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2007 J. Phys.: Condens. Matter 19 365228

(http://iopscience.iop.org/0953-8984/19/36/365228)

IOP PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER

J. Phys.: Condens. Matter **19** (2007) 365228 (7pp) doi:10.1088/0953-8984/19/36/365228

Coherent tunnelling conductance in magnetic tunnel junctions of half-metallic full Heusler alloys with MgO barriers

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Received 21 December 2006, in final form 2 January 2007
Published 24 August 2007
Online at stacks.iop.org/JPhysCM/19/365228

Abstract

We have carried out electronic structure and transport calculations for magnetic tunnel junctions (MTJ) composed of MgO and a half-metallic full Heusler alloy Co_2MnSi on the basis of the density functional theory and the Landauer formula. We find that the density of states of Co atoms at the Co_2MnSi/MgO(001) interface shifts toward the higher energy side due to the reduced symmetry, leading to a reduction of the spin polarization at the interface. Furthermore, we show that the majority-spin transmittance as a function of the in-plane wavevector $k_{\parallel}$ has a broad peak centred at $k_{\parallel} = (0, 0)$ due to the tunnelling from the Δ_1 channel of Co_2MnSi, while the transmittance from the Δ_5 channel is three orders of magnitude smaller than that of the Δ_1 channel. These results indicate that coherent tunnelling through the Δ_1 band is dominant also in an MTJ with Co_2MnSi and an MgO barrier, like in Fe/MgO/Fe(001) MTJ and related systems.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

The challenge of utilizing the spin degree of freedom of electrons as well as their charge in electronic applications (spintronics) has drawn much attention in recent years [1]. A prototype phenomenon of this concept is the tunnelling magnetoresistance (TMR) effect which is essential for spintronics devices, such as the magnetoresistive random access memory (MRAM). There are two main scenarios for realizing much larger TMR. One is the use of half-metallic ferromagnets (HMF) as the electrodes. Here, the HMF is metallic for the majority-spin band and semiconducting with an energy gap at the Fermi level for the minority-spin band, leading to complete (=100%) spin polarization. While there are many theoretical predictions for the HMF [2–8], the Co-based full Heusler alloys Co_2YZ (Y: transition metal; Z: sp atom) are

the best prospective candidates for application in the spintronics devices. This is due to a high Curie temperature beyond room temperature [9] and the robustness of the spin polarization against B2-type atomic disorder [10, 11]. A lot of experimental results on TMR for MTJ using Co_2YZ, have been reported for alumina barriers [12–19], and a huge TMR (570%) was obtained at low temperature. However, the TMR decreases rapidly with increasing temperature in experiments [16].

The other scenario for obtaining much larger TMR was the use of single-crystalline MgO as the barrier [20, 21]. Butler *et al* [20] predicted a much larger TMR ratio, as high as 6000%, for the Fe/MgO/Fe(001) MTJ using the first-principles layer KKR approach. They found that the coherent tunnelling of highly spin-polarized Fe s-like states (Δ_1 states) propagating along the direction perpendicular to the plane, i.e. $k_\parallel = (0, 0)$, make the main contribution to the large magnetoresistance because of their symmetry matching with MgO complex Δ_1 bands within the energy gap and the slow decay in MgO. Indeed, a larger TMR ($\sim$410%) ratio was obtained at room temperature for the MTJ of Fe/MgO/Fe(001) and related systems [22–25]. Although the high TMR observed in Fe/MgO/Fe(001) MTJ and related systems overcomes some problems in the MRAM, larger TMR beyond 1000% will be required for further development of the MRAM and other spintronics devices. To achieve this, we have to suppress the interfacial resonant tunnelling between Fe/MgO interfacial states at a particular $k_\parallel \neq (0, 0)$ in the minority-spin channel, because the upper bounds of the TMR in Fe/MgO/Fe(001) are determined by the resonant transmission. The use of the HMF as the electrodes together with the MgO barrier can be expected to eliminate the resonant transmission, and to provide a much larger TMR ratio. In fact, experimentally observed TMR in the MTJ of Co_2YZ/MgO/Co_2YZ has been improved steadily [26–29], although the temperature dependence of the TMR is also very large.

