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Numerical calculation model for spin-dependent transport of photoexcited electrons across Fe/GaAs(0 0 1) interfaces

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Abstract
Spin-dependent transport of photogenerated electrons across Fe/GaAs(0 0 1) interfaces is calculated using a one-dimensional electron transport model. Creation of spin-polarized electrons by photoexcitation in this model is defined by the band structure of GaAs along the [0 0 1] direction and the optical selection rules. The tunnel probability across the interface is obtained from Chang's model and first principles calculations are employed to calculate the spin polarization of Fe for electrons propagating along the [0 0 1] direction. By combining the above ingredients, the spin-filtering current, I_{SF}, was calculated for different parameter values, including Schottky barrier height and photon energy. The model is used to fit with experimental results of the photoexcitation technique, yielding qualitative agreement especially for the observed sign switching of the spin-filtering current.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Spintronics is a multi-disciplinary field combining expertise from magnetic, semiconductor and optical physics with the aim of utilizing the spin degree of freedom in novel electronic/optical devices [1]. As a key building block of such devices, a ferromagnetic metal (FM)/semiconductor (SC) interface is expected to serve as input (injection) and output (detection) parts of spin-polarized current in semiconductors. However, there has not been developed an efficient way of spin injection/detection at room temperature yet, and therefore it is indispensable to reveal detailed physics on both spin injection and detection in FM/SC interfaces. A useful technique that enables investigation of spin-dependent electron transport across FM/SC interface is spin-polarized photoexcitation [2]. In this measurement, circularly polarized light creates spin-polarized electrons in GaAs via the optical selection rules [3] and an FM/SC interface is employed to measure the spin polarization electrically. Despite a large number of investigations using this technique [4–10], there are no theoretical calculations supporting them, to the authors' knowledge, except for recent tight-binding calculations on an Fe/GaAs interface by Honda *et al* [11]. Here, we present a phenomenological model designed for these photoexcitation experiments. Our model is simple and empirical, but we found that calculated results using the model fit well with our measured data. Furthermore, the dependence of the spin-filtering effect on various parameters is presented.

2. Calculation model

Our model for spin-dependent transport of photoexcited electrons across FM/SC interfaces is based on a one-dimensional stack of an Fe/Schottky barrier/GaAs(0 0 1) interface, schematics of which are shown in figure 1. Spin-polarized electrons are created in GaAs (part 1) and tunnel through the Schottky barrier (part 2) into the Fe DOS (part 3). Each part of the process was calculated individually and used to calculate the overall spin-dependent transport of such photoexcited electrons, assuming that the electron energy and spin orientation are conserved between the processes.

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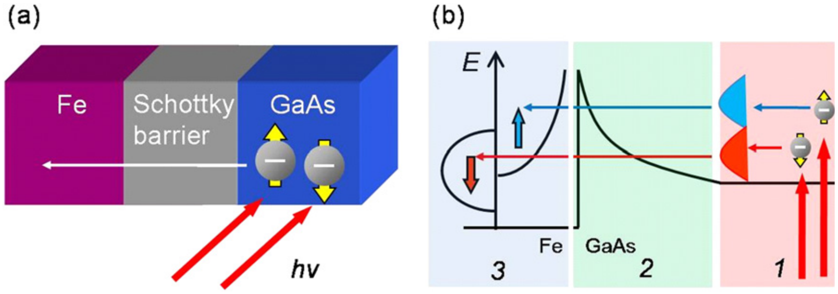

Figure 1. (*a*) Block diagram and (*b*) energy diagram schematic for the calculation model of spin-dependent transport across an Fe/GaAs(0 0 1) interface.

