

Theoretical Investigation on Magnetic Tunnel Junctions with 4-Valued Conductances: Application to Carbon Nanotube Encapsulating Magnetic Atoms

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Magnetic tunnel junctions (MTJ) like ferromagnet(FM)/barrier/FM junctions [1] are recently applied to elements in magnetic random access memories because of their large tunnel magnetoresistance effect. As for the MTJ, compared with elements in other memories such as the Flash memory, few studies have been done on multiple valued (or multi-level) cell property [2], which allows the plural bits to be stored in each memory cell, and reduces the memory cell size by 1/(the number of bits). If such the property is added in the MTJ, they will function as a memory cell more efficient than the conventional one.

In this paper, we theoretically investigate the multiple valued cell property in the MTJ, which is in principle realized by sensing conductances of four states recorded with magnetization configurations of two FMs; (up,up), (up,down), (down,up), (down,down). Then, in order to sense all the states, 4-valued conductances corresponding to the respective states are necessary. Paying attention to magnitude of magnetization in the whole system for the respective configurations, we propose FM1/spin-polarized barrier(SPB)/FM2 junctions, where the FM1 and FM2 are different ferromagnets, and the barrier depends on spin [3]. In actual calculations, the FM1/SPB/FM2 junctions explicitly exhibit 4-valued conductances. Also, as applications, we consider the conductances in the cases of the SPB having the localized spins, that is, Fe-doped oxide barrier [4] and carbon nanotube encapsulating magnetic atoms [5].

Now, we simply investigate the conductance of the FM1/SPB/FM2 junctions, where the SPB merely has spin dependent barrier height due to the pinned magnetization, and its material is not specified for general discussions. The conductance is calculated within the nonequilibrium Green's function technique [3], $\Gamma = \frac{4\pi^2 e^2}{h} \sum_{\sigma=\uparrow,\downarrow} \sum_{\sigma'=\uparrow,\downarrow} T_{\sigma,\sigma'} D_{1,\sigma} D_{2,\sigma'}$, where σ is spin of the tunnel electron, and $D_{1(2),\sigma}$ denotes the density-of-states of FM1(2) at the Fermi level. Further, $T_{\sigma,\sigma'}$ is spin dependent transmission coefficient based on conduction band of the SPB, and includes spin-flip tunneling process with $\sigma \neq \sigma'$. When spin conserved tunneling process with $\sigma = \sigma'$, $D_{1,\downarrow}/D_{1,\uparrow}=0.38$, and $D_{2,\downarrow}/D_{2,\uparrow}=0.58$ are taken into account, we obtain $1 - \delta$ ($= 1 - T_{\downarrow,\downarrow}/T_{\uparrow,\uparrow}$) dependence of $\gamma_{m1,m2} = \Gamma_{m1,m2}/\Gamma_{\uparrow,\uparrow}$ as shown in Fig. 1(a), where $m1$ ($m2$) is magnetization state of the FM1 (FM2) represented by \uparrow or \downarrow . At $1 - \delta=0$, difference of $\gamma_{m1,m2}$ exists only between parallel (P) and antiparallel (AP) configurations. Near $1 - \delta=1$, the differences among all $\gamma_{m1,m2}$ become large, and 4-valued conductances are obviously found.

As applied examples which embody $T_{\sigma,\sigma'}$ in real systems, we focus on the MTJ with the Fe-doped oxide barrier [4] and the carbon nanotube encasing the magnetic atoms [5]. We use a single orbital tight-binding model with nearest neighbor transfer integrals and take into account of the exchange interaction between the tunnel electron spin and the localized spin; $-J\sigma \cdot \mathbf{S}$, where J is an exchange integral, σ is the Pauli matrix, and \mathbf{S} is regarded as a classical spin with $|\mathbf{S}| = S$.

First, we analyze the MTJ with the barrier having n localized spins configured linearly, which may be suitable for a simple model of the Fe-doped oxide barrier [see Fig. 1(b)]. It is assumed that J is a ferromagnetic exchange integral with positive value [4], and direction of the localized spins is parallel to z -axis. Figure 1(c) shows $\gamma_{m1,m2} = \Gamma_{m1,m2}/\Gamma_{\uparrow,\uparrow}$ vs. $|JS/t|$, where t is the transfer integral. With increasing $|JS/t|$, $\gamma_{m1,m2}$ approaches to respective saturation values. In particular, $\gamma_{m1,m2}$ for $n=8$ saturate more rapidly than those for $n=2$, because δ for $n=8$ decreases with $|JS/t|$ more drastically than that for $n=2$ according to $\delta \approx e^{-\Delta_{\kappa n}}$ [3],

where $\Delta\kappa$, the quantity related to the spin dependent conduction band, increases with $|JS/t|$.