In this work, we theoretically investigate electronic structures and transport properties of Co_2MnSi/MgO/Co_2MnSi(001) MTJ (abbreviated as CMS/MgO/CMS hereafter) in order to clarify their possibilities of showing much larger TMR. In particular, we focus on electronic properties of the interface between CMS and MgO (CMS/MgO) and a symmetry matching between propagating states and decaying states in CMS/MgO/CMS for the parallel magnetization case. To this end, we perform first-principles electronic structure and transport calculations using the quantum ESPRESSO code [30].

2. Computational details

For conductance calculations, we consider an open quantum system consisting of a scattering region corresponding to MgO and a junction with CMS attached to left and right semi-infinite electrodes corresponding to bulk CMS. Conductance is obtained by solving a scattering equation with an infinite boundary condition in which the wavefunction of the scattering region and its derivative are connected to the Bloch states of each of the electrodes. The potential in the scattering equation can be obtained from the first-principles electronic structure calculations for a supercell which contains a left electrode and a scattering region. (A right electrode can be removed from the supercell, because we consider MTJ with parallel magnetization.) The first-principles calculations are performed by the ultrasoft pseudopotential method with the generalized gradient approximation for the exchange–correlation energy [31].

Since our system is repeated periodically in the xy plane and propagating states can be classified with an in-plane wavevector $k_\parallel = (k_x, k_y)$ index, different $k_\parallel$ do not mix and can be treated separately. Furthermore, our approach neglects the spin–orbit interaction and noncollinear spin configuration; therefore electrons with different spin move independently in different potentials. Thus, we solve scattering equations at some fixed $k_\parallel$ and spin index on the

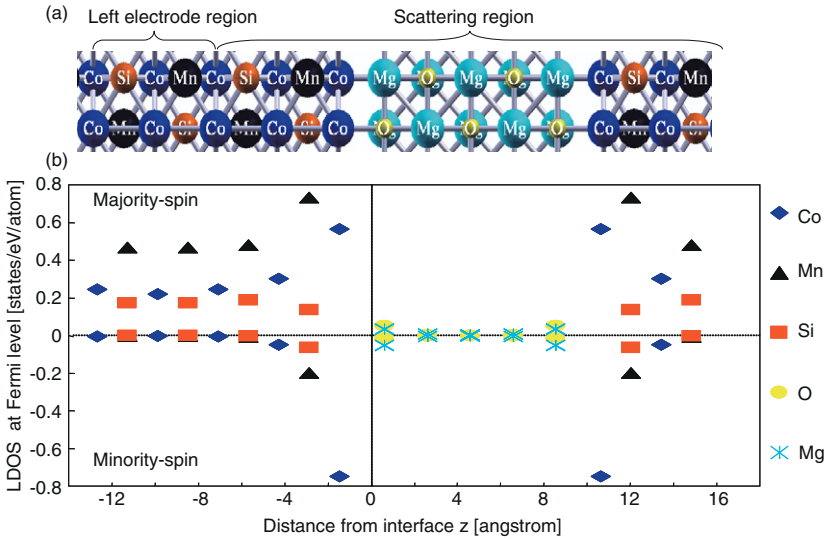

Figure 1. (a) A supercell of the Co_2MnSi/MgO/Co_2MnSi MTJ with the Co-terminated O-top configuration, and the corresponding left electrode and scattering regions assumed in conductance calculations. (b) Local density of states at the Fermi level projected onto each atomic sphere as a function of the distance from the left-hand side of the Co_2MnSi/MgO interface, where the sign of the LDOS indicates majority spin (positive) and minority spin (negative).

basis of the approach proposed by Choi and Ihm [32, 33]. Finally, we evaluate the zero-bias limit conductance (at the Fermi level) from the Landauer formula [34].

