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Tunnel Conductance in Strong Disordered Limit

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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 surface densities of states of metals separated by the spacer when the disorder is strong.

Key words: tunnel conductance, liner response theory, substitutional disorder, band gap, CPA

1. Introduction

Ferromagnetic tunnel junctions comprised of two ferromagnetic metals separated by thin insulating spacer exhibit large magnetoresistance (TMR). Although TMR was observed more than one decade ago, the magnitude of the effect was only a few %.[1),2)] Recently, TMR up to 40% is observed in $Fe/Al_2O_3/Fe$[3)] and $CoFe/Al_2O_3/Co$[4)] systems.

This noble phenomenon originates from the spin dependent tunneling across the insulating spacer. Theoretical explanations of TMR are based on the tunneling Hamiltonian theory or scattering theory for one-body potential barrier. In the tunneling Hamiltonian theory, the tunnel conductance is proportional to the product of the densities of states (DOS's) of metals separated by the spacer.[5)] By applying the tunneling Hamiltonian theory to the ferromagnetic tunnel junctions, TMR ratio is expressed in terms of the spin polarization (P) of ferromagnetic metals as $TMR = 2P^2/(1+P^2)$.[1),2)] When we use the observed values of P,[6)] TMR ratio obtained in experiments can be explained semi-quantitatively. On the other hand, Slonczewski[7)] solved the Schrödinger equation of the pseudo 1-dimensional rectangular potential barrier in the free electron model and discussed the dependence of TMR ratio on the barrier height. The dependences of TMR ratio on the barrier thickness and the applied bias voltage have also been discussed.[8)–10)]

In the tunneling Hamiltonian theory, the phase memory of the wave function is assumed to be lost during tunnel process due to the inelastic scatterings. In Slonczewski's approach, on the other hand, the wave function of the tunneling electron is treated explicitly. However, disorder is not taken into account in his theory.

Actual materials must include disorder, especially around interfaces between insulating spacer and metals. In this work, the conductance is calculated for a model including strong disorder keeping the band gap open in the spacer. We use scattering theory to treat the wave function correctly and clarify the important ingredients which govern the tunnel conductance through the disordered spacer. Linear response theory, *i.e.*, Kubo formula and coherent potential approximation are used to calculate the conductance at zero temperature and at zero bias limit. It will be shown that the conductance is proportional to the product of the *surface* DOS's of metals separated by the spacer.

2. Model and Method

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 (001) axis is taken for stacking a layers. In order to take into account the disorder and band gap, we assume following substitutional-type disorder in the spacer. The Hamiltonian of the system is

$$\hat{H} = -t \sum_{\langle(\mathbf{i},l),(\mathbf{j},l')\rangle,\sigma} \left(c^\dagger_{\mathbf{i},l,\sigma} c_{\mathbf{j},l',\sigma} + H.c. \right) + \sum_{\mathbf{i},l\sigma} u_{\mathbf{i},l} c^\dagger_{\mathbf{i},l,\sigma} c_{\mathbf{i},l,\sigma} , \tag{1}$$

where $c^{(\dagger)}_{\mathbf{i},\sigma}$ is annihilation (creation) operator of electron at site $\mathbf{i}$ in l-th plane with spin σ. Here, l labels the layer plane normal to the (001) axis and $\mathbf{i}$ denotes the site within the layer plane. In Eq.(1), t is transfer integral and the summation $\langle(\mathbf{i},l),(\mathbf{j},l')\rangle$ runs over nearest-neighbor sites. The on-site potential $u_{\mathbf{i},l}$ at site $\mathbf{i}$ in l-th plane takes constant value u_0 in both left ($l \leq 0$) and right ($l \geq L+1$) leads while it takes u or $-u$ randomly with equal probability in the spacer ($1 \leq l \leq L$). 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. One of the advantages of the CPA is that the band gap of the spacer can be reproduced for large u. The conductance through the disordered spacer is calculated by using Kubo formula[12)] at zero temperature. Because there is no translational invariance in the current direction, the vertex correction to the conductance does not disappear. The vertex correction is calculated by the approximation consistent with the CPA in order to satisfy the current conservation.[13)] Since we concentrate ourselves on the transport property at the zero bias limit, the inelastic scattering (see, *e.g.*, Zhang and Levy[14]) is not included in our calculation.

