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Effect of magnetic impurities on TMR at finite bias voltage

S. Nonoyama[a,*], H. Itoh[b], A. Oguri[c], J. Inoue[b], P. Bruno[d]

[a]*Faculty of Education, Yamagata University, Yamagata 990-8560, Japan*
[b]*Department of Applied Physics, Nagoya University, Nagoya 464-8603, Japan*
[c]*Department of Materials Science, Faculty of Science, Osaka City University, Osaka 558-8585, Japan*
[d]*Institute d'Électronique Fondamentale, CNRS URA 22, Université Paris-Sud, Orsay, France*

Abstract

Transport phenomena through a ferromagnetic tunneling junction in the presence of magnetic impurities are investigated at a finite bias voltage. We have found that the feature of the reduction of the tunnel magnetoresistance (TMR) with increasing bias voltage changes by the impurity effect.

Keywords: Non-linear response; Tunnel magnetoresistance; Impurity effect

Spin-polarized transport phenomena in ferromagnetic metal (FM)/insulator/FM tunnel junctions have attracted current interest [1–4]. In recent years, the transport phenomena in such systems are studied extensively, and large magnetoresistance ratios have been reported for $Fe/Al_2O_3/Fe$ [3] and $CoFe/Al_2O_3/Co$ [4]. Although a great progress has been made in the experimental study, there remain some unsolved problems about tunnel magnetoresistance (TMR), which are more or less related to the randomness [5–7].

In this study, to examine these problems, we have used a microscopic model which can be applicable to the complex structure of the sample geometry *under finite bias voltages*. In spite of the importance of studying transport *under the finite bias voltages*, theoretical approaches seem to be still in a developing stage because of the difficulty in treating the non-equilibrium systems. Previously, we presented the numerical method, which can treat the non-linear response, using a recursive Green-function method based on the Keldysh formalism [8]. Using the method, in this study, we have performed numerical calculations to investigate the current–voltage (I–V) characteristics and TMR. We have also investigated the effect of the randomness in the insulating layer on the current and TMR. We concentrate ourselves on the zero-temperature case for simplicity throughout this work.

We consider a metal/insulator/metal trilayer structure, in which the parameter l is introduced as a label of the layer in the z-direction (stacking direction). The regions where $l \leqslant 0$ and $l \geqslant N+1$ are the semi-infinite metallic leads and the region where $1 \leqslant l \leqslant N$ is the insulating layer. The thickness of the insulating layer is Na with a being the lattice constant and the cross section of the system is $Ma \times Ma$. Periodic boundary conditions are adopted in the x- and y-directions. The parameters N and M are set to be three and five in this work, respectively. The Hamiltonian $\mathscr{H}$ is given by

$$\mathscr{H} = -t \sum_{\langle (i,l),(i',l') \rangle,\sigma} (c^{\dagger}_{i,l,\sigma} c_{i',l',\sigma} + \text{H.c.}) + \sum_{i,l,\sigma} V_{l,\sigma}(\boldsymbol{r}_i) c^{\dagger}_{i,l,\sigma} c_{i,l,\sigma} + \sum_{i,\sigma} \sum_{l=1}^{N} \Phi_l c^{\dagger}_{i,l,\sigma} c_{i,l,\sigma}, \quad (1)$$

where $\boldsymbol{r}$ denotes the positional vector in the x–y planes, $c^{\dagger}_{i,l,\sigma}$ is the creation operator for an electron at the site $(\boldsymbol{r}_i, l)$ with spin σ, and $V_{l,\sigma}(\boldsymbol{r}_i)$ is the potential energy. The last term appears when the bias voltage eV along the z-direction is applied to the insulating layer, and we assume the electrostatic potential to be $\Phi_l \equiv eV$ in the left lead, and $\Phi_l \equiv 0$ in the right lead. For $1 \leqslant l \leqslant N$, it is

* Corresponding author.

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assumed to be $\Phi_l = eV(N+1-l)/(N+1)$ when the electric field is uniform. The total current flowing along the z-direction can be obtained by the method described in Ref. [8]. The detailed description for the calculation of the interlayer Green's function is also given in Ref. [8].

Now we discuss the transport phenomena through an insulating layer. In what follows, we take the transfer integral t as a unit of the energy. The chemical potential in the right lead μ_R is set to be $-5t$. We consider the case where the leads and impurity atoms are made of a ferromagnet. Inside the insulating barrier ($1 \leqslant l \leqslant 3$), $V_{l,\sigma}(\boldsymbol{r}_i)$ is chosen to be the barrier height $1.5t$, except the impurity site. At the impurity site and at the lead wire, $V_{l,\pm}(\boldsymbol{r}_i)$ is taken to be $\mp V_{ex}$ with V_{ex} being the exchange energy. The alignment of the magnetization of the left and right leads are assumed to be parallel (P) and anti-parallel (AP), respectively. Correspondingly, we define I_P and I_{AP} as the currents in the parallel and antiparallel configurations, respectively. The TMR ratio is defined as $(I_P - I_{AP})/I_P$.