3. Results and discussion

3.1. Electronic structure of the interface

We consider a tetragonal CMS/MgO/CMS supercell, where the in-plane lattice constant of the supercell is fixed at 3.96 Å which corresponds to $a_0/\sqrt{2}$ with a_0 being the lattice constant of bulk CMS (5.63 Å) on a 45° in-plane rotation, and is smaller by 4% than the lattice constant of bulk rock-salt MgO (4.22 Å). The CMS/MgO(001) interface has two types of termination on CMS: one is the Co termination and the other is the MnSi termination. Furthermore, each has three possible structures, in which atoms terminating the CMS are positioned on top of O atoms (O-top), Mg atoms (Mg-top) or hollow sites of MgO(001) surface. We adopted the Co-terminated O-top configuration as a CMS/MgO interface structure, because this interface has larger adhesion energy than other interface structures [35], where the adhesion energy is defined as the ideal work for separating an interface [36]. The supercell is composed of nine atomic layers of CMS, five layers of MgO and four atomic layers of CMS along the [001] direction. The number of atomic layers between the right edge of the left electrode and the left-hand side of the CMS/MgO interface is chosen large enough to reproduce bulk properties of CMS in the electrode region. This feature is essential for applying the infinite boundary condition. We checked that four atomic layers are necessary from the right edge of the left electrode to the left-hand side of CMS/MgO interface so that CMS in the left electrode shows bulk-like electronic structure. Schematic diagrams of the supercell and corresponding left electrode and scattering region are shown in figure 1(a).

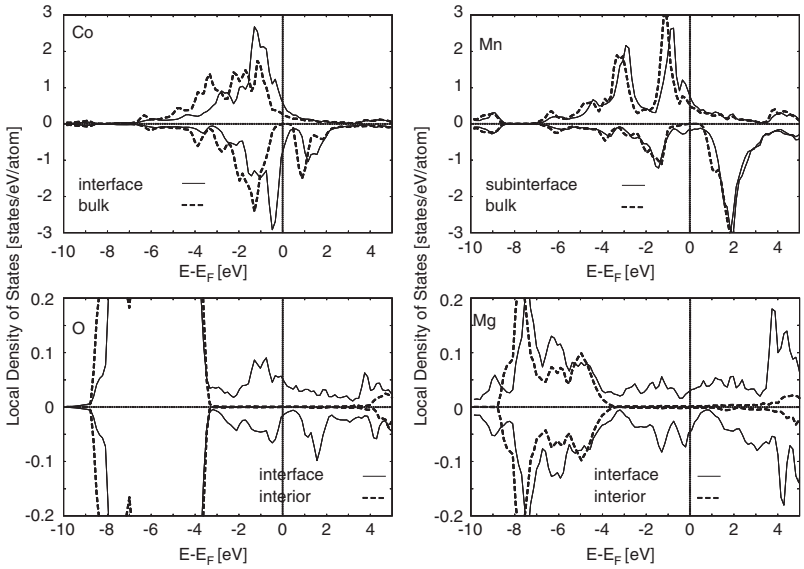

Figure 2. LDOS of interface Co, O, Mg and subinterface Mn in the Co-terminated O-top configuration of the Co_2MnSi/MgO interface as a function of energy relative to the Fermi energy. The sign of the LDOS indicates majority spin (positive) and minority spin (negative). For comparison, the LDOS in the bulk-like or interior region is also presented, as a dashed line.

Figure 1(b) shows the majority-spin and the minority-spin local density of states (LDOS) at the Fermi level projected onto each atomic sphere as a function of the distance z from the left-hand side of the CMS/MgO interface. It is found that the minority-spin LDOS is almost zero in the left electrode region of the MTJ ($z = -12.7$ to -7.07 Å). This confirms that the thickness of the CMS layer is large enough for recovering the half-metallicity of bulk CMS. On the other hand, minority-spin interface states are observed around the CMS/MgO interface, which significantly degrades the spin polarization at the interface.