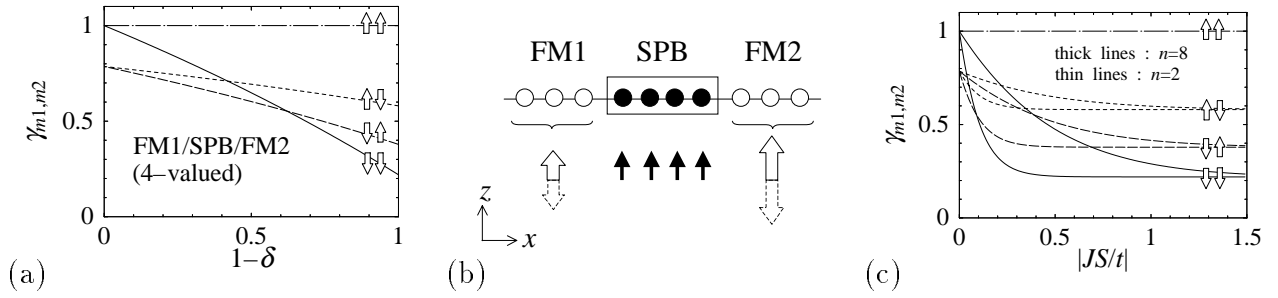


Figure 1: (a) $\gamma_{m1,m2}$ vs. $1 - \delta$. Sets of two arrows are the magnetization states of two FMs. (b) An illustration of the MTJ with the barrier having the localized spins ($n=4$). (c) $\gamma_{m1,m2}$ vs. $|JS/t|$ for the system (b).

Second, the single-walled zigzag carbon nanotube, which encapsulates the magnetic atoms at one side tip, is considered as the SPB. Such the nanotubes were actually fabricated using transition metals of Fe, Co, and Ni as the metallic catalysts [5]. In Fig. 2(a), we show a simplified model, in which the magnetic atoms are arrayed along two zigzag lines and coupled with only respective nearest carbons. Here, J is set to be an antiferromagnetic exchange integral with the negative sign [6], $D_{1,\downarrow}/D_{1,\uparrow}=0.8$ and $D_{2,\downarrow}/D_{2,\uparrow}=0.65$ are adopted, and \mathbf{S} is given by $(S \sin \theta, 0, S \cos \theta)$, where θ is a angle between the spins and the z -axis. In Fig. 2(b), the differences among all $\gamma_{m1,m2} = \Gamma_{m1,m2}/\Gamma_{\downarrow,\downarrow}$ increase with increasing $|JS/t|$, and also $\Gamma_{\downarrow,\downarrow}$ is largest in all $\gamma_{m1,m2}$ owing to $J < 0$. In Fig. 2(c), there is the difference of $\gamma_{m1,m2}$ only between the P and AP configurations at $\theta = -0.5\pi$ because of $T_{\downarrow,\downarrow} = T_{\uparrow,\uparrow}$ and $T_{\uparrow,\downarrow} = T_{\downarrow,\uparrow}$, while the differences among all $\gamma_{m1,m2}$ become large for $\theta \sim 0$ reflecting large difference between $T_{\downarrow,\downarrow}$ and $T_{\uparrow,\uparrow}$.

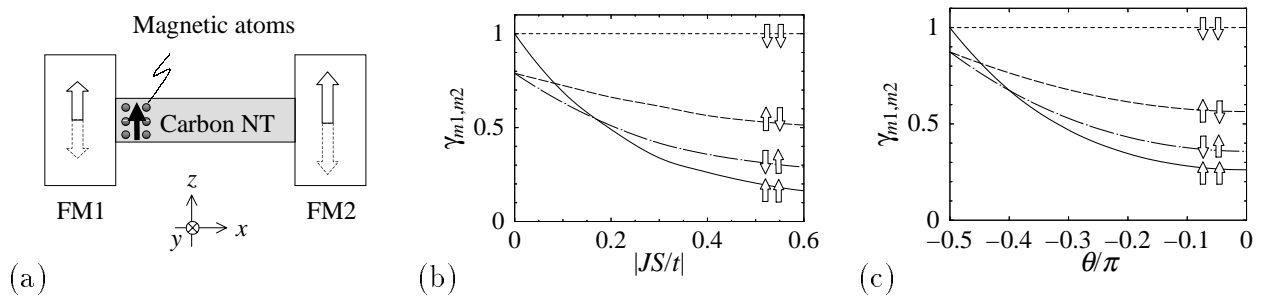


Figure 2: (a) An illustration of the MTJ with the carbon nanotube interacting with the magnetic atoms. (b) $\gamma_{m1,m2}$ vs. $|JS/t|$ in the case of $\theta=0$. (c) $\gamma_{m1,m2}$ vs. θ in the case of $|JS/t|=0.4$. Here, we put $t=-2.5$ eV.

- [1] T. Miyazaki *et al.*, J. Magn. Magn. Mater. **139**, L231 (1995); J. S. Moodera *et al.*, Phys. Rev. Lett. **74**, 3273 (1995); M. Tsunoda *et al.*, Appl. Phys. Lett. **80**, 3135 (2002).
- [2] R. V. Girdhar, Jpn. J. Appl. Phys. **35**, 6347 (1996); N. Takahashi *et al.*, Appl. Phys. Lett. **76**, 209 (2000).
- [3] S. Kokado *et al.*, preprint.
- [4] R. Jansen *et al.*, Appl. Phys. Lett. **75**, 400 (1999); J. Inoue *et al.*, Phys. Rev. B **65**, 104433 (2002).
- [5] X. X. Zhang *et al.*, J. Magn. Magn. Mater. **231**, L9 (2001).
- [6] J. R. Schrieffer *et al.*, Phys. Rev. **149**, 491 (1966).