2.1. Optical spin excitation in GaAs

To calculate the creation of spin-polarized electrons in GaAs, we assume that electrons are excited by a pure circularly polarized light around the Γ point and the kinetic energy of the photoexcited electrons is obtained using the effective mass approximation for the GaAs band structure as follows:

$$h\nu = E_g + \frac{\hbar^2 k_0^2}{2m_e^*} + \frac{\hbar^2 k_0^2}{2m_h^*}, \tag{1}$$

where E_g, $\hbar$, k_0, m_e^* and m_h^* are the energy gap, the reduced Planck constant, the wavevectors of the photoexcited electrons/holes and the effective masses of electrons and holes in GaAs. Since the creation of spin-polarized electrons takes place close to an FM/SC interface in the spin-polarized photoexcitation measurements, we assume that the electron energy is not fully relaxed down to those of equilibrium electrons during the electron transport in GaAs; a typical electron thermalization time is a few picoseconds [12], which is longer than an electron transport time in GaAs after photoexcitation (estimated to be about 1 ps for our experiment [13]) and the tunnelling time (estimated to be shorter than 1 ps [14, 15]). However, processes of this thermalization are difficult to treat analytically [12] and the exact description of the energy-distribution function for non-equilibrium electrons is unknown. We therefore model the spread of the energy distribution as a Gaussian function with standard deviation σ_s around the excitation energy; we set $\sigma_s = k_B T(300\,\mathrm{K}) = 26\,\mathrm{meV}$ for our calculations and later σ_s was used as a fitting parameter. Under this assumption the energy distribution of the spin polarization packet, $N_{\mathrm{GaAs,i}}(E, V)$, of the photoexcited electrons for a given transition i can be written as

$$N^{\mathrm{i}}_{\mathrm{GaAs}}(E, V) = \frac{1}{\sigma_s\sqrt{2\pi}} \exp\left(-\frac{\left(E + qV - \frac{\hbar^2 k_0^2}{2m_e^*}\right)^2}{2\sigma_s^2}\right). \tag{2}$$

Here, $N_{\mathrm{GaAs,i}}(E, V)$ is a function of the electron energy E, q is the electron charge and V is the applied bias. In our model, $E = 0$ is defined to correspond to the Fermi level of Fe. GaAs has three optical transitions across the bandgap, the heavy-hole (hh), light-hole (lh) and split-off hole (sh) bands to the conduction (c) band. The transition probabilities and the kinetic energies of photoexcited electrons for these transitions are different due to the optical selection rules [3] and the effective masses of holes, respectively. By taking into account the transition probabilities, the total spin polarization created around the Γ-point of GaAs is given by

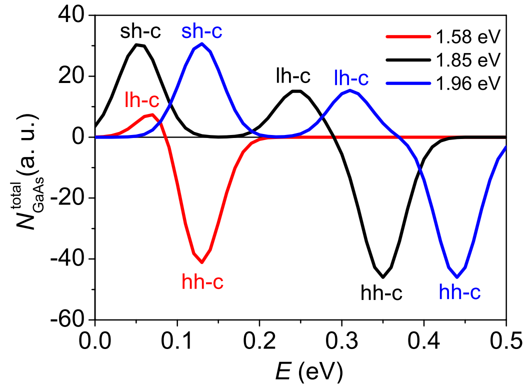

Figure 2. $N_{\mathrm{GaAs,total}}$ for different light energies, 1.58, 1.85 and 1.96 eV, at $V = 0$.

$$N^{\mathrm{total}}_{\mathrm{GaAs}}(E, V) = -3N^{\mathrm{hh-c}}_{\mathrm{GaAs}}(E, V) + N^{\mathrm{lh-c}}_{\mathrm{GaAs}}(E, V) + 2N^{\mathrm{sh-c}}_{\mathrm{GaAs}}(E, V). \tag{3}$$

Calculation results from this equation for three different photon energies using $\sigma_s = 26\,\mathrm{meV}$ are shown in figure 2. The curve for 1.96 eV consists of two peaks at around 0.12 and 0.32 eV and one trough at 0.44 eV. They are attributed to the hh–c transition for 0.44 eV, the lh–c transition for 0.32 eV and the sh–c transition for 0.12 eV. The energy positions decrease when the photon energy is decreased, following a similar overall trend.

