Initial/final state selection of the spin polarization in electron tunneling across an epitaxial Fe/GaAs(001) interface

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Spin dependent electron transport across epitaxial Fe/GaAs(001) interfaces has been investigated using photoexcitation techniques. Spin filtering is observed in the forward bias regime and its sign is switched by using different photon energies. First principles calculations suggest that the spin polarization of the Fe layer is positive within the energy region into which spin polarized electrons tunnel. The authors attribute this sign switching to the initial and final states of the electrons tunneling across the interface, whose spin polarizations are determined by the selection rules in GaAs during photoexcitation and spin polarization of the Fe(001) layer, respectively.
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A significant amount of research has recently been carried out on spin dependent charge transport in semiconductors (SCs) for use in future generations of electronic devices.[1] In order to fully exploit the spin transport properties in SCs, it is crucial to develop adequate external spin injectors and detectors since the carriers in widely used commercial semiconductors are not intrinsically spin polarized. Some of the most promising materials for spin injector and detector are ferromagnetic metals (FMs) because their high Curie temperatures make them suitable for room temperature (RT) operation. Several remarkable results have been reported on spin injection (where spin-polarized electrons travel from a FM into a SC) using the electroluminescence technique. For instance, Hanbicki *et al.* have reported a spin polarization of 32% in a GaAs quantum well with an abrupt Fe/AlGaAs interface,[2] and also Jiang *et al.* reported 57% using a CoFe/MgO(100) spin injector.[3] Despite these reports of high spin injection efficiencies, there has been no robust demonstration of three-terminal semiconductor-based spintronic devices. One major issue here is the lack of a comprehensive understanding of spin detection. It is noteworthy that the underlying physics of spin injection and detection are not identical for several reasons. The Schottky barrier at the interface is an asymmetric barrier which is abrupt on the FM side and decays exponentially towards the bulk SC. In addition, the available energy states of a FM layer are different for spin injection and detection. During spin injection, electrons at the Fermi level in the FM propagate into the SC, while electrons travel into the unoccupied states above the Fermi level of the FM in the case of spin detection. This is due to a finite voltage for the device operation, which elevates the conduction band minimum of the SC higher than the Fermi level of the detecting FM. Therefore, intensive studies of spin detection are required in order to develop three-terminal spintronic devices. One of the most useful approaches to the investigation of spin detection phenomena is that of spin-polarized photoexcitation.[4–6] In this letter, we present our recent observation of the bias dependence in spin filtering for electron tunneling across an epitaxial Fe/GaAs(001) interface followed by an explanation of the underlying physics.

A Si-doped ($n=1\times10^{24}$ m^{-3}) GaAs layer was grown on a GaAs(001) substrate, followed by As capping layer growth in a semiconductor molecular beam epitaxy (MBE) chamber. Prior to the preparation of the Fe/GaAs interface, an Ohmic GePd layer was prepared on the bottom of the sample by thermal evaporation. The GaAs substrate was then loaded into a metal MBE chamber with a base pressure of 3.0×10^{-10} mbar. After dissolving the As layer, a 5 nm thick Fe layer was grown at RT, monitored by reflection high-energy electron diffraction (RHEED), and capped with 3 nm Au. The magnetic properties of the sample were investigated by using magneto-optical Kerr effect (MOKE) magnetometry. Photoexcitation measurements were performed at RT in a conventional setup in an in-plane geometry[6] using a He-Ne laser with a wavelength of 632.8 nm ($h\nu=1.96$ eV) and two laser diodes with wavelengths of 670 nm (1.85 eV) and 785 nm (1.58 eV), respectively (for more details of the setup, please see Ref. 5).

