# Theoretical studies on spin-dependent conductance in FePt/MgO/FePt(001) magnetic tunnel junctions



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# Theoretical Studies on Spin-Dependent Conductance in FePt/MgO/FePt(001) Magnetic Tunnel Junctions

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**The spin-dependent transport properties of FePt/MgO/FePt(001) magnetic tunnel junctions have been investigated on the basis of first-principles electronic structure calculations. The totally symmetric $\Delta_1$-band predominantly contributes to the tunneling conductance for both the majority and the minority-spin channels. In the parallel magnetization configuration, the tunneling conductance via the majority-spin channel shows almost the same values for the junctions with the Fe- and Pt-terminated interfaces. On the other hand, the tunneling conductance via the minority-spin channel for the Fe-terminated interface is two orders of magnitude smaller than that through the Pt-terminated interface. The tunneling magnetoresistance ratio evaluated for the junction with the Fe-terminated interface exceeds 380%, which is in contrast to about 70% for that with the Pt-terminated interface.**

*Index Terms*—**First-principles calculation, $L1_0$-ordered alloy, spintronics, tunnel magnetoresistance.**

## I. Introduction

RECENTLY, extensive research activities have been devoted to nonvolatile magnetoresistive random access memories (MRAMs) which exploit magnetic tunnel junctions (MTJs) as memory cells. When each cell-size is reduced in order to fabricate ultrahigh-density MRAMs, it is inevitable to improve the stability of the magnetization direction at each MTJ against thermal fluctuations at finite temperatures. A possible way to overcome the problem is adopting ferromagnetic materials possessing large magneto-crystalline anisotropy, such as $L1_0$-ordered FePt, as electrodes of MTJs. So far, a tunneling magnetoresistance (TMR) ratio of 18% has been observed at room temperature in the MTJ with an ordered FePt electrode and an amorphous Al-O barrier [1]. The spin polarization deduced from the density of states at the Fermi level is 72% and $-45\%$ for $s$- and $d$-electrons, respectively, in ordered FePt [2]. According to the Jullier model, the uppermost TMR ratio expected is about 220% for FePt/Al-O/FePt MTJs.

On the other hand, huge TMR ratios over 400% at room temperature have been reported for MTJs with use of single-crystalline MgO as a barrier material [3], [4]. The huge TMR can be attributed to gradual decay of the totally symmetric $\Delta_1$ evanescent state in the MgO barrier together with the absence of the $\Delta_1$-band at the Fermi level in the minority-spin state of electrode materials [5], [6]. Thus, it is worthwhile to investigate the possibility to improve the TMR ratio by using the MgO barrier in the MTJs with FePt electrodes. In this study, we investigate electronic structures and spin-dependent transport properties of FePt/MgO/FePt(001) MTJs theoretically on the basis of first-principles density-functional calculations.

## II. Computational Procedure

Actual calculations have been carried out by using a first-principles ultrasoft pseudopotential method implemented in the quantum ESPRESSO code [7]. We adopt plane-wave basis sets with cutoff energies, 30 and 300 Ryd, for expanding wavefunctions and the charge density in the system, respectively, and a generalized gradient approximation for the exchange-correlation energy [8]. The spin-orbit interaction is not considered in this work.

For transport calculations, we consider an open quantum system consisting of an electron-scattering region and left and right semi-infinite electrode regions. The scattering region corresponds to the MTJ including several monatomic layers (MLs) of FePt attached to the both side of the MgO barrier. On the other hand, the electrode region has the same electronic potential energy with that of bulk FePt. The electronic transmittance can be obtained by solving a scattering equation under the boundary condition, i.e. the propagating wavefunction in the scattering region should be continuously smooth with the Bloch states in each electrode region [9], [10]. Since we assume atomically flat FePt/MgO(001) interfaces, the in-plane wave-vector $\boldsymbol{k}_{//} = (k_x, k_y)$ of each propagating state is conserved throughout the MTJ. Furthermore, no inelastic scattering as well as no spin-flip process is considered in the transport calculations.

## III. Result and Discussion

First, we have calculated the electronic band-structure of bulk FePt. The dispersion curves along the [001] direction are depicted for the majority- and the minority-spin states in Fig. 1(a) and (c), respectively. It is found that the totally symmetric $\Delta_1$-band in FePt crosses the Fermi level both in the majority- and minority-spin states, in contrast to ferromagnetic transition metals such as bcc Fe. The minority-spin $\Delta_1$-band is predominantly composed of Fe and Pt $d(3z^2 - r^2)$ orbital at the Fermi level, while the majority-spin $\Delta_1$-band is mainly constructed from Fe and Pt $p(z)$ orbital. Since the $\Delta_1$-band electrons predominantly transmit the MgO barier [5], [6], huge TMR ratios cannot be expected in the FePt/MgO/FePt(001) MTJs from the viewpoint of symmetry compatibility between the electronic band-structure in the bulk FePt and MgO. However, it is too hasty to conclude the inefficient TMR performance in FePt/MgO/FePt(001) MTJs, as will be discussed later.