2.2. Tunnel probability through the Schottky barrier and Fe spin polarization

The calculation of tunnel probabilities in Fe/GaAs(0 0 1) interfaces is carried out with Chang's model [16]. The proposed tunnel probability, P_{tunnel}, as a function of the electron energy, E, and applied bias, V, in a Schottky barrier is given by

$$P_{\mathrm{tunnel}}(V, E) = \exp\{-R\sqrt{(\Phi_{\mathrm{Bn}} - qV)(\Phi_{\mathrm{Bn}} - E)}\} \times \exp\left\{\frac{R(E - qV)}{2}\ln\left[\frac{E - qV}{2\Phi_{\mathrm{Bn}} - qV - E}\right]\right\}, \tag{4}$$

$$R = \frac{2}{q\hbar}\sqrt{\frac{m_e^*\epsilon_S}{N_d}}, \tag{5}$$

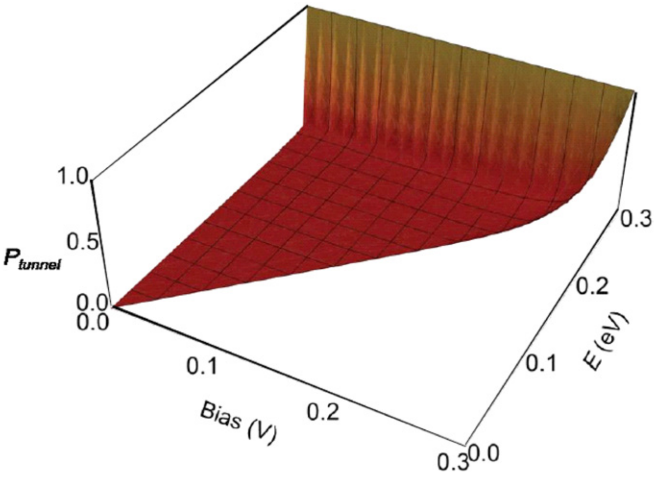

Figure 3. Three-dimensional plot of P_{tunnel} as a function of V and E for $\Phi_{\mathrm{Bn}} = 0.30\,\mathrm{eV}$.

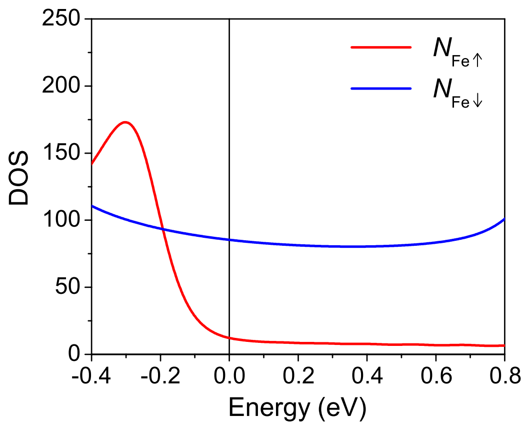

Figure 4. Calculated DOS of bulk Fe along the [0 0 1] direction for spin-up and down-spin.

where ϵ_{S}, Φ_{Bn} and N_{d} are the dielectric constant of GaAs, the Schottky barrier height and the carrier density, respectively. Calculation results of $P_{\mathrm{tunnel}}(V, E)$ are shown in figure 3. An increase in $P_{\mathrm{tunnel}}(V, E)$ is seen when E is close to Φ_{Bn}. This is because the effective barrier width for electrons in this energy region is thin, leading to the high tunnel probabilities. In order to calculate electrons travelling across an epitaxial Fe/GaAs(0 0 1) interface, the spin polarization of Fe for our model is calculated by integrating DOS of bulk bcc Fe band structure along the electron transport orientation. The Fe bulk DOS was calculated by density functional theory with a generalized gradient approximation [17–20]. These DOS for up-spin ($N_{\mathrm{Fe}\uparrow}$) and for down-spin ($N_{\mathrm{Fe}\downarrow}$) are shown in figure 4.