3. Results

First, we show the calculated results of the DOS's of spacer and lead in Figs. 1(a) and (b), respectively. Here, the chemical potential (Fermi energy) is chosen at $E = 0$. In Fig. 1(a), the gap appears around the chemical potential as the random potential u increases. However, the DOS is finite even if the gap (pseudo-gap) appears for large u. This is because the electron penetrates into spacer from the leads due to the proximity effect. The DOS's of the lead near the interface shows the oscillatory behavior. This behavior for large u is almost the same as that of the surface DOS.

In Fig. 2, the calculated results of the conductance Γ are shown in logarithmic scale for various thicknesses L of the spacer as functions of u. Here, we take the on-site potential u_0 of the leads zero. It can be seen that Γ decreases as the gap appears in the DOS of the spacer with increasing u. It is also seen that Γ decrease with increasing L.

In order to examine the relation between the electronic structure of the leads and Γ, we shift the DOS's of the leads by changing u_0. We define the energy ϵ as $\epsilon \equiv 6t - u_0$ that denotes the relative energy between the chemical potential and the bottom of the band of the leads. In Fig. 3(a), the calculated results of the normalized conductance $\Gamma(\epsilon)/\Gamma(6t)$ are shown for various values of u. Here, the dependence of $\Gamma(6t)$ on u has been already shown in Fig. 2. In Fig. 3(b), the channel number N_c and the square of the surface DOS (D_{SF}) of the semi-infinite metallic lead normalized with respect to those values at $\epsilon = 6t$ are shown. In the ballistic limit, the conductance is known to be proportional to the channel number N_c that is the number of the states contributing to the transport.

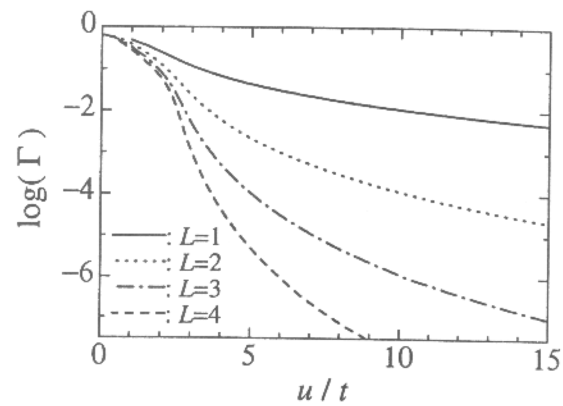

Fig. 2 Calculated results of the conductance as functions of u for various values of L. Here, we take $u_0 = 0$. Solid, dotted, chained and broken curves are Γ for $L = 1, 2, 3$ and 4, respectively.

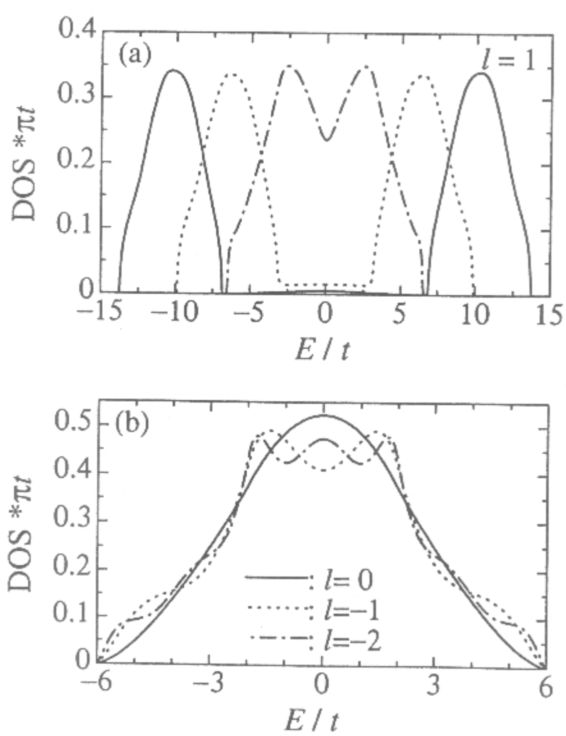

Fig. 1 Calculated results of the local DOS's of (a) the spacer and (b) the lead. Here, we take $L = 2$ and $u_0 = 0$. (a) Chained, dotted and solid curves are the DOS's for $u/t = 2, 6$ and 10, respectively. (b) Solid, dotted and chained curves are the DOS's at $l = 0, -1$ and -2, respectively for $u/t = 10$.

