Large magnetoresistance in planar Fe/MoS₂/Fe tunnel junction

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Abstract

We report a large magnetoresistance observed in a Fe/MoS₂/Fe tunnel junction, where iron electrodes are attached to the edges of MoS₂ nanoribbon (i.e. the current is flowing in the plane of the MoS₂ 2D monolayer). Using non-equilibrium Green's functions in the framework of density functional approach, our calculations show a large magnetoresistance in Fe/MoS₂/Fe junction, with the values up to 150%. The strong coupling between states of Mo atoms at the edge of the MoS₂ monolayer and those at the Fe surface have a dramatic effect on the conductance property of the material as well as the MR of the Fe/MoS₂/Fe tunnel junction. We conclude that the Fe electrodes polarize the spin states of MoS₂ near the interface and efficiently inject carriers into MoS₂. We find that the atomically-thin spacers are metallic due to a strong hybridization between the Fe and Mo states at the interface. MoS₂ spacers of a larger width remain insulating. We also find that the magnetoresistance of thin MoS₂ ribbons (three atomic layers wide) is negative and has a small value. Notably however, as the width of the MoS₂ spacer increases, this value turns positive and increases in magnitude.

Introduction

Recently, spin-valve devices have attracted the attention of the scientific community as promising candidate in designing next-generation magnetic random-access-memories (MRAM)¹, magnetic sensors², and novel programmable logic devices³. Spin-valve structures used in modern hard-drive read heads and magnetic random access memories comprise two ferromagnetic electrodes whose relative magnetization orientations can be switched between parallel and antiparallel configurations, yielding the desired giant or tunneling magnetoresistance effect. For example, Fe/Mo multilayers⁴ with Mo as a spacer exhibit Giant magnetoresistance (GMR), while molecular contact Au/Mo₂Fe₂/Au shows a magnetoresistance at low bias voltage⁵. Wide-gap oxide is typically used as an insulating spacer in current spin valve devices such as Fe/MgO/Fe⁶. Recently, 2D materials with atomically-thin layers have been examined as useful ultrathin nonmagnetic spacer layers in spin-valve devices. Recently, magnetic tunnel junctions (MTJ) have been fabricated with graphene^{7,8} and Boron Nitride (BN)⁹ as the tunnel layers. These devices show considerable tunnel magnetoresistance.

The transition metal dichalcogenides (TMDs) are 2D materials that potentially may lead to the development of spintronic devices. Molybdenum disulfide (MoS₂) is one of the most studied TMDs. MoS₂ has drawn attention due to its distinctive electronic and optical properties such as electrostatic coupling¹⁰, large carrier mobility¹¹, high current carrying capacity¹², and high thermal stability¹³. It has a tunable bandgap that changes from an indirect 1.2 eV¹⁴ in the bulk to a direct 1.8 eV^{15,16} for monolayers, exhibiting conventional semiconducting behavior. Structurally, bulk

MoS₂ is a layered semiconducting material constructed of stacked S-Mo-S composite 2D monolayers. The adjacent monolayers in MoS₂ bulk crystals are weakly bound through van der Waals interactions¹⁷. Due to the weak interlayer coupling and wave function overlap MoS₂ displays a relatively poor conductivity in the vertical direction (perpendicular to the MoS₂ sheet plane).

Recent theoretical studies promise a large magnetoresistance when MoS₂ is sandwiched between two Fe electrodes owing to the efficient spin injection, thus rendering the possibility of realizing tunable spin-valve devices based on 2D-TMDs.¹⁸ However, this study focuses on the vertical transport properties of MoS₂, i.e. the current flows in a direction perpendicular to the plane of the MoS₂.

The monolayer of MoS₂ is typically produced by the micromechanical exfoliation method^{19,20}. Although MoS₂ monolayer has a direct band gap, the mobility of its charge carriers is low compared to graphene¹⁰. However, it has recently been shown that the mobility of the MoS₂ monolayer can be increased by several times by bringing MoS₂ in contact with metallic electrodes (metal/MoS₂)²¹. Considerable efforts have been directed to investigate the electrical transport properties of metal/MoS₂ structures such as NiFe/MoS₂²² and Fe/MoS₂¹⁸.