2.3. Spin-filtering effect calculations across Fe/GaAs interfaces

We focused our calculations in the case of using highly doped n-GaAs in which the bottom of the conduction band is close to the Fermi level. Therefore, for simplicity, we set the conduction edge equal to the Fermi level. Following the two-current model proposed by Mott [21], the currents for up- and down-spin channels are calculated separately, and the spin polarization of the photoexcited current is obtained by taking the difference of spin-up and spin-down currents. By multiplying the three functions, $N_{\mathrm{Fe}\uparrow,\downarrow}(E)$, $P_{\mathrm{tunnel}}(E, V)$ and $N_{\mathrm{GaAs}\uparrow,\downarrow}(E, V)$, the current for electrons with the specific energy and voltage in the interface $S_{\uparrow,\downarrow}(E, V)$ is obtained for the up-spin channel:

$$S_{\uparrow}(E, V) = N_{\mathrm{Fe}\uparrow}(E) \times P_{\mathrm{tunnel}}(E, V) \times N_{\mathrm{GaAs}\uparrow}(E, V), \qquad (6)$$

with an equivalent expression for the down-spin channel. $S_{\uparrow,\downarrow}(E, V)$ for $\sigma_{\mathrm{s}} = 26\,\mathrm{meV}$, $h\nu = 1.58\,\mathrm{eV}$, $\Phi_{\mathrm{Bn}} = 0.30\,\mathrm{eV}$ and $N_{\mathrm{d}} = 10^{24}\,\mathrm{m}^{-3}$ is shown in figure 5. In both graphs the largest S values are for electrons tunnelling at the high energy region especially at E close to 0.30 eV, following the $P_{\mathrm{tunnel}}(E, V)$ component. The total spin-filtering currents ($I_{\mathrm{SF}}(V)$) were obtained from the difference of two integrals, $S_{\uparrow,\downarrow}(E, V)$, over the energy range available for electron tunnelling across the interface as

$$I_{\mathrm{SF}}(V) = \int_{qV}^{\Phi_{\mathrm{Bn}}} S_{\uparrow}(E, V) - S_{\downarrow}(E, V)\,\mathrm{d}E. \qquad (7)$$

I_{SF} calculated with the previous parameter values is shown in figure 6. Upon increasing the bias from zero, I_{SF} starts to decrease in the negative region, exhibits a trough at 0.17 V and eventually increases back to zero. This trend is very similar to typical photoexcitation results (with an opposite sign) [2] and therefore this calculation model can successfully represent the experimental results observed in the photoexcitation measurements. In the later sections, predictions for spin-dependent transport using this model and the comparison between the calculated and experimental results for the spin-filtering current are shown and discussed in detail.

3. Parameter dependence of the spin-filtering current

In order to further understand the physics of the spin-filtering effect, the model was used to generate the photoexcitation results with varying parameter values. In this paper, we particularly present the Schottky barrier height and the photon energy dependence of the spin-filtering current. Figure 7 shows a set of calculation results with a variation of Φ_{Bn} ranged from 0.2 to 0.8 eV. Normally, it is difficult to engineer Φ_{Bn} when fabricating Schottky interface devices, and it is therefore very useful to be able to predict the Φ_{Bn} dependence of spin-dependent electron transport across Schottky interfaces. The other calculation parameters used here are $\sigma_{\mathrm{s}} = 26\,\mathrm{meV}$, $h\nu = 1.58\,\mathrm{eV}$ and $N_{\mathrm{d}} = 10^{24}\,\mathrm{m}^{-3}$. From the results, it is clarified that Φ_{Bn} controls the peak position of I_{SF}. Increasing Φ_{Bn} shifts the peak towards the higher bias regions with an approximately linear relationship. This is because by increasing Φ_{Bn} electron tunnelling at the higher energy regions is now allowed, where the tunnel probabilities are greater than those of the lower part of the barrier. Therefore, changing Φ_{Bn} is found to be a very useful method to control the output signal of spin devices with Schottky interfaces. This finding is consistent with experimental work which compares the photoexcitation results for different doping densities of

