The electronic band structure of ferromagnets with spin injection and extraction

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We study spin injection and spin extraction signals in lateral spin-valve structures consisting of ferromagnetic Co2FeSi contacts on n-type GaAs transport channels. The dependence of the spin-valve signals on the bias current is found to strongly depend on the degree of ordering in the Co2FeSi lattice. For the fully ordered L21 phase, the signal is equal for injection and extraction and independent of the bias current. In contrast, a strong dependence of the relative signal strengths (spin injection versus extraction) on the bias current is observed for the partially disordered B2 phase. We explain the strongly different behavior by the crucial influence of the respective electronic band structure on the spin generation processes.

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I. INTRODUCTION

For semiconductor spintronics, the generation of spin-polarized carriers in nonmagnetic semiconductors by electrical means is regarded as a major building block [1]. One promising approach to realize such building blocks is the utilization of ferromagnetic contacts acting as spin-polarized sources in ferromagnet/semiconductor (FM/SC) or FM/insulator/SC hybrid structures. Two processes are considered for the generation of a spin accumulation in the SC when driving an electrical current through the interface(s). For n-type SCs, spin injection refers to the case of a net electron flow from the FM into the SC (reverse bias for Schottky contacts). In contrast, an electron flow from the SC into the FM (forward bias for Schottky contacts) leads to the process of spin extraction, resulting in a spin polarization in the SC which is of opposite sign compared to that created by spin injection [2,3].

In a nonlocal spin valve (NLSV) consisting of FM contact strips on a nonmagnetic (n-type SC, metal, graphene) lateral transport channel, both spin generation processes can be observed [3–12]. Nonlinear dependences of the NLSV signals on the bias current were discussed in some reports in terms of an exchange-split energy band in the FM assuming a parabolic dispersion [10], or localized electron states near (at) the FM/SC interface [4,5,9,13].

We have previously demonstrated that the hybrid system consisting of the Heusler alloy Co2FeSi on n-type GaAs transport channels holds promise for potential spintronic applications [3,14]. Co2FeSi in the fully ordered L21 phase is considered to be half metallic and, hence, an ideal candidate for electrical spin injection [15]. Disorder drastically modifies the electronic band structure [16]. The partially disordered B2 phase, for example, not only lacks half metallicity, but also exhibits an opposite spin polarization at the Fermi level. In this paper, we investigate the bias-current dependence of spin generation in Co2FeSi/GaAs NLSVs and compare our experimental results with the expectations derived from the bulk band structures obtained by first-principles calculations for the two different Co2FeSi phases.

II. EXPERIMENT

The investigated samples were grown by molecular beam epitaxy on semi-insulating GaAs(001) substrates. The layer sequence consists of a 1500-nm-thick, lightly n-type doped (nt= 2 × 1016 cm−2) GaAs spin transport layer, followed by a 15-nm-thick layer with a linearly increasing doping density ranging from nt to nH= 5 × 1018 cm−2 and a heavily doped (nH) 15-nm-thick layer leading to a narrow Schottky barrier. After transfer in ultrahigh vacuum into a growth chamber for metals, a 16-nm-thick layer of the ferromagnetic Heusler alloy Co2FeSi was deposited epitaxially. Detailed information on the growth of the Heusler alloy Co2FeSi is provided elsewhere [17,18]. Most important for our investigation is the fact that the crystal phase in the Co2FeSi layers can be controlled by the choice of the appropriate substrate temperature (Tg) during growth [16,19,20]. Layers consisting dominantly of the L21 (B2) phase were grown at Tg= 280 °C (Tg≈ 60 °C).

The lateral transport devices were processed by wet chemical etching as well as photolithography, and finally by the evaporation of Au bond pads. The device structure comprises a 50 × 400 μm2 conductive mesa region with Co2FeSi strip contacts and is described in more detail in Ref. [14]. For the present experiments, a center-to-center separation between the spin generation (injection or extraction) and detection contact strips was chosen to lie between 6.5 and 12.5 μm. All measurements were performed at 20 K in a He exchange gas cryostat with the electrical signals recorded by a standard dc method. The NLSV experiments were conducted in the same manner as described, e.g., in Refs. [4,6,14].