The observed RHEED image [inset in Fig. 1(b)] indicates epitaxial growth of Fe on the clean GaAs substrate. The magnetic field dependence of the helicity dependent photocurrent ΔI (which is the difference in photocurrent for illumination with right and left circularly polarized light) using the He-Ne laser at zero electrical bias is shown in Fig. 1. Both ΔI loops, measured along different crystallographic directions, closely follow the results of MOKE measurements (inset in Fig. 1) in terms of coercivity as well as the shape of the hysteresis, thereby signifying clearly that the ΔI signals are entirely controlled by the magnetization of the Fe layer and that any helicity dependent effects in GaAs can be ruled out in our measurements. As ΔI is known to be a superposition of spin filtering at the FM/SC interface and magnetic circular dichroism (MCD) in the FM layer,[6,7] we subtracted the MCD contribution from the net ΔI (as shown in detail in Refs. 6 and 7) in order to obtain the current contributed by the spin filtering effect (ΔI_{SF}). Figure 2 shows the typical bias dependences of ΔI_{SF} for the epitaxial Fe/GaAs(001) interface measured using lasers with different photon energies. It is important to note that only the shapes of the ΔI_{SF}

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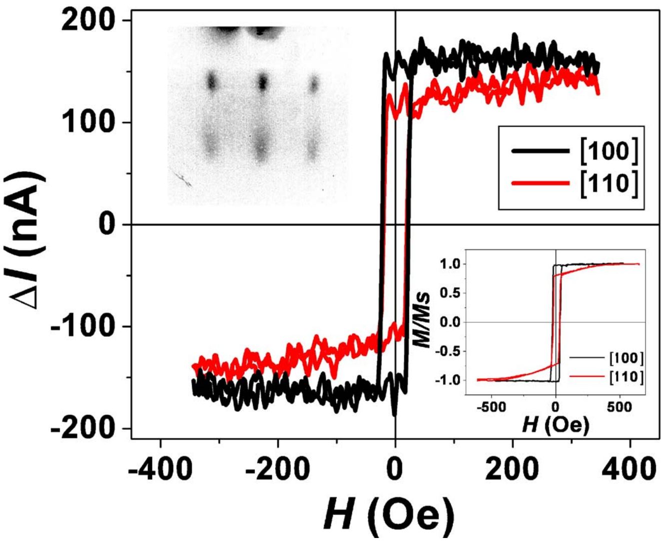

FIG. 1. (Color online) Magnetic field dependence of ΔI for a sample with an epitaxial Fe/GaAs(001) interface using a photon energy of 1.96 eV. The sample was measured at zero bias and along different magnetic field directions. The observed RHEED pattern for the Fe layer along the [110] direction and MOKE loops for the same sample are shown in the inset.

curves can be discussed due to the difference in the laser intensities, which creates different numbers of excited electrons in GaAs. For $h\nu = 1.96$ eV, in the reverse bias region, where most electrons travel into the bulk of the GaAs, ΔI_{SF} is nearly zero, implying that the MCD effect in the Fe layer predominantly contributes to ΔI. On the other hand, a distinct peak is observed in the forward bias region, which is in good agreement with previous photoexcitation measurements.[6,7] The fact that ΔI_{SF} rapidly decreases above a certain positive bias value strongly suggests that electron tunneling is responsible for the observed spin filtering effect: if electrons traveling over the Schottky barrier are responsible for the measured spin filtering effect, the monotonic increase in ΔI_{SF} with increasing bias would be expected. A similar behavior can be seen for the case of using photons with $h\nu = 1.85$ eV. However, when decreasing the photon energy down to $h\nu = 1.58$ eV, ΔI_{SF} is found to change its sign in the forward bias region; this sign change in ΔI_{SF} was also demonstrated for other samples with an epitaxial Fe/GaAs interface (not shown here). Here, the negative ΔI_{SF} suggests that the conductance of minority spin electrons is larger than that of majority electrons at the interface. We now describe an interpretation of how the photon energy dependence of the spin filtering occurs at the Fe/GaAs(001) interface.