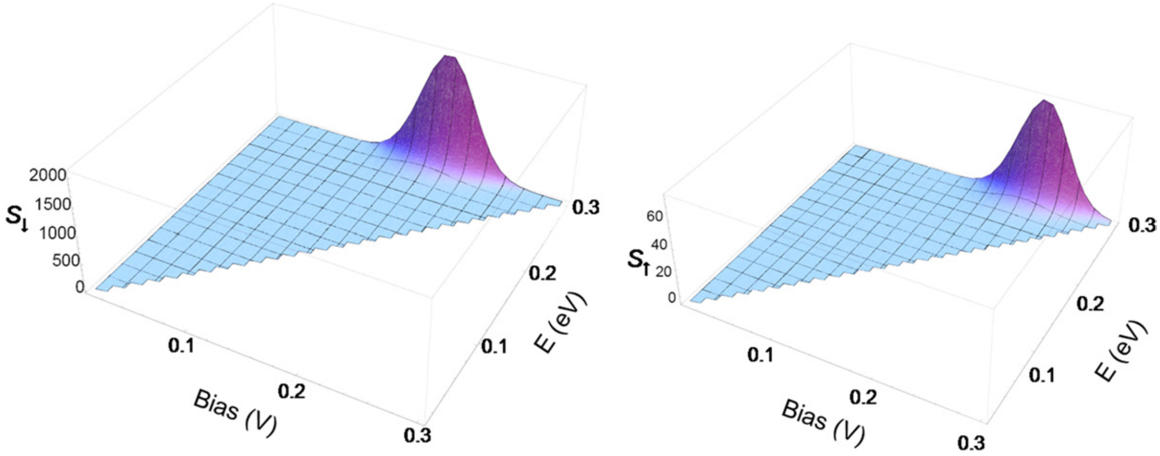

Figure 5. Three-dimensional plots of $S_\downarrow(E, V)$ (left panel) and $S_\uparrow(E, V)$ (right panel) calculated for $\sigma_s = 26$ meV, $h\nu = 1.58$ eV, $\Phi_{Bn} = 0.30$ eV and $N_d = 10^{24}$ m^{-3}.

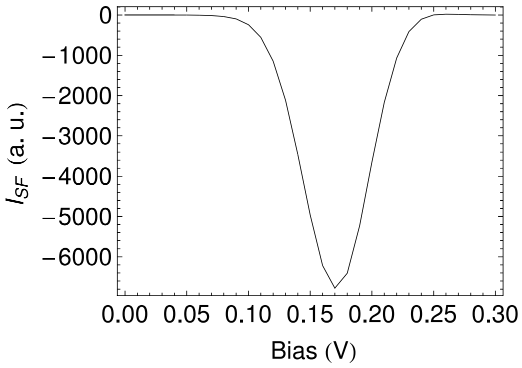

Figure 6. Plot of I_{SF} calculated with the parameters: $\sigma_s = 26$ meV, $h\nu = 1.58$ eV, $\Phi_{Bn} = 0.30$ eV and $N_d = 10^{24}$ m^{-3}.

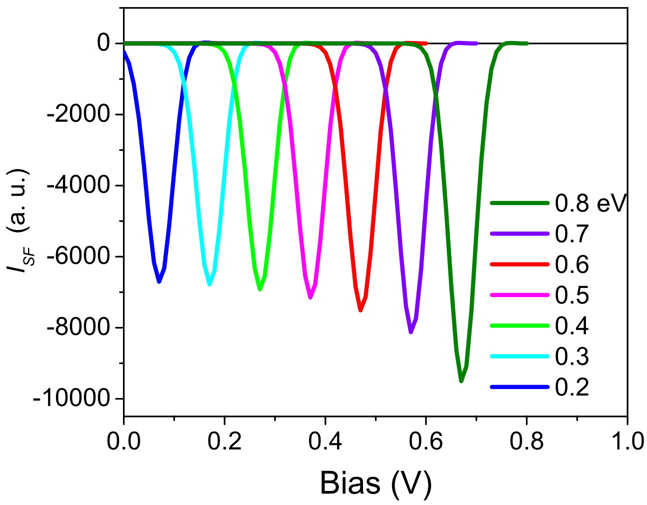

Figure 7. Φ_{Bn} dependence of I_{SF}. Φ_{Bn} is in the range of 0.2 to 0.8 eV. The other parameters used are $\sigma_s = 26$ meV, $h\nu = 1.58$ eV and $N_d = 10^{24}$ m^{-3}.