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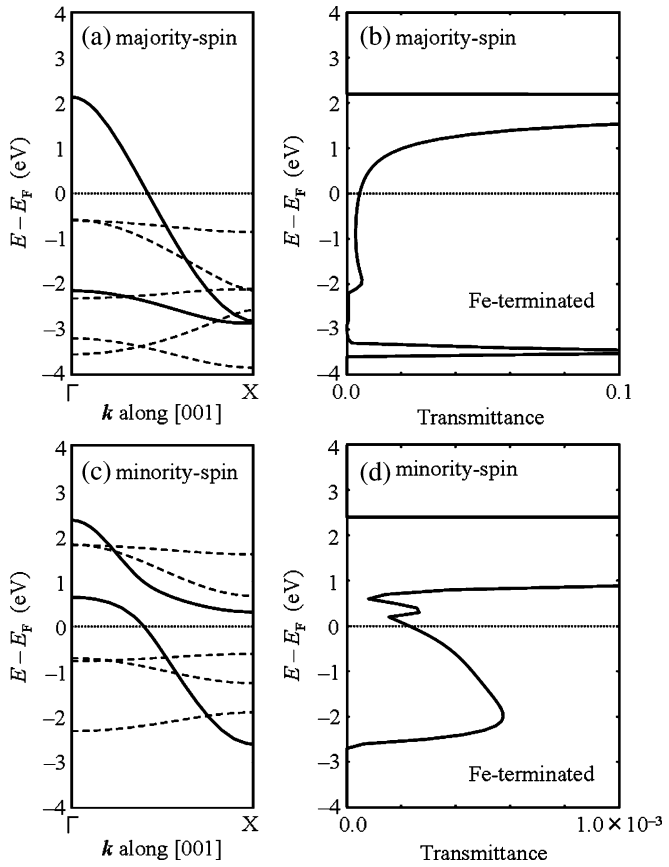


Fig. 1. Left: the electronic band dispersion curves of bulk FePt as a function of wave-vector $\boldsymbol{k}$ along the [001] direction: (a) the majority-spin state and (c) the minority-spin state. Full and broken curves represent the bands with the $\Delta_1$ and the other symmetries, respectively. Right: tunneling transmittance for $\boldsymbol{k}_{//} = (0, 0)$ as a function of incident electron energy relative to the Fermi level $E_{\rm F}$ for the Fe-terminated FePt/MgO/FePt MTJ in the parallel magnetization configuration: (b) the majority-spin channel and (d) the minority-spin channel. It is noted that the scale of the transmittance in (d) is two orders of magnitude smaller than that in (b).

Next, we have investigated the energetically favorable atomic structure of the FePt/MgO(001) interface. The lattice constant of bulk MgO, 0.422 nm, is larger by about 9% than that of bulk FePt, 0.386 nm. In this study, we assume that the in-plane lattice constant of the MTJ is identical with that of bulk FePt. The interlayer separations in the MTJs are fully relaxed so as to minimize the total energy of the system. Comparing the adhesion energy of the interface, we found that the Fe-terminated interface, in which the Fe atom is located on top of the O atom, has strong bonding with MgO layer, as compared with the other structures including the Pt-terminated interfaces. Moreover, the formation energy is lower for the Fe-terminated interface than that for the Pt-terminated interface. These results clearly show that the Fe-terminated interface to MgO is more stable than the Pt-terminated one. In contrast to this, for the free surface, the Pt termination is energetically favorable. The formation of Fe-O bonding significantly contributes to the stability of the Fe-terminated FePt/MgO(001) interface. In fact, the Fe-O distance at the Fe-terminated interface is 0.22 nm, which is much shorter than the Pt-O distance, 0.26 nm, in the Pt-terminated interface.

Finally, we have investigated the tunneling conductance of FePt/MgO/FePt (001) MTJs with 5-ML MgO thickness. In Fig. 1(b) and (d), tunneling transmittance calculated for the in-plane wave-vector $\boldsymbol{k}_{//} = (0, 0)$ is depicted as a function of incident electron energy relative to the Fermi level for the Fe-terminated FePt/MgO/FePt MTJ in the parallel magnetization configuration via the majority- and the minority-spin channels, respectively. It is confirmed that the $\Delta_1$-band predominantly contributes to the tunneling transmittance for both the majority- and the minority-spin channels. Furthermore, it is noted that the tunneling transmittance via the minority-spin channel is almost two orders of magnitude smaller than that via the majority-spin channel at the Fermi level.