III. RESULTS AND DISCUSSION

A. Spin-valve signals

The operation of NLSVs containing L21 Co2FeSi contact strips has already been demonstrated in Ref. [14]. For a NLSV structure with B2 Co2FeSi contact strips, the absolute value of the nonlocal spin voltage (VNL) is shown in Fig. 1 as a function of the external magnetic field (μ0H) for the two opposite bias-current directions. The observed voltage jumps ΔVnj and ΔVextr correspond to the switching between parallel and antiparallel magnetization of the spin generating and detecting strips during an upward sweep of the magnetic field. These

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characteristic spin-valve signatures provide clear evidence for both electrical injection and extraction of spin-polarized electrons in Co$_2$FeSi/GaAs transport structures. Note that the $V_{NL}$ jumps for spin extraction and injection are of opposite sign. $\Delta V_{\text{extr}}$ and $\Delta V_{\text{inj}}$ are defined as their absolute values. The complete NLSV characteristics including both upward and downward sweeps of the magnetic field are shown for both a net electron flow into (dark blue circles: $\Delta V_{\text{inj}}$) and out of (green squares: $\Delta V_{\text{extr}}$) the contact strip used for spin generation. Note that the $V_{NL}$ jumps for spin extraction and injection are of opposite sign. $\Delta V_{\text{extr}}$ and $\Delta V_{\text{inj}}$ are defined as their absolute values. Inset: NLSV signal induced by spin injection during upward and downward sweeps of the magnetic field.

B. Current-voltage characteristics

To clarify whether or not the electrical Co$_2$FeSi/GaAs contact properties are the origin of the different behavior found for the spin generation induced by the $B2$ and $L2_1$ phases (cf. Fig. 2), we measured the current-voltage characteristics of the respective contacts in a three-terminal arrangement described, e.g., in Ref. [23]. The obtained voltage drop at the FM/SC interface ($V_{BL}$) is shown in Fig. 3 as a function of bias current ($I_B$) for $L2_1$- and $B2$-phase contacts. Both current-voltage curves are not fully symmetric with respect to the forward and reverse current directions, i.e., for spin extraction and injection conditions, respectively. However, the observed asymmetries are very similar for $L2_1$- and $B2$-phase contacts. Consequently, we exclude the electrical contact properties as the major reason for the strongly different current dependences of $\Delta V_{\text{inj}}/\Delta V_{\text{extr}}$ observed for $L2_1$ and $B2$ Co$_2$FeSi contacts (cf. Fig. 2). Nevertheless, it is worth noting that the asymmetry in the current-voltage curve is presumably the reason for $\Delta V_{\text{inj}}/\Delta V_{\text{extr}}$ being larger than unity at the lowest current values in the case of $B2$-phase contacts (cf. Fig. 2). The signal ratios shown in Fig. 2 have been determined at fixed absolute current values which correspond to somewhat different interface voltages $V_{NL}$ in forward (extraction) and reverse (injection) directions. For example, a fixed bias current of 100 $\mu$A corresponds to interface voltages of 218 and 285 mV in the forward and reverse directions, respectively (cf. Fig. 3).
However, for B2-phase contacts, the individual signals $\Delta V_{\text{inj}}$ and $\Delta V_{\text{extr}}$ depend in a very different manner on the interface voltage $V_B$, as will be shown in the discussion below.

C. Simulation of spin generation

In order to understand the strongly different behavior of the two Co$_2$FeSi phases revealed in Fig. 2, we have to consider the bias voltage dependence of the spin generation processes with regard to the specific electronic band structure in the ferromagnetic contacts. The two different spin generation processes, spin injection and extraction, are illustrated in Fig. 4 and have to be distinguished in the following way. The transmission of free carriers through a FM/SC interface is spin dependent for either direction of the electrical current due to the spin-dependent density of states (DOS) in the conduction band of the FM. Spin injection (reverse bias) takes place mainly at the (quasi-) Fermi energy ($E_F$) in the FM, considering tunneling through the Schottky barrier being much less efficient for electrons at lower energies. In a more accurate approach, we include the contribution of electron states at energies ($E$) below the Fermi level in Co$_2$FeSi and use the following low-temperature approximation for the transmission coefficients of spin-up ($T^\uparrow$) and spin-down ($T^\downarrow$) electrons at the FM/SC interface:

$$T^{\uparrow\downarrow}(\Delta E) \propto \int_{E_F-\Delta E}^{E_F} W(E)D^{\uparrow\downarrow}(E)\,dE,$$