GaAs [22] and the theoretical results reported by Honda *et al* [11]. In addition, another important factor in the photoexcitation measurements, the photon energy, is varied in order to influence I_{SF}. As can be seen in figure 2, changing the photon energy provides different energy distributions of the spin polarization in the GaAs conduction band. The photon energy dependence of I_{SF} has been calculated and shown in figure 8. For $h\nu$ below the energy of 1.78 eV, where the sh–c transition is forbidden, I_{SF} is characterized by the trough originating from the hh–c transition; the contribution from electrons excited via the lh–c transition is small due to the lower optical transition probability as well as lower available DOS for tunnelling into the Fe layer for these electrons. The trough shifts towards a lower bias region with increasing $h\nu$. On the other hand, for $h\nu$ above 1.78 eV, a positive I_{SF} emerges in the high bias region. The positive contribution of I_{SF} is attributed to the sh–c transition and the position of the peak moves towards a lower bias region with increasing $h\nu$. In the I_{SF} curve for $h\nu = 2.0$ eV, the lower negative I_{SF} has been pushed away and only the positive part of I_{SF} exists in the forward bias region. This explains that most of the excited electrons from the hh–c transitions for $h\nu = 2.0$ eV are unable to tunnel across the interface since these electrons are excited into energy states of the GaAs conduction band higher than the top of the Schottky barrier. Therefore, the main contribution

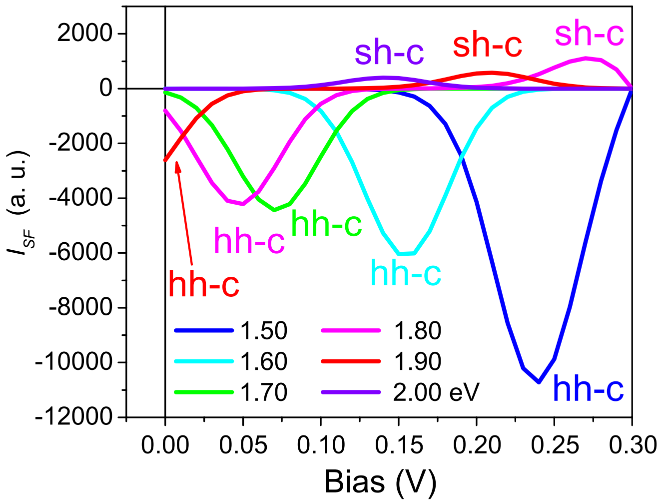

Figure 8. $h\nu$ dependence of I_{SF}. $h\nu$ is in the range from 1.5 to 2.0 eV. The other calculation parameters used are $\sigma_s = 26$ meV, $\Phi_{Bn} = 0.3$ eV and $N_d = 10^{24}$ m^{-3}.