We first consider the ferromagnetic junction with no impurity atoms in the insulating layer. Fig. 1 shows the calculated results of the bias voltage dependence of the current I_P and I_{AP} for $V_{ex} = 0.2$. As can be seen from Fig. 1, the slopes of the current curves increase with increasing bias voltage because the effective width of the barrier becomes narrower as eV increases. Around $eV = 1$, the slopes of the current curves change slightly in Fig. 1. Here, we have evaluated the TMR as a function of eV (see the solid line in Fig. 2). The TMR ratio in this case decreases with increasing bias voltage, as depicted in Fig. 2 (solid curve). Note that the TMR ratio decreases with decreasing V_{ex}, monotonically, e.g., the TMR ratio for $V_{ex} = 0.2$ is about four times as large as that for $V_{ex} = 0.1$ for $0 \leqslant eV \leqslant 1.5$. The TMR ratios in these results seem to be small, compared with that reported in the experiment, which are due to the smallness of μ_R and V_{ex}, although decreasing features of TMR with increasing eV are reproduced in this calculation. To compare the calculated TMR with those in the experiment exactly, we should perform a calculation in the case where the sample size, the chemical potential, and the exchange splitting are enlarged.

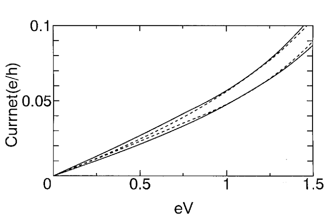

Fig. 1. The bias voltage dependence of the current for the case of the ferromagnetic tunneling junction with no impurity. The exchange splitting V_{ex} is 0.2. The solid and dotted curves represent the calculated currents I_P and I_{AP}, respectively.

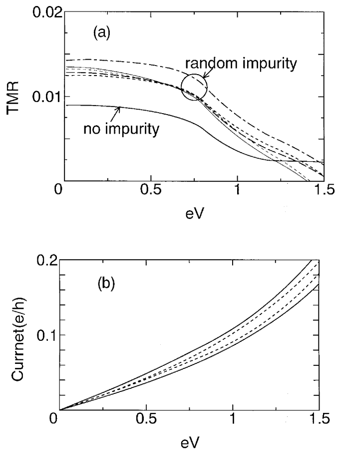

Fig. 2. (a) The bias voltage dependence of the TMR for the case of the ferromagnetic tunneling junction with or without the random impurities. Each curve except the thick solid curve shows the calculated result for the diffferent impurity configurations. The thick solid curve shows the calculated TMR ratio for the case without impurities. (b) The bias voltage dependence of the current for the case of the ferromagnetic tunnel junction with random impurities. The solid and dotted curves represent the calculated currents I_P and I_{AP}. The impurity configuration in this case corresponds to that in the case of the thick dotted curve in (a).

Secondly, we consider the impurity effect on the current and TMR. In this case, we consider the tunnel conduction through an insulating layer containing random magnetic impurities. We use a simple model for considering the randomness which can be seen in the experiment. In the present case, the locations of the impurities in the insulating layer are determined by the uniform random numbers. We take $V_{ex} = 0.2$ and the impurity concentration is $c = 0.1$. For the computation of I_{AP}, the concentrations of the magnetic impurities with $+V_{ex}$ and $-V_{ex}$ are taken to be equal. Fig. 2(a) gives the typical examples of the eV dependence of the TMR for five different impurity configurations. We also plot the bias voltage dependence of the current for the typical impurity configuration in Fig. 2(b). In Fig. 2(a), we can see the similar decreasing characters in the five sample geometries. At $eV = 0$, the TMR ratios in these cases are larger than that in the non-impurity case and those in the random impurity cases decrease rapidly with increasing bias voltage [see Fig. 2(a)]. The reduction of the TMR by the bias voltage is enhanced by the impurity effect in this calculation.

In summary, we have investigated the bias voltage dependence of the I–V characteristics and TMR by using the rescursive Green function method. We have also studied the impurity effect on the TMR. We have found that the TMR ratio decreases with increasing bias voltage and the feature of the reduction with increasing bias voltage changes by the impurity effect.

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References

[1] M. Julliere, Phys. Lett. A 54 (1975) 225.
[2] S. Maekawa, U. Gefvert, IEEE Trans. Magn. IMAG-18 (1982) 707.
[3] T. Miyazaki, N. Tezuka, J. Magn. Magn. Mater. 139 (1995) L231.
[4] J.S. Moodera, L.R. Kinder, T.M. Wong, R. Meservey, Phys. Rev. Lett. 74 (1995) 3273.
[5] N. Tezuka, Y. Ando, T. Miyazaki, J. Mag. Soc. Japan 19 (1995) 369.
[6] N. Tezuka, T. Miyazaki, J. Appl. Phys. 79 (1996) 6262.
[7] H. Itoh, T. Kumazaki, J. Inoue, S. Maekawa, Jpn. J. Appl. Phys. 37 (1998) 5554.
[8] S. Nonoyama, A. Oguri, Phys. Rev. B 57 (1998) 8797.