Journal of Magnetism and Magnetic Materials 198–199 (1999) 545–547

Theory of tunnel conductance through a strongly disordered spacer

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Abstract

The tunnel conductance through a disordered spacer is studied in the linear response theory at zero temperature. It is shown that the conductance is proportional to the product of the surface densities of states of metals separated by the spacer and tunnel magnetoresistance ratio is expressed in terms of spin polarization of the surface density of states of ferromagnetic metals when the disorder is strong. © 1999 Elsevier Science B.V. All rights reserved.

Keywords: Tunnel conductance; TMR; Disorder; Spin polarization; Surface density of states

Since the discovery of giant magnetoresistance in magnetic multilayers [1], a considerable number of studies have been made on the spin dependent transport phenomena in magnetic nano-structures. One of the examples is the tunnel magnetoresistance (TMR) in ferromagnetic tunnel junctions. Recently, a large TMR ratio as much as 30% has been observed in $Fe/Al_2O_3/Fe$ [2] and $CoFe/Al_2O_3/Co$ [3] systems.

There are several theoretical works to explain the TMR. They can be classified into two approaches according to the treatment of the wave function of tunnel electrons. One is based on the tunnel Hamiltonian theory. In the tunnel Hamiltonian theory, the tunnel conductance is proportional to the product of the densities of states (DOSs) of metals separated by an insulating spacer and the resultant expression of TMR ratio (*TMR*) is given as [4,5]

$$TMR = 2P^2/(1 + P^2), \quad (1)$$

where P denotes the spin polarization of DOS of the ferromagnetic metals. When we use the observed values of P [6], TMR ratio obtained in experiments can be explained semi-quantitatively. The other is based on the scattering theory of the one-body potential barrier. Slonczewski [7] solved the Schrödinger equation of the rectangular potential barrier without disorder in the free electron model and discussed the dependence of TMR ratio on the barrier height. In his theory, TMR ratio has not been given by a simple expression as Eq. (1). However, the dependences of TMR ratio on the barrier thickness and the applied bias voltage can be calculated [8–10].

Real systems, on the other hand, include disorder, especially near interfaces between the insulating spacer and the metallic leads. In this work, we clarify the effect of elastic scatterings due to strong disorder on the tunnel conductance and the TMR. We adopt a model which includes strong disorder but keeps the band gap open in the insulating spacer and treat the wave function properly.

We consider a trilayer consisting of two semi-infinite metallic leads separated by a spacer of L atomic layers. This trilayer is described by the single orbital tight-binding model on a simple cubic lattice and the (0 0 1)

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0304-8853/99/$ – see front matter
PII: S0304-8853(98)01228-1

axis is taken as the stacking direction. In order to take into account the disorder and band gap, we assume the following substitutional-type disorder in the spacer. The Hamiltonian of the system is

$$\hat{H} = -t \sum_{\langle (i,l),(j,l') \rangle, \sigma} (c^{\dagger}_{i,l,\sigma} c_{j,l',\sigma} + \text{H.c.}) + \sum_{i,l,\sigma} u^{\sigma}_{i,l} c^{\dagger}_{i,l,\sigma}, \quad (2)$$

where $c^{(\dagger)}_{i,l,\sigma}$ is the annihilation (creation) operator of the electron at site $\boldsymbol{i}$ in l-th plane with spin σ. Here, l labels the layer plane normal to the (0 0 1) axis and $\boldsymbol{i}$ denotes the site within the layer plane. In Eq. (2), t is transfer integral and the summation $\langle (\boldsymbol{i}, l), (\boldsymbol{j}, l') \rangle$ runs over the nearest-neighbor sites. The on-site potential $u^{\sigma}_{i,l}$ at site $\boldsymbol{i}$ in lth plane takes constant value u^{σ}_{L} in left ($l \leqslant 0$) and u^{σ}_{R} right ($l \geqslant L+1$) leads while it takes u or $-u$ randomly with equal probability in the spacer ($1 \leqslant l \leqslant L$). We take the random potential u large to open the gap in the band of the spacer.

In order to treat the disorder, the single site coherent potential approximation (CPA) [11] is adopted. The conductance through the disordered spacer is calculated by using Kubo formula [12] at zero temperature. The vertex correction, which depends on the layer, to the conductance is calculated by evaluating the ladder diagrams consistently with the coherent potential in order to satisfy the current conservation [13]. We ignore spin flip scatterings and calculate the TMR ratio by using the two current model.

First, we show the calculated results of the DOSs of the spacer and the lead in Fig. 1. Here, both u^{σ}_{L} and u^{σ}_{R} are taken to be zero and the chemical potential (Fermi energy) is chosen at $E = 0$. As the random potential u increases, the gap appears in the DOS of the spacer around the chemical potential. However, the DOS is finite even if the gap (pseudo-gap) appears for large u. This is because the electron penetrates into the spacer from the leads due to the proximity effect. The DOS of the lead at the interface is almost the same as the surface DOS of semi-infinite metallic lead for large u.