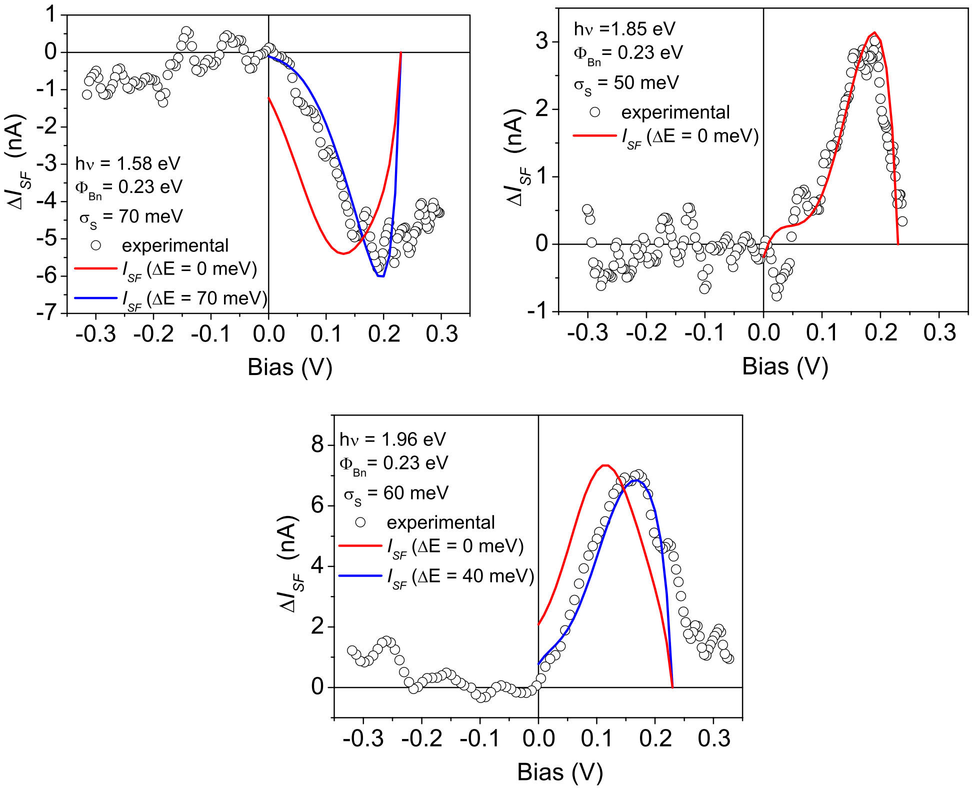

Figure 9. Comparisons of ΔI_{SF} and I_{SF} for the three different $h\nu$. The parameter values used are shown in each figure.

to the spin-filtering effect results from electrons created by the sh–c transition.

4. Comparison with experimental observation

As presented above, our calculation model can be successfully used for a large number of cases of photoexcitation experiments by changing the calculation parameters. By varying these parameter values, we fit the calculations to experimental data of the spin-filtering effect (ΔI_{SF}) [20], results of which are shown in figure 9. For these fittings, the experimentally deduced Φ_{Bn} (=0.23 eV) from the sample was used (detailed characterization of Fe/GaAs Schottky can be found in [23]) as well as $N_{\mathrm{d}} = 10^{24}\,\mathrm{m}^{-3}$, and the fitting parameters were σ_{s} and the peak heights of I_{SF}. Best fit calculation data are shown as red lines in the figures; the blue lines will be explained below. The most important point for the comparison is that the fitting curves represent the sign change in ΔI_{SF}. The origin of the sign change in the calculated results can be understood by the difference of the photoexcitation transition types which contribute to I_{SF} when changing the photon energy as already explained in the last section. The spin-polarized electrons that dominate the I_{SF} curve of 1.58 eV are generated via the hh–c transition, whereas the I_{SF} curves for 1.85 and 1.96 eV result from the sh–c transition. I_{SF} fits very well with ΔI_{SF} for 1.85 eV, while for the other two energies there are slight shifts between ΔI_{SF} and I_{SF}. A possible origin of the shifts is the lowering of energy peak position due to different electron-energy relaxation rates. The calculated kinetic energies of photoexcited electrons contributing the peak are 125 meV (from the hh–c transition), 54 meV (from the sh–c transition) and 129 meV (from the sh–c transition) for 1.58 eV, 1.85 eV and 1.96 eV, respectively. Since high energetic electrons relax their energies faster, it would be a case that the peak position of electron-energy distribution would be slightly lowered for 1.58 and 1.96 eV. In order to confirm this hypothesis, we introduce an additional factor to shift the electron energy (ΔE) in the energy part of equation (2). The calculation results with appropriate ΔE values are shown in figure 9. These better fits indicate that our hypothesis is a possible reason and more realistic definition for the electron-energy distribution is needed to improve our model. This improvement is one of our future plans for developing a better model of the experiments.

