Spin Injection and Filtering in Halfmetal/Semiconductor
(CrAs/GaAs) Heterostructures

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Abstract. We present theoretical investigations of the spin-dependent transport properties of a Halfmetal/Semiconductor (CrAs/GaAs) heterostructure, which indicate that the structure is a probable candidate for efficient room temperature spin injection and filtering. The spin dependent electronic structure of zinc blende CrAs and the band offset between GaAs and CrAs are determined by ab initio calculations within the method of linear muffin tin orbitals (LMTO). The obtained band structures of the bulk materials are mapped onto an effective sp$^3$d$^5$s$^*$ nearest neighbor tight binding (TB) model and the steady state transport characteristics are calculated within the non-equilibrium Green’s function approach. We find current spin polarizations at room temperature up to ??%.

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INTRODUCTION

Theoretical investigations of bulk CrAs by means of density functional theory (DFT) revealed that, as a bulk material, CrAs crystallizes in an orthorhombic structure and shows antiferromagnetic behavior [1]. Interestingly, when epitaxially grown on GaAs, CrAs can crystallize in the zinc-blende (zb) structure showing half-metallic ferromagnetic behavior, i.e., 100% spin polarization at the Fermi energy, with a Curie temperature well above room temperature [2]. These findings suggest that CrAs might be an interesting material to realize room temperature spin injection into semiconductor materials. Here, we study the current-voltage (IV) characteristics of a CrAs single barrier consisting of 10 atomic layers sandwiched between two GaAs leads. Our theoretical results reveal that GaAs/CrAs heterostructures can act as efficient room temperature spin filters.

THEORETICAL APPROACH AND RESULTS

The theoretical approach consists of three major steps: (i) the calculation of the ab initio electronic structure of the materials involved and the determination of the band offset between those materials, (ii) the mapping of the electronic structure onto an effective sp$^3$d$^5$s$^*$ nearest neighbor TB model, and (iii) the calculation of the IV characteristic within the framework of the non-equilibrium Green’s function approach.

(i) Electronic Structure and Band Offset. The electronic structure of bulk zb GaAs, bulk zb CrAs and a (GaAs)$_6$(CrAs)$_6$ supercell was calculated with the LMTO-ASA code as developed by Jepsen and Andersen [3]. Based on these calculations we determine the band offset $\Delta$ between bulk GaAs and bulk CrAs by using almost flat, deep lying As-s band as the reference state [4]. With respect to the center of mass of this band we obtain $\Delta_1 = 0.601$ and $\Delta_2 = 0.545$ eV for the majority and minority spin, respectively.

(ii) Effective sp$^3$d$^5$s$^*$ Tight Binding Model. The part of the ab initio CrAs band structure, which contributes to the transport, is fitted within a nearest neighbor sp$^3$d$^5$s$^*$ TB Hamiltonian by minimizing the cost functional

$$K(\xi) = \sqrt{\sum_{nk} a_n(k) |\epsilon_n^{LSM}(k) - \epsilon_n^{TB}(k, \xi)|^2},$$

using a genetic algorithm. Here, $\xi$ are the TB-parameters, $n$ denotes the band index, $k$ is the $k$-vector, $a_n(k)$ are normalized weights and $\epsilon_n^{LSM}(k)$ and $\epsilon_n^{TB}(k, \xi)$ denote the ab initio and the tight binding band structure, respectively. The fit procedure will be discussed in more detail elsewhere. The ab initio electronic structures of majority and minority spin CrAs, the respective fits, and the fitted band structure of GaAs are plotted in Figs. 1 and 2.

(iii) Steady State Transport. The space-dependent transport Hamiltonian of the GaAs/CrAs/GaAs structure is set up by performing a partial Wannier transform of the basis states from the wave-vector $\mathbf{k}$ to $(x, k_{\parallel})$ [5], where
FIGURE 1. (Color online) Majority spin CrAs ab initio band structure (red solid line), CrAs TB fit (green dashed line), and GaAs TB fit (blue dash-dotted line). The Fermi energy $E_F = 0.01 \text{ eV}$ above the conduction band minimum of GaAs is indicated by the horizontal solid line.

FIGURE 2. (Color online) Minority spin CrAs ab initio band structure (red solid line), CrAs TB fit (green dashed line) and GaAs TB fit (blue dash-dotted line). The Fermi energy is indicated by the horizontal solid line.

$x$ denotes the growth direction of the crystal and $k_\parallel$ is the in-plane momentum, yielding

$$H(k_\parallel) = \sum_{i,\sigma\sigma'} c_{i,\sigma}^{(i)} \epsilon^{(i)}_{\sigma\sigma'} c_{i,\sigma'}^{\dagger} + \sum_{i,\sigma\sigma'} t^{(i)}_{\sigma\sigma'} c_{i+1,\sigma}^{\dagger} c_{i,\sigma'} + \text{h.c.},$$

with $c_{i,\sigma}^{\dagger}$ denoting the creation operator for site $i$ and orbital $\sigma$, $\epsilon^{(i)}_{\sigma\sigma'}(k_\parallel)$ and $t^{(i)}_{\sigma\sigma'}(k_\parallel)$ are onsite and hopping matrices, respectively. The transmission function is calculated from the system’s retarded (R) and advanced (A) Green’s functions $G^R/A$ and the coupling functions $\Gamma_{L/R}$ functions of the left (L) and right (R) leads, respectively,

$$T(E, k_\parallel) = \text{Tr} \left[ \Gamma_R G^R \Gamma_L G^A \right],$$

where $E$ is the total energy and $\text{Tr} [\cdot]$ denotes the trace operation. The steady state current $J$ is then calculated by the Landauer-Büttiker formula:

$$J = \frac{2e}{h} \sum_{k_\parallel} \int dE \ T(E, k_\parallel) \left[ f_L(E) - f_R(E) \right].$$

Here, $e$ is the elementary charge, $h$ is Planck’s constant, and $f_{L/R}$ denote the Fermi-Dirac distributions of the left and right lead, respectively. The IV-characteristics of the single barrier GaAs/CrAs/GaAs system for different temperatures is shown in Fig. 3, where a linear voltage drop from the left to the right lead is assumed. Even at room temperature the current of one spin species remains strongly suppressed compared to the other, which leads to the desired spin filtering and spin injection into the right GaAs lead.

Based on our tight-binding transport model a detailed investigation of the dependence of this effect on the properties and modeling of the interface will be given in near future.

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REFERENCES