) layer V atom to the interface. The Fermi level $E_f$ is set to zero and positive and negative values are relative to the majority and the minority spin states, respectively. The vertical dotted line serve as an indicator.
Figure 3. The in-plane (solid line) and the macroscopic (dashed line) averaged electrostatic potentials (a) and the energy alignment (b) based on (a). Unit: eV.

Figure 1 shows the spin polarized band structure of zinc-blende VAs with lattice constant slightly expanded to that of GaAs along with energies of band edges with respect to the averaged electrostatic potential of the bulk materials. The majority and the minority spin band structures of VAs show that the half metallic nature remains unchanged upon strain effect. The minority spin has a band gap of 1.41 eV. Due to the inefficiency for the conduction bands calculatin by DFT in LDA, this value should be lower than actual one and can only serve as a very rough estimation. The Fermi level lies at 1.26 eV over the VBM of the minority spin. This value should be sufficient to prevent the minority spin at VBM from being injected to semiconductors by thermal excitation should it be maintained at the interface.

To study the electronic properties of the V layers near the interface, we show the density of states (DOS) of the V layer considered in the supercell in Fig. 2. A cutoff radius of 1.45 Å and dense 12×12×1 k-mesh are used for the DOS calculation. As shown in the figure, the bulk property is recovered at the second V layer from the interface. For the V layer nearest to the interface, the DOS is slightly different. The energy gap between the Fermi level and VBM of the minority spin is reduced to around 1.0 eV (See the vertical dotted line). This value is larger than those of common Heusler compound semiconductors and high enough to prevent active thermal excitation of the minority spin.

The energy alignment at the interface is evaluated by the well established ”bulk plus lineup” method in which the macroscopic averaged electrostatic potentials are used as reference energies as proposed by van de Walle et al. [19]. The macroscopic averaged electrostatic potential (dashed line) along the c direction is plotted in Fig. 3 (a) along with its in-plane average (solid line). The difference between the two macroscopic averaged electrostatic potentials ∆V is estimated to be 0.69 eV. Base on this lineup, we plot the energy alignment in Fig. 3 (b). Here the experimental value of 1.42 eV for the band gap of GaAs is used to correct the CBM. For the majority spins, the energy difference between the Fermi level and the CBM of GaAs which is the Schottky barrier height (SHB) of n-type GaAs, is estimated to be 1.09 eV. This means that an equivallent bias should be applied for the majority spin current to be injected to n-type GaAs. This bias is still acceptable compared to the band gap of GaAs.

4. Conclusion
The spin density functional theory calculations have been carried out to study the VAs/GaAs interface. Electronic properties and energy alignment at the interface have been obtained. DOS calculation revealed that the VAs can maitain its half-metallicity at the interface and the Fermi level lies well above the VBM of the minority spin under strain effect. These results suggest that
VAs is a promising candidate for spin injection to GaAs semiconductor. High polarized spin current injection can be expected for the VAs/GaAs heterostructure. Schottky barrier height is only 1.09 eV for $n$-type GaAs which is suitable for GaAs IC technological application.

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