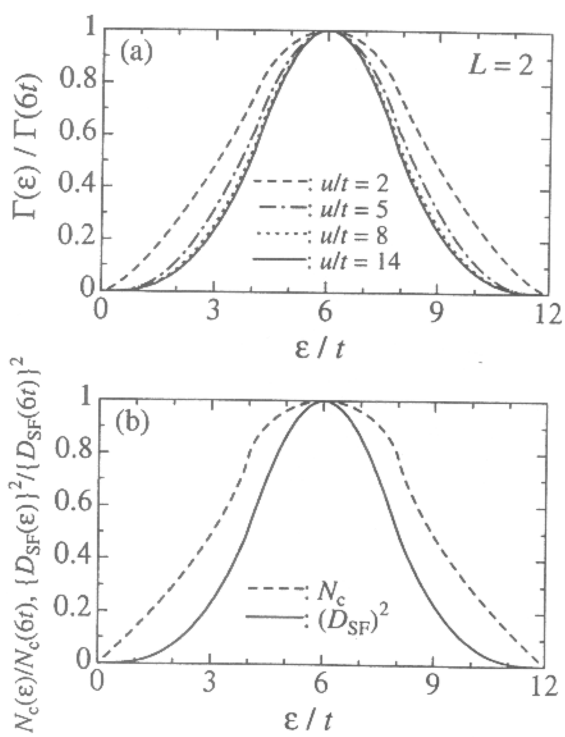

Fig. 3 Calculated results of (a) the normalized conductance for various values of u and (b) the channel number (broken curve) and the square of the surface DOS of the semi-infinite metallic lead (solid curve) as functions of ϵ. In (a), broken, chained, dotted and solid curves are normalized Γ for $u/t = 2, 5, 8$ and 14, respectively.

When u is small, the shape of $\Gamma(\epsilon)/\Gamma(6t)$ is similar to that of $N_c(\epsilon)/N_c(6t)$. As u increases, the shape of $\Gamma(\epsilon)/\Gamma(6t)$ becomes narrow and $\Gamma(\epsilon)/\Gamma(6t)$ converges to $\{D_{SF}(\epsilon)\}^2/\{D_{SF}(6t)\}^2$. Therefore, it is considered that $\Gamma \propto {D_{SF}}^2$ in strong disordered limit.

4. Discussion and Conclusion

In the linear response theory, the conductance at zero temperature is expressed as[13),15)]

$$\Gamma = \frac{2e^2}{h} \sum_{\mathbf{k},\mathbf{k}'} 4t^4 \langle |G_{1,L}^{\mathbf{k},\mathbf{k}'}|^2 \rangle \, \mathrm{Im} f_{\mathrm{L}}^{\mathbf{k}} \, \mathrm{Im} f_{\mathrm{R}}^{\mathbf{k}'} . \tag{2}$$

where $G_{1,L}^{\mathbf{k},\mathbf{k}'}$ is the interlayer Green's function between 1-st and L-th planes and $f_{\mathrm{L(R)}}$ is the surface Green's function of the left (right) lead. Here, $\mathbf{k} = (k_x, k_y)$ is the element of the wave vector parallel to the layer planes and the bracket $\langle \cdots \rangle$ denotes the statistical average due to the disorder. If the $\mathbf{k}, \mathbf{k}'$ dependence of $\langle |G_{1,L}^{\mathbf{k},\mathbf{k}'}|^2 \rangle$ is neglected, the summations over $\mathbf{k}$ and $\mathbf{k}'$ run independently, then, the conductance is proportional to the product of the surface DOS's of the leads. In our results, Γ is also proportional to ${D_{SF}}^2$ when u is large. Then, it is considered that $\langle |G_{1,L}^{\mathbf{k},\mathbf{k}'}|^2 \rangle$ in Eq.(2) becomes independent of $\mathbf{k}$ and $\mathbf{k}'$ in strong disordered limit.

In conclusion, the conductance through the strong disordered spacer is proportional to the products of the *surface* DOS's of the leads. Our results suggest that the spin polarization in the expression of TMR ratio should be interpreted as the spin polarization of the *surface* DOS of ferromagnetic metals for strong disordered tunnel junctions.

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