To look at electronic structures at interfaces in a little more detail, we present in figure 2 the LDOS of interface Co, Mg and O atoms and subinterface Mn atoms as a function of energy relative to the Fermi energy. The LDOS of the same atoms in the corresponding bulk-like region are shown as a reference. It is found that the LDOS of Co atoms shifts toward the higher energy side, and the Fermi level falls at the right edge of the Co minority valence bands. Since a Co atom loses half of its first neighbours at the interface, non-bonding d states can appear around the Fermi level. This makes a shift of the LDOS of the Co atom and degrades the half-metallicity at the interface. Similar behaviour can be observed in the LDOS of Co atoms in the Co-terminated *surface* of Co_2MnSi and Co_2MnGe [37]. In contrast, the LDOS of Mn atoms at the subinterface layer behaves similarly to that of the bulk, because a subinterface Mn atom has four Co atoms as first neighbours and retains the local coordination of bulk Co_2MnSi. The small DOS appearing in the half-metallic gap of minority-spin states are due to hybridization with interface Co atoms.

The LDOS of the interior MgO layers in the vicinity of the Fermi energy shows a wide gap, where sp states of O and Mg atoms are located between 3 and 9 eV below the Fermi level. It is noticeable that metal induced gap states (MIGS) are observed in the LDOS of O and Mg atoms at the interface due to the Co–O and Co–Mg interactions. However, the LDOS of the MIGS appearing in the energy gap are rather small as compared with the LDOS of O atoms

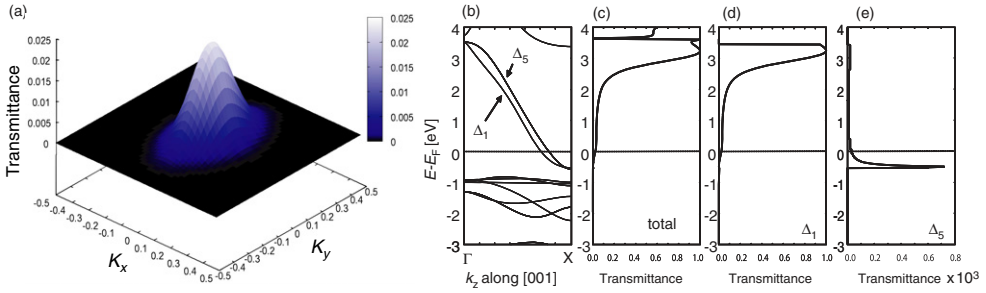

Figure 3. (a) Majority-spin transmittance as a function of $k_\parallel = (k_x, k_y)$ at the Fermi level for $Co_2MnSi/MgO/Co_2MnSi(001)$ MTJ. (b) The band structure of bulk Co_2MnSi along the [001] direction at $k_\parallel = (0, 0)$. (c)–(e) The total and band resolved transmittances at $k_\parallel = (0, 0)$ as a function of energy relative to the Fermi energy.

between −8 eV and −4 eV, indicating weak hybridization between Co and O at the interface. In the CMS/MgO/CMS, the position of the O p states is much lower than the Fermi level, while the Co d states are located mainly in the vicinity of the Fermi level. Therefore, the Co d orbital cannot hybridize strongly with the O p orbital due to their large orbital energy difference.

3.2. Conductance of $Co_2MnSi/MgO/Co_2MnSi$

In figure 3(a), we show the majority-spin transmittance at the Fermi level as a function of $k_\parallel$ for the Co-terminated interface of CMS/MgO/CMS. The result shows a broad peak centred at $k_\parallel = (0, 0)$ like for the tunnelling transmission in a free electron model. A broad peak centred at $k_\parallel = (0, 0)$ was also observed in the tunnelling transmission for Fe/MgO/Fe(001) MTJ [20]. We show in figure 3(c) the majority-spin transmittance at $k_\parallel = (0, 0)$ as a function of incident electron energy. The band structure of bulk CMS along the [001] direction at $k_\parallel = (0, 0)$ is also presented in figure 1(b) for comparison. It is found that the transmittance increases with increasing energy and the threshold coincides with the bottom of the broad conduction bands of bulk CMS. This means that the conduction bands make the main contributions to the transmittance at $k_\parallel = (0, 0)$.