(1)

where $D^{\uparrow\downarrow}(E)$ is the spin-dependent density of states in the Co$_2$FeSi conduction band (see the left panel of Fig. 4 for the B2 phase). The quasi-Fermi level $E_F$ on the FM side is chosen as the point of reference for the energy scale ($E = 0$). As a tunneling weighting factor, we use $W(E) = \exp[-(\phi_B - E)/E_0]$ with reasonable values for the Schottky barrier height $\phi_B = 0.7$ eV and the characteristic tunneling energy $E_0 = 0.1$ eV. In the lightly doped semiconductor channel, a very narrow ($\delta$-like) energy distribution of occupied states is assumed with the Fermi energy lying only a few meV above the conduction band edge.

For spin extraction (forward bias), we have to consider the DOS in the FM at an energy $\Delta E = eV_B$ above the (quasi-) Fermi energy (cf. Fig. 4). Finally, we arrive at following relations for the spin polarizations $P_{\text{inj}}$ and $P_{\text{extr}}$ created in the semiconductor by spin injection and extraction, respectively:

$$P_{\text{inj}}(\Delta E) \propto T^\uparrow(\Delta E) - T^\downarrow(\Delta E) \propto \frac{\Delta E}{E_F},$$

(2)

$$P_{\text{extr}}(\Delta E) \propto \frac{\Delta E}{E_F + \Delta E},$$

(3)

$$\Pi(E) = \frac{D^\uparrow(E) - D^\downarrow(E)}{D^\uparrow(E) + D^\downarrow(E)}.$$  

(4)

In fact, both the injected and extracted spin polarizations depend in a combined manner on the voltage $V_B = \Delta E/e$ and the energy-dependent spin polarization $\Pi(E)$ in the conduction band of Co$_2$FeSi. Since the NLSV signals ($\Delta V_{\text{inj}}$ and $\Delta V_{\text{extr}}$) are both proportional to the generated spin polarizations in the SC ($P_{\text{inj}}$ and $P_{\text{extr}}$), we use the following relations for the comparison between experiment and simulation (see, e.g., Ref. [14]),

$$\Delta V_{\text{inj( extr)}} = \gamma P_{\text{inj( extr)}}I_B,$$

(5)

$$\frac{\Delta V_{\text{inj}}}{\Delta V_{\text{extr}}} = \frac{P_{\text{inj}}}{P_{\text{extr}}},$$

(6)

FIG. 3. (Color online) Absolute value of the FM/SC interface voltage ($V_B$) as a function of the bias current measured in a three-terminal arrangement for L2$_1$- and B2-phase Co$_2$FeSi contacts.

FIG. 4. (Color online) Left panel: Spin-dependent (spin-up and spin-down) density of states for the B2 phase of Co$_2$FeSi obtained by first-principles calculations [16]. Right: Conduction band edge in GaAs as a function of position for the cases of spin injection (lower green curve) and spin extraction (upper dark blue curve) conditions. The directions of the net electron flow are indicated by the dark blue leftwards and green rightwards arrows for spin injection and spin extraction conditions, respectively.
where \( y \) represents a constant (bias-independent) factor for a given NLSV configuration. For the calculation of \( P_{\text{inj}} \) and \( P_{\text{extr}} \) based on Eqs. (1)–(3), we used the spin-dependent density of states \( D_{\uparrow\downarrow}(E) \) of Co₂FeSi given in Ref. [16] as a result of first-principles calculations (see the left panel of Fig. 4 for the B₂ phase).