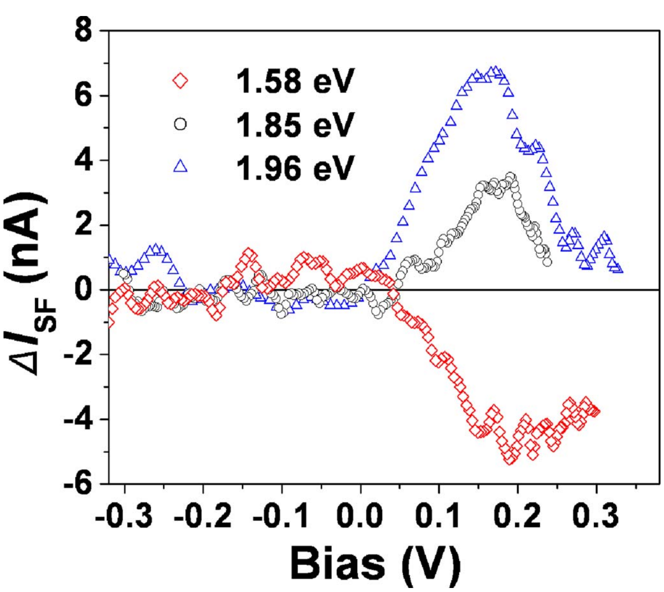

FIG. 2. (Color online) Bias dependence of ΔI_{SF} for an epitaxial Fe/GaAs(001) interface for different photon energies.

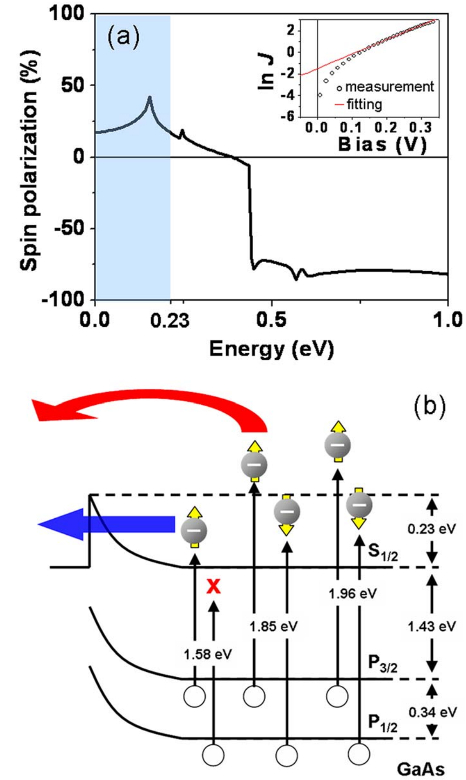

FIG. 3. (Color online) (a) Computational calculation for the spin polarization of Fe(001) as a function of the energy, where the zero energy indicates the Fermi level. The Schottky barrier height is estimated to be 0.23 eV from ln J vs bias plot (inset): circle and red line represent experimental results and fitting line, respectively. The states between the Fermi level and the Schottky barrier height (the blue region) are available for electrons to travel into. (b) A schematic energy diagram for different photoexcitation processes according to the selection rules.

It has been shown both experimentally[2,3,6,7] and theoretically[8,9] that electron tunneling can be responsible for spin dependent electron transport across FM/SC interfaces. When an electron tunnels through a barrier, the initial and final electron states play key roles in determining the tunneling probability. In this section, the spin polarizations of both initial and final states for tunneling are discussed in order to clarify the observed spin filtering effects. Using density functional theory,[10] a generalized gradient approximation,[11] and the method introduced in Ref. 12, we calculated the spin polarization of bulk Fe(001) states (Fig. 3), which is to be the final states for the tunneling process. By fitting the J-V characteristics [inset in Fig. 3(a)] using the thermionic emission theory,[13] the height of the Schottky barrier (Φ_B) for the sample is estimated to be ~0.23 eV, assuming that most electrons travel across the interface via thermionic emission (however, a small but finite number of electrons tunnel through the interface[6]). Therefore the energy levels into which the tunneling electrons travel are in the range from the Fermi level up to 0.23 eV of the Fe layer (here, we assume that the conduction band minimum is at the same level as the Fermi level in the GaAs due to the high Si doping of the GaAs). The calculation results point out that the spin polarization of the Fe layer in this region remains positive.