The tunneling transmittance of electrons at the Fermi level as a function of the in-plane wave-vector $\boldsymbol{k}_{//} = (k_x, k_y)$ shows a sharp peak around the center of the two-dimensional (2-D) Brillouin zone, as shown in Fig. 2. It is a typical behavior for coherent tunneling transmittance of the $\Delta_1$-band electrons found in the MgO-based MTJs [5], [6], [11]. In the parallel magnetization configuration, the tunneling transmittance via the majority-spin channel is in the same order of magnitude for the MTJs with the Fe- and Pt-terminated interfaces, as shown in Fig. 2(a) and (c). On the other hand, the tunneling conductance via the minority-spin channel depends remarkably on the interface structure of the MTJ, i.e. the conductance for the Fe-terminated interface is two orders of magnitude smaller than that through the Pt-terminated interface as shown in Fig. 2(b) and (d).

The significant reduction of the tunneling transmittance can be attributed to the scattering of the minority-spin electrons at the Fe-terminated FePt/MgO(001) interface. Fig. 3 shows the tunneling electron density of the $\Delta_1$-band at the Fermi level as a function of each atomic site through the Fe-terminated FePt/MgO/FePt(001) MTJ in the parallel magnetization configuration. The decay rate of the tunneling electron density in the interior region of the MgO barrier is almost the same for both the majority- and the minority-spin channels. The abrupt reduction of the tunneling electron density is found in the interfacial region between the left FePt electrode and the MgO barrier for the minority-spin channel as shown in Fig. 3(b). It is a clear evidence of significant interfacial scattering of the minority-spin electrons in the Fe-terminated FePt/MgO(001) interface. It is noted that the the minority-spin $\Delta_1$-band in FePt is predominantly composed of Fe and Pt $d(3z^2 - r^2)$ orbital at the Fermi level. Thus the interfacial scattering can be originated from small transfer probability between the Fe $d(3z^2 - r^2)$ and the O $p(z)$ orbitals at the Fe-terminated interface. The interfacial scattering is pronounced only for the Fe-terminated interface, since the Fe $d(3z^2 - r^2)$ orbital is much more localized than the Pt $d(3z^2 - r^2)$ orbital.

The interfacial scattering reduces the tunneling transmittance of both the spin-up and spin-down electrons in the antiparallel magnetization configuration for the Fe-terminated FePt/MgO/FePt(001) MTJ, since the tunneling electrons must be in the minority-spin bands of the left or right FePt electrodes. The tunneling transmittance averaged over the in-plane wavevector is $1.76 \times 10^{-4}$ and $3.66 \times 10^{-5}$ in the parallel and antiparallel magnetization configuration, respectively, for the Fe-terminated