In this paper, we analyze the magnetoresistance in Fe/MoS₂/Fe devices in planar geometry. Fe electrodes were attached to the edges of the MoS₂ nanoribbon. The electric current flows in the plane of the MoS₂ monolayer. Using Density Functional Theory (DFT) calculations, we predict a large magnetoresistance (MR) effect in Fe/MoS₂/Fe junctions, with a maximum MR of 150%. The calculations reveal that atomically-thin spacers are metallic as a result of the strong hybridization between states of atoms at the edge of the MoS₂ structures and those on the Fe surface. We find that Fe electrodes efficiently inject carriers into atomically-thin MoS₂ spacers. Spacers having a larger width remain insulating with higher MR. The effect of the interface states on the conductance of MoS₂ is discussed.

Figure 1. [(a) top view and (b) side view] The structure of $(\text{Fe}/\text{MoS}_2(n)/\text{Fe})$ tunnel junctions. MoS_2 armchair terminated monolayers of varied widths (shown as green, Mo, and black, S) is attached to the Fe (100) bulk electrodes (shown in red). The region within the two dashed lines is the scattering region and the remaining parts are the semi-infinite left and right electrodes.

Computational Method

The Fe (100)/ MoS_2 interface was optimized within the density functional theory (DFT),²³ as implemented in the SIESTA package²⁴. Troullier–Martins type norm-conserving pseudopotentials²⁵ were used in our calculations. All pseudopotential calculations include f-states, core radii for S (s- 1.63, p- 1.76, d- and f-1.94 a_0 , where a_0 is a Bohr radius), Mo (s- 2.75, p-2.89, d-,f-2.49 a_0), and Fe (s- 2.41, p-2.53, d-,f- 2.29 a_0). The generalized gradient approximation (GGA) of the Perdew–Burke–Ernzerhof (PBE)²⁶ form is used to describe the exchange-correlation energy. Self-consistent calculations are performed with a 400 Ry mesh cut off. A linear combination of numerical atomic orbitals with double- ξ polarizations (DZP) basis set is used. The conjugate gradient method is used to relax the ionic coordinates until the force on each atom is less than 0.03 eV/Å and the difference of the total energy between two consecutive ionic steps is less than 10^{-5} eV.

The two probe transmission in $\text{Fe}(100)/\text{MoS}_2/\text{Fe}(100)$ junctions is calculated by the non-equilibrium Green's function (NEGF) technique within the Keldysh formalism, as implemented in the TranSIESTA. The current flows in the plane of MoS_2 ribbon. The computational parameters in case of the electronic transport calculations are the same as those for the above DFT calculations.

A 5X6 $k_{\parallel}$ -mesh is used to converge the charge density matrix for the quantum transport calculation, but a denser $k_{\parallel}$ mesh, typically of 11X17 $k_{\parallel}$ points, is used to evaluate transmission coefficients. It was found that the calculated transmission coefficient do not change significantly at denser k-point sampling. At zero bias, the conductance G is evaluated by the transmission coefficients $T(E)$ at the Fermi energy, E_F , as follows

$$G = G_0 T(E_F), \quad (1)$$

where $G_0 = 2e^2/h$ is the unit of quantum conductance. The MR ratio is defined as

$$MR = \frac{G_P - G_{AP}}{G_{AP}} \times 100\%, \quad (2)$$

where G_P and G_{AP} are the total conductance for two ferromagnetic (FM) leads with parallel (P) and antiparallel configurations (AP), respectively.

At non-zero bias NEGF approach $I(V)$ curve is evaluated using the Landauer-Buttiker equation²⁷

$$I(V_b) = \frac{2e^2}{h} \int_{-\infty}^{\infty} T(E, V_b) [f_L(E - \mu_L) - f_R(E - \mu_R)] dE, \quad (3)$$

Where $T(E, V_b)$ is the transmission probability of electrons incident at an energy E through the device with external voltage V_b , $f_{L(R)}$ is the Fermi-Dirac distribution function for left (right) lead, and $\mu_{L(R)}$ is the electrochemical potential of the left (right) lead.