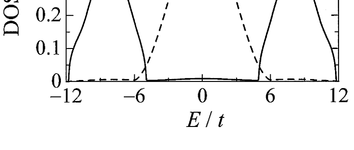

Fig. 1. Calculated results of the local DOSs of the spacer (solid curve) and the lead (broken curve). Here, we take $L = 2$, $u/t = 10$ and $u^{\sigma}_{\mathrm{L}} = u^{\sigma}_{\mathrm{R}} = 0$.

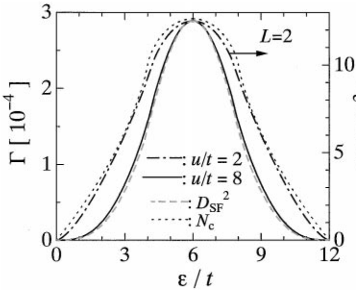

Fig. 2. Calculated results of the conductance in units of $2e^2/h$. Chained and solid curves are Γ for $u/t = 2$ and 8, respectively. The channel number and the product of the surface DOSs of semi-infinite metallic lead are also shown by dotted and broken curves in arbitrary units.

In order to examine the relation between the electronic structure of the leads and Γ, we shift the DOSs of the leads by changing $u_0 (= u^{\sigma}_{\mathrm{L}} = u^{\sigma}_{\mathrm{R}})$. We define the energy ε as $\varepsilon \equiv 6t - u_0$ that denotes the relative energy between the chemical potential and the bottom of the band of the leads. In Fig. 2, the calculated results of the conductance Γ are shown with channel number N_{c} and square of the surface DOS (D_{SF}) of the metallic leads. In the ballistic limit ($u \to 0$), the conductance is known to be proportional to the channel number which is the number of the states contributing to the transport. When u is small, the shape of Γ is similar to that of N_{c}. As u increases, the shape of Γ becomes narrow and converges to that of D^2_{SF}. Therefore, it is considered that Γ is proportional to D^2_{SF} in strong disordered limit.

Next, we consider the ferromagnetic leads by introducing the spin dependent u^{σ}_{L} and u^{σ}_{R}. We adopt the local spin quantization axis for each ferromagnetic lead and define the spin $+$ and $-$ to be the majority and minority spin states for each ferromagnetic lead, respectively. The potentials of the ferromagnetic leads are chosen as $u^{\pm}_{\mathrm{L(R)}} = u_0 \mp \Delta/2$ where Δ denotes the exchange splitting. The conductance Γ_{P} in the parallel alignment is given by $\Gamma_{\mathrm{P}} = \Gamma_{++} + \Gamma_{--}$ by using the two current model. Similarly, the conductance Γ_{AP} in the anti-parallel alignment is given by $\Gamma_{\mathrm{AP}} = \Gamma_{+-} + \Gamma_{-+}$. The TMR ratio is defined as

$$TMR \equiv (\Gamma_{\mathrm{P}} - \Gamma_{\mathrm{AP}})/\Gamma_{\mathrm{P}}. \quad (3)$$

Calculated results of *TMR* as functions of ε are shown in Fig. 3 for several values of u. As u increases, *TMR* becomes close to $2P^2_{\mathrm{SF}}/(1 + P^2_{\mathrm{SF}})$ where P_{SF} is the spin polarization of the surface DOS of the metallic leads defined as $P_{\mathrm{SF}} \equiv (D^{+}_{\mathrm{SF}} - D^{-}_{\mathrm{SF}})/(D^{+}_{\mathrm{SF}} + D^{-}_{\mathrm{SF}})$.

Results obtained in strong disordered limit are similar to those obtained by using the tunnel Hamiltonian theory but the conductance is proportional to the product of

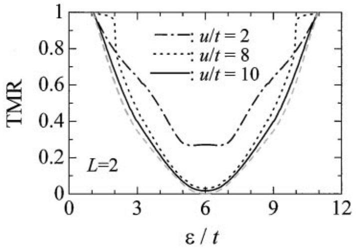

Fig. 3. Calculated results of the TMR ratio for several values of random potential u. Chained, dotted and solid curves are *TMR* for $u/t = 2$, 8 and 10, respectively. The broken curve shows the evaluated value of *TMR* from Eq. (1) with the spin polarization of surface DOS instead of that of the DOS of ferromagnetic leads.

the *surface* DOSs of metallic leads. As for the TMR, P in Eq. (1) should be interpreted as the spin polarization of the *surface* DOS of the ferromagnetic metals for strongly disordered junctions.

This work was supported by Grant-in-Aid for Scientific Research on Priority Area, Ministry of Education, Science, Sports and Culture and also Monbusho International Scientific Research Program: Joint Research. P.B. thanks JSSP Fellowship for Research in Japan. A part of the numerical calculation was performed by using facilities of the Computer Centre, the Institute for Molecular Science, Okazaki and the Super Computer Centre, Institute for Solid State Physics, University of Tokyo.

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