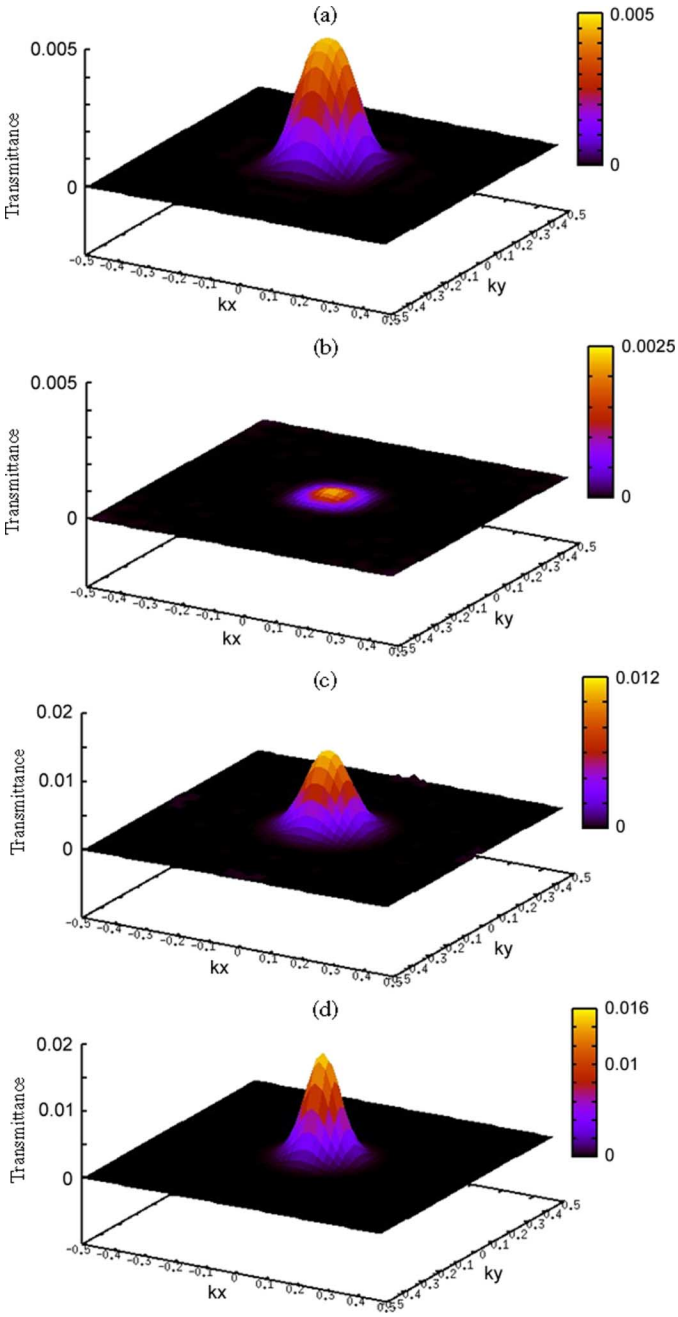


Fig. 2. Tunneling transmittance of electrons at the Fermi level as a function of the in-plane wave-vector $\boldsymbol{k}_{//} = (k_x, k_y)$ for the FePt/MgO/FePt MTJs in the parallel magnetization configuration: (a) the majority-spin and (b) the minority-spin channel for the MTJ with the Fe-terminated interface and (c) the majority-spin and (d) the minority-spin channel for the MTJ with the Pt-terminated interface, respectively.

MTJ. As the consequence, the TMR ratio evaluated for the MTJ with the Fe-terminated interface exceeds 380%, which is in contrast to that of about 70% for the MTJ with the Pt-terminated interface. It is noted that the TMR ratio over 100% has been observed experimentally for FePt/MgO/Fe/FePt(001) MTJs [12]. The effect of inserting Fe layer is unclear at the present stage, however, the large TMR ratio observed could be attributed to the existence of the Fe-terminated FePt/MgO(001) interface in the MTJs.

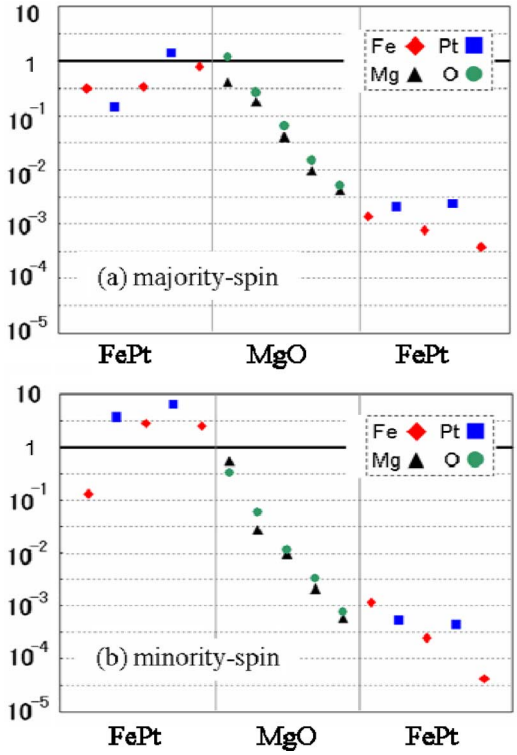


Fig. 3. Tunneling electron density of the $\Delta_1$ band at the Fermi level as a function of each atomic site through the Fe-terminated FePt/MgO/FePt(001) MTJ in the parallel magnetization configuration: (a) the majority-spin channel and (b) the minority-spin channel.

## IV. Conclusion

The Fe-terminated interface is more desirable for obtaining larger TMR ratio in the FePt/MgO/FePt(001) MTJs. The Fe-terminated FePt/MgO(001) interface is found to be favorable energetically and thus it can be realized for appropriate growth conditions. Recently, spin injection from FePt/MgO (001) junctions into GaAs has been succeeded at room temperature [13]. The Fe-terminated interface can also be expected to improve the efficiency of spin injection from the FePt/MgO(001) junctions, since it possesses spin-filtering functionality originated from the interfacial scattering of tunneling electrons.

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