Since it is of great importance to assess the symmetry matching between propagating states of CMS and decaying states of MgO in CMS/MgO/CMS, we show in figures 3(d) and (e) band resolved transmittances as a function of incident electron energy. It is noted that the lower conduction band in figure 3(b) has Δ_1 symmetry and is composed of Si s (69%) and Mn s (25%) at the Γ point and of Co d_{z^2} and $d_{x^2-y^2}$ (76%) at the X point. Furthermore, the upper conduction bands which correspond to Δ_5 symmetry are doubly degenerate and composed of Si p (78%) at the Γ point and of Mn d_{xy}, d_{yz}, and d_{zx} (51%) at the X point. In figure 3(d), we find that the Δ_1 channel in the lower conduction band dominates the tunnelling and the energy dependence of the transmittance is almost the same as that of the total transmittance, indicating the symmetry matching of the Δ_1 wavefunction in CMS/MgO/CMS. A steep increase of the transmittance above 2 eV is attributed to the presence of the conduction band of MgO, i.e. the incident electron energy is higher than the potential barrier in MgO. On the other hand, the transmittance from the Δ_5 channel in doubly degenerate upper conduction bands is three orders of magnitude smaller than that from the Δ_1 channel due to the rapid decay of the Δ_5 wavefunction in the MgO energy gap [20]. These results indicate that the presence of the Δ_1 band across the Fermi level in CMS is crucial for a larger transmittance in CMS/MgO/CMS.

In figure 1(b), the minority-spin DOS at the Fermi level appears around the CMS/MgO interface due to the reduced symmetry. These minority-spin interface states do not contribute

to the transmittance, because there are no minority-spin Bloch states in the electrode region due to the half-metallic character of bulk CMS. Thus, all minority-spin transmittance around the Fermi energy becomes zero by definition in the MTJ with the parallel magnetization, leading to in total zero transmittance around the Fermi energy for the MTJ with anti-parallel magnetization. However, as is pointed out by Mavropoulos *et al* [38], if spin mixing processes such as spin–orbit interaction, noncollinear spin and thermal spin fluctuation are included in transport calculations, the minority-spin interface states can contribute to the transmittance, which gives rise to finite transmittance for MTJ with the anti-parallel magnetization. In the present system, the minority-spin interface states around the Fermi level are composed mainly of Co d non-bonding states. Therefore, these states will undergo rapid decay in the MgO barrier and make little contribution to the transmittance of minority-spin state as compared with the majority-spin Δ_1 state.

In conclusion, we investigated electronic structures and transport properties of CMS/MgO/CMS with parallel magnetization. We found that in the Co-terminated O-top interface, the LDOS of Co atoms shifts toward the higher energy side due to the reduced symmetry, and the Fermi level falls at the right edge of the Co minority valence bands, leading to a reduction of the spin polarization. Furthermore, we found that the majority-spin transmittance as a function of $k_\parallel$ has a broad peak centred at $k_\parallel = (0, 0)$ due to the tunnelling from the Δ_1 band of CMS, while the transmittance from the Δ_5 channel is three orders of magnitude smaller than that of the Δ_1 channel. This means that coherent tunnelling through the Δ_1 band, as for Fe/MgO/Fe(001) MTJ and related systems, can be expected also in the present system. All these findings suggest that the MTJ with MgO and CMS (and possibly other full Heusler alloys) will show huge magnetoresistance and are worth further investigation.

Acknowledgments

This work was supported in part by a Grant-in-Aid for Scientific Research from the MEXT (Grant Nos 16310081, 17064001, 18740172 and 18760227) and also by the IT programme of Research Revolution 2002 from the MEXT.

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