On the other hand, the spin polarization of the photoexcited electrons in GaAs prior to tunneling is mainly determined by the selection rules (outlined in Ref. 14). The spin-orbit interaction in GaAs splits the sixfold p states into fourfold $P_{3/2}$ and twofold $P_{1/2}$ states with a 0.34 eV gap at the Γ point and, most importantly, electrons photoexcited from the $P_{3/2}$ states are oppositely spin polarized to those from the $P_{1/2}$ states due to the selection rules. We now define the energy $E_H = h\nu - E_t$, which represents the energy height from the bottom of the conduction band to the states into which electrons are photoexcited at Γ, where E_t is the minimum energy necessary for a given transition from either $P_{3/2}$ and $P_{1/2}$ states into the bottom of the conduction band. For the photoexcitation with $h\nu = 1.58$ eV, only the transitions from the $P_{3/2}$ states are allowed to occur with $E_H = 0.15$ eV. Using photons with $h\nu = 1.85$ (1.96) eV, both transitions are allowed, with $E_H = 0.42$ (0.53) eV for $P_{3/2}$ states and 0.08 (0.19) eV for $P_{1/2}$ states, respectively. For the two higher photon energies, the electrons photoexcited from the $P_{3/2}$ states are excited with higher $E_H (> \Phi_B)$ and hence travel thermionically across the interface, thereby losing their spin polarization. However, the electrons photoexcited from the $P_{1/2}$ states with lower $E_H (< \Phi_B)$ predominantly contribute to the spin dependent electron transport by tunneling. As a result, electrons photoexcited from the $P_{3/2}$ states give rise to the spin polarization at the interface only for the measurement with $h\nu = 1.58$ eV. Since the electrons photoexcited from the two states of the valence band are oppositely spin polarized to each other, the spin polarizations of initial electron states for tunneling across the interface change its sign when altering the photon energy down to 1.58 eV. As mentioned previously, the spin polarization of the Fe layer for the tunneling process is positive, and therefore, the combination of the spin polarizations of the initial and final states for the tunneling process across the interface clearly reflects the observed sign change in ΔI_{SF} as a function of the excitation energy.

Further support to our interpretation is given by the photoemission measurements of spin-polarized electrons from p-type GaAs by Pierce and Meier.[14] They measured the spin polarization of electrons photoemitted from GaAs(011) by Mott scattering and observed the onset of $P_{1/2}$ states contribution in GaAs as a function of the photon energy. Although they observed the change of the total net spin polarization only, the difference between their and our findings is explained by the different type of interface. Their observation is based on a vacuum/CsO/SC interface with a negative electron affinity, where the whole range of excited electrons may contribute to the spin polarization. In our case, the spin dependent electron transport at the FM/SC interface is more sensitive to the energy of electrons because the Schottky barrier acts as a spin selective barrier.

In conclusion, we have studied the spin filtering behavior at epitaxial Fe/GaAs(001) interfaces with photoexcitation techniques and observed that the spin filtering effect is strongly dependent on the photon energy. In particular, a sign change of the spin filtering is observed when decreasing the photon energy to 1.58 eV. We ascribe this sign change to the influence of the spin polarizations of available initial/final states for tunneling electrons represented by the selection rules in GaAs and the spin polarization of the Fe(001) layer, respectively. This finding underlines the importance of initial/final states for tunneling during spin dependent electron transport at FM/SC interfaces and especially offers possibilities for developing useful functionality in spintronic device architectures where spin dependent conductance can be controlled by altering the states available for electrons tunneling at the FM/SC interface.

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