Figure 5 displays the simulated ratios \( P_{\text{inj}}/P_{\text{extr}} \) as a function of the absolute value of the voltage \( V_B = \Delta E/e \) for both the \( L₂_1 \) and the B₂ phase. Because of the half-metallic characteristic of the \( L₂_1 \) phase, the spin polarization \( \Pi(E) \) is 100% in the vicinity of the Fermi energy resulting in constant polarizations \( P_{\text{inj}} = P_{\text{extr}} = 1 \) as well as a constant ratio \( P_{\text{inj}}/P_{\text{extr}} = 1 \) in almost the whole energy range between 0 and 300 meV. In contrast, for the B₂ phase, the injected (extracted) spin polarization \( P_{\text{inj}} (P_{\text{extr}}) \) decreases (increases) with increasing voltage \( V_B = \Delta E/e \). As a consequence, the ratio \( P_{\text{inj}}/P_{\text{extr}} \) exhibits a strong energy (voltage) dependence. The qualitative behavior obtained for B₂-phase contacts can be easily deduced from the corresponding electronic band structure shown in Fig. 4. For the \( L₂_1 \) phase, the spin-dependent density of states is given in Ref. [16]. The band structure obtained by first-principles calculations reveals a half-metallic gap which extends from 800 meV below to about 300 meV above the Fermi energy. As a consequence, the polarization \( P_{\text{extr}} \) starts to decrease when approaching \( V_B = 300 \) meV (\( \Delta E = 300 \) meV), which is manifested in Fig. 5 by an increase in the ratio \( P_{\text{inj}}/P_{\text{extr}} \). Since the voltage \( V_B \) is a monotonic function of the current applied during the NLSV experiments (cf. Fig. 3), it is justified to directly compare the experimental data in Fig. 2 with the simulated results in Fig. 5. Indeed, the simulated voltage (current) dependence of \( P_{\text{inj}}/P_{\text{extr}} \) (cf. Fig. 5) reproduces the strong difference in the behavior of the NLSV signal ratio \( \Delta V_{\text{inj}}/\Delta V_{\text{extr}} \) observed for the two Co₂FeSi phases (cf. Fig. 2). In contrast to the simulation for \( L₂_1\)-phase contacts, the measured signal ratio exhibits no increase when approaching \( V_B = 300 \) meV. This finding indicates that the actual half-metallic gap extends to even more than 300 meV above the Fermi energy. Note that a constant ratio \( P_{\text{inj}}/P_{\text{extr}} \) (or \( \Delta V_{\text{inj}}/\Delta V_{\text{extr}} \)) could also be obtained by a ferromagnetic band structure with exactly the same energy dependence of a finite density of states for both spin subsystems (above and below the Fermi level) which, however, constitutes an extremely unlikely case.

In order to directly compare our simulations with the measured NLSV data, we display in Fig. 6 the individual signals \( \Delta V_{\text{inj}} \) and \( \Delta V_{\text{extr}} \) as a function of the interface voltage \( V_B \). For the simulations according to Eq. (5) as well as for the presentation of the experimental data, the relation between the bias current \( I_B \) and the interface voltage \( V_B \) has been taken from the current-voltage curves shown in Fig. 3. Note that the absolute signal strengths depend on the actual device dimensions chosen for the NLSV measurements with the \( L₂_1 \)- or B₂-phase contacts. For the voltage dependences of all individual NLSV signals, a good agreement is found between experiment and simulation. In the case of B₂-phase contacts, different scaling factors \( y \) have to be used for injection and extraction conditions in order to account for the experimentally observed relative signal strengths. Most strikingly, the spin injection signals of the two different Co₂FeSi phases reveal strongly different voltage dependences. Remarkably, no decrease of the spin injection signal \( \Delta V_{\text{inj}} \) is observed for voltages up to 450 mV in the case of \( L₂_1 \)-phase contacts. This finding indicates that voltage-dependent spin relaxation processes in the GaAs channel under reverse-bias conditions are here of minor importance [9,22].
IV. CONCLUSIONS

Our observations demonstrate that the specific characteristics of the electronic band structures in the FM contacts indeed manifest themselves in the current dependences of the spin generation processes. With this knowledge, we have a tool at hand to probe details of the spin-polarized electronic band structure of ferromagnetic materials. In this way, our experimental findings confirm the results of the first-principles calculations reported in Ref. [16]. In particular, for the $L_2^1$ phase of Co$_2$FeSi, the prediction of a half-metallic character is strongly supported, an important material property which is otherwise very difficult to access experimentally.

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