5. Conclusion

In this paper, spin-dependent electron transport of photogenerated electrons across Fe/GaAs(0 0 1) interfaces is calculated using a one-dimensional transport model for an Fe/GaAs(0 0 1) interface. The spin-filtering current I_{SF} is calculated by changing Schottky barrier height and photon energy. The calculated results provide useful predictions for spin-polarized transport of photoexcited electrons across Fe/GaAs(0 0 1) interfaces. The comparison of the calculated I_{SF} with the experimental results of the photoexcitation measurements reveals that the calculation model using realistic parameter values can provide qualitative agreement with the experimental observations. This model therefore is useful for understanding and predicting spin-polarized photoexcitation measurements for investigating spin-dependent electron transport across FM/SC interfaces.

References

[1] Wolf S A, Awschalom D D, Buhrman R A, Daughton J M, von Molnar S, Roukes M L, Chtchelkanova A Y and Treger D M 2001 *Science* **294** 1488
[2] Bland J A C, Steinmuller S J, Hirohata A and Taniyama T 2005 *Ultrathin Magnetic Structures IV* ed J A C Bland and B Heinrich (Berlin: Springer) Chapter 4
[3] Dyakonov M I and Perel V I 1984 *Optical Orientation* ed F Meier and B P Zakharchenya (Amsterdam: North-Holland)
[4] Hirohata A, Xu Y B, Guertler C M and Bland J A C 1999 *J. Appl. Phys.* **85** 5804
[5] Isakovic A F, Carr D M, Strand J, Schultz B D, Palmstrom C J and Crowell P A 2001 *Phys. Rev.* B **64** 161304R
[6] Taniyama T, Mori T, Watanabe K, Wada E, Itoh M and Yanagihara H 2008 *J. Appl. Phys.* **103** 07D705
[7] Trypiniotis T, Tse D H Y, Steinmuller S J, Cho W S and Bland J A C 2007 *IEEE Trans. Magn.* **43** 2872
[8] Wada E, Itoh M and Taniyama T 2008 *J. Appl. Phys.* **103** 07A702
[9] Isber S, Park Y J, Moodera J S and Heiman D 2008 *J. Appl. Phys.* **103** 07D713
[10] Kurebayashi H, Trypiniotis T, Lee K, Easton S, Ionescu A, Farrer I, Ritchie D A, Bland J A C and Barnes C H W 2010 *Appl. Phys. Lett.* **96** 022505
[11] Honda S, Itoh H, Inoue J, Kurebayashi H, Trypiniotis T, Barnes C H W, Hirohata A and Bland J A C 2008 *Phys. Rev.* B **78** 245316
[12] Shah J 1999 *Ultrafast Spectroscopy of Semiconductors and Semiconductor Nanostructures* (Berlin: Springer)
[13] Kurebayashi H 2009 *PhD Thesis* University of Cambridge
[14] Davies P C W 2005 *Am. J. Phys.* **73** 23
[15] Averin D V and Likharev K K 1991 *Mesoscpic Phenomena Solids* (Amsterdam: Elsevier)
[16] Chang C Y and Sze S M 1970 *Solid State Electron.* **13** 727
[17] Payne M C, Teter M P, Allen D C, Arias T A and Joannopoulos J D 1992 *Rev. Mod. Phys.* **64** 1045
[18] Perdew J P, Burke K and Ernzerhof M 1996 *Phys. Rev. Lett.* **77** 3865
[19] Yates J R, Wang X, Vanderbilt D and Souza I 2007 *Phys. Rev.* B **75** 195121
[20] Kurebayashi H, Steinmuller S J, Laloe J B, Trypiniotis T, Easton S, Ionescu A, Yates J R and Bland J A C 2007 *Appl. Phys. Lett.* **91** 102114
[21] Mott N H 1936 *Proc. R. Soc.* A **153** 699
[22] Steinmuller S J, Gurtler C M, Wastlbauer G and Bland J A C 2005 *Phys. Rev.* B **72** 045301
[23] Fleet L R, Yoshida K, Kobayashi H, Ohno Y, Kurebayashi H, Kim J-Y, Barnes C H W and Hirohata A 2010 *IEEE Trans. Magn.* **46** 1737