Device Model

The two-probe structural models used in our calculation are illustrated in Figure 1. A MoS₂ nanoribbon is symmetrically sandwiched between two Fe (100) electrodes. The electrode cell was set up with 3x2 repeats of unit cell of Fe (100) and aligned with the edge of an armchair terminated MoS₂ nanoribbon. The scattering region includes a monolayer of MoS₂ together with three screening Fe (100) layers on the left and four layers on the right, to improve the stability of the calculation (by reducing scattering at the lead-barrier interface). The calculated in-plane lattice parameter of the MoS₂ ribbon is 5.47 Å, ensuring a good lattice parameter match at the Fe/MoS₂ interface. In order to compensate for the lattice mismatch across the Fe/MoS₂ interface (~ 3.5%), the Fe unit cell was subjected to a small amount of stress so that it matched the MoS₂ lattice parameter. The width of the MoS₂ monolayer varied from 3 atomic layers (1.5 unit cell) to 11 atomic layers (5.5 unit cells) as shown in Figure 1. The width of the nanoribbon is represented by the value of the number of layers, n , in Figure 1. The different geometries are denoted by Fe/MoS₂(n)/Fe ($n = 3, 5, 7, 9, 11$).

The width, c , of the MoS₂ spacer interfaced with the Fe (100) electrodes was optimized. The total energy of the Fe/MoS₂ supercell as a function of c for each of the considered geometries (i.e. $n = 3, 5, 7, 9, 11$) was calculated. A structural relaxation of the Fe/MoS₂/Fe structure was performed for each width. The c values corresponding to the minimum energy Fe/MoS₂ supercells are presented in Figure 1. These supercells were used to build the two-probe Fe/MoS₂(n)/Fe device in the conductance calculations.

Result and Discussion

The conductance, in the linear regime, is proportional to the transmission calculated at the Fermi level (Eq. 1). Figure 2 presents the calculated transmissions of Fe/MoS₂(n)/Fe junctions, with $n=3, 5, 7, 9$ and 11 atomic layers perpendicular to MoS₂ monolayer in the scattering region, with magnetizations of Fe (100) electrodes are parallel (P), or anti-parallel (AP). As can be seen in Figure 2, at Fermi energy, the transmission through a Fe/MoS₂(3)/Fe is about four times larger than that of Fe/MoS₂(5)/Fe. The transmission through Fe/MoS₂(n)/Fe is high for $n=3$ and 5 . Therefore, the spacer is metallic for these ribbon widths. The transmission values at Fermi energy for Fe/MoS₂(7)/Fe, Fe/MoS₂(9)/Fe and Fe/MoS₂(11)/Fe are very small. For these wide spacer configurations ($n=7, 9$ and 11) a band gap emerges in MoS₂ spacer, recovering the semiconducting behavior of the MoS₂ sheet. This suggests that there is a tunneling regime of conductance in the wider junctions. The majority and minority spin conductance are equal in the AP state for each system due to symmetry. In the P state the minority-spin electrons dominate the conductance if the spacer width is larger than three atomic layers ($n>3$) as illustrated in Figure 3.

The transmission, T , across the MoS₂ ribbon was analyzed as function of the reciprocal k_y vector component. Figure 4 shows $T(k_y)$ from the Γ point to the band edge, point X, in parallel, P, and antiparallel, AP, alignment of the electrode's magnetizations. (There is little dispersion in the k_x direction due to the lack of translation in this direction.) Compared with the wider insulating ribbons ($n=7$ and larger), there is a marked difference in transmission through the narrow conducting ribbon ($n=3$). In the latter case ($n=3$), the transmission is dominated by the reciprocal vectors of larger k_y in majority spin channels, while it is largest near Γ -point in minority spin channels. In the former case ($n=7$), the transmission is dominated by the reciprocal vectors of small k_y near Γ -point for both majority and minority spin channels. The maximum conductance in the AP alignment is near the Γ -point both for the wider ($n=7$) and narrower ($n=3$) MoS₂ spacers. However, the transmission is more localized at lower k_y values in wider ribbons.

Figure 2. The total transmission as a function of energy for $\text{Fe}/\text{MoS}_2(n)/\text{Fe}$ geometries at $V=0$. The red and black curves show transmissions in the parallel (P) and anti-parallel (AP) alignments of the electrode magnetizations, respectively. The Fermi energy is set at zero. The inset figures are shown in logarithmic scale.

Figure 3. Spin-resolved transmission as a function of energy for $\text{Fe}/\text{MoS}_2(n)/\text{Fe}$ geometries at $V=0$ in the parallel alignment of electrode magnetizations. The Fermi energy is set to zero. In the figure, majority (up) and minority (down) spins transmissions are denoted in black and red, respectively. The inset figures are shown in logarithmic scale.

Figure 4. k -resolved transmission through the MoS_2 spacer in the $\text{Fe}/\text{MoS}_2(n)/\text{Fe}$ tunnel junctions. Only the region from the Γ point to the band edge is shown along the k_y direction: (a) $n=3$, (b) $n=7$.

Figure 5. MR of the MoS_2 as a function of the spacer width, n , in $(\text{Fe}/\text{MoS}_2(n)/\text{Fe})$.

Figure 5 illustrates the dependence of the MR as a function of the width of the MoS_2 nanoribbon. The MR is negative in the case of narrowest spacer ($\text{Fe}/\text{MoS}_2(3)/\text{Fe}$) implying larger conductance for an AP state. Such negative MR is realized when the spacer possesses a localized

state near the E_F . Then, if the resonant tunneling occurs in the AP configuration, mediated by this state, the transmission is larger in AP than in P state²⁸.

Another important feature is that the MR increases in magnitude as the width of the MoS₂ spacer increases. Although the absolute value of transmission decreases with the increasing width of MoS₂ monolayers, a wider MoS₂ monolayer slab shows a greater asymmetry in transmission. For example, a greater transmission value for the minority spin channel in the P state is observed with respect to the transmission value in the majority spin channel at E_F . There is no asymmetry in transmission in the spin channels in the AP state. The transmission value in the AP state is smaller than that in the minority channel in the P state.

Figure 6. Local magnetic moments (in μ_B/atom) of the Fe and Mo surfaces as a function of the layer position, m ($m=0$ indicates the Fe layer at the interface).

Figure 7. Calculated site-projected DOSs of the Fe/MoS₂(11)/Fe tunnel junction as function of the site position. (a) $m=-5$, (c) and (d) $m=0$, (e) $m=5$, (f) $m=1$. (b) DOS of free Fe (100) surface (for reference). m is the layer notation as shown in Figure 1.

The local electronic properties of atoms located at the interface of the Fe and MoS₂ spacer differ considerably from that of their bulk counterparts. More specifically, the magnetization from Fe electrodes propagates into the MoS₂ spacer. Figure 6 gives the calculated local magnetic moments (LMM) in each layer of the Fe/MoS₂(n)/Fe. The LMMs of the Fe atoms in the 7 atomic layers closest to the interface and the 3 or 6 Mo atoms in the MoS₂ spacer are shown for $n=5$ and 11, respectively. The local magnetic moment at the central layer of the Fe slab is $2.25 \mu_B$, a value that agrees well with the experimental values of $2.17 \mu_B$ ²⁹, $2.22 \mu_B$ ³⁰, the theoretical value of $2.17 \mu_B$ ³¹ for the bulk Fe. The agreement with the bulk magnetic moments indicates that the magnetic properties converge with respect to the width of the slab regardless of the lattice elastic stress due to the Fe/MoS₂ interface. Fe atoms located closest to the interface have a larger LMM ($\sim 3 \mu_B$) compared to the value of the bulk Fe atom.

Importantly, the large local magnetic moments appear on interfacial Mo atoms (magnitude $0.8 \mu_B$). This is due to the strong hybridization between the Fe and Mo states as can be seen from the projected densities of states (DOS) as shown in Figure 7. Particularly, DOSs of the Fe(100) surface are significantly modified due to bonding with the MoS₂ ribbon (Figures 7b-d). Furthermore, the Mo in the second atomic layer ($m=2$ in Figure 1) shows substantial LMM of $\sim 0.5 \mu_B$ due to the indirect hybridization of the Fe and Mo states through interfacial S and Mo atom

states. There is a small induced moment on Mo in the third atomic layer of the MoS₂ structure. The atoms located farthest from the interface are not spin polarized.

The induced magnetization on the Mo atoms near interface is due to the strong overlap of its states with the states of the Fe electrodes. Figures 7 shows that DOS of iron and molybdenum disulfide are strongly modified due to hybridization between the Fe and Mo states at the interface. Remarkably, the DOSs of Mo exhibits significant broadening of the peak of DOSs at ~1.5eV above and 1eV below the Fermi energy resulting in the closing of the bandgap (Figure 7f). The DOS of iron bonded to Mo is also modified at the interface compared to the DOS of bulk or pristine Fe(100) surface as can be clearly seen from Figures 7a-d. Particularly, the minority states near Fermi energy are noticeably modified both for S- and Mo-bonded Fe atoms. Furthermore, while the interfacial Mo does not show a band gap at E_F making this layer metallic, the central (“bulk”) portion of the MoS₂ slab exhibits a well-pronounced bandgap (of width ~1.8eV) as can be seen in Figure 7e.

As a consequence of the discussed earlier overlap of states at the interface, the MoS₂ spacer of 3 atomic layers does not exhibit bandgap and can be considered as metallic. This is reflected in noticeable ~ $2G_0$ conductance (see Figure 2a). As the width of the spacer increases, the MoS₂ bandgap is restored as reflected in the DOS of the inner Mo/S atoms. The spacer exhibits insulating properties and the transmission becomes very small at E_F . The tunneling MR is much larger than the MR of “metallic” spacer case resulting in abrupt increase in MR when thickness of the MoS₂ spacer increases from 5 to 7 or more layers.

It is very important that the DOS of interfacial Mo at the E_F becomes spin polarized, suggesting possible spin injection into MoS₂ with an efficiency $\eta = \frac{N(E_F)^\uparrow - N(E_F)^\downarrow}{N(E_F)^\uparrow + N(E_F)^\downarrow} = 18\%$ at the interface. The spin-polarized current can be injected in a lateral spin-valve geometry. However, the wider MoS₂ spacer does not show spin asymmetry in $N(E_F)$ for the atomic layers located farther away from the interface ($m > 3$). Thus, the spin injection will be most efficient in the thin MoS₂ spacers.

MR can be tuned by varying the gate or source-drain bias. The plot of MR with respect to the bias voltage (V_b) for the Fe/MoS₂(11)/Fe is shown in Figure 8. MR declines with the increase of the bias voltage. From Figure 8, we can see that the MR is about 50% when $V_b = 20$ mV. The MR declines to around 40% at $V_b = 40$ mV, and further to 35% at $V_b = 60$ mV. MR reduction is expected from the analysis of the transmission coefficient (Figures 2 and 3) where the spin asymmetry is maximum near the Fermi energy. The application of the bias voltage reduces this asymmetry somewhat.

Figure 8. MR as a function of the bias voltage for the Fe/MoS₂(11)/Fe tunnel junction.

Conclusion.

The transport properties of the Fe/MoS₂/Fe tunnel junction using non-equilibrium Green's functions calculations were analyzed using density functional approach. Fe electrodes were attached to the edges of the nanoribbon and the current was considered in the plane of the MoS₂ 2D monolayer. A large magnetoresistance was found in the Fe/MoS₂/Fe junctions, the largest value being 150%. The calculations reveal that atomically-thin spacers are metallic and have a large transmission value as a result of strong coupling between atoms at the MoS₂ edge and ones at the surface of the Fe. The results revealed that the spin injection into MoS₂ had an 18% efficiency at the interface as calculated from the spin polarized DOS at the E_F . The MoS₂ spacers that had a larger width remained insulating. Finally, it was concluded that the magnetoresistance increased as the width of the MoS₂ spacer increased.

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[(a) top view and (b) side view] The structure of (Fe/MoS₂(n)/Fe) spin-valve junctions. The MoS₂ armchair terminated monolayer of various widths (shown in green (Mo) and black (S)) is attached to the Fe (100) bulk electrodes (shown in red). The region within the two dashed lines is the scattering region and the remaining parts are the semi-infinite left and right electrodes.

Magnetoresistance of the MoS₂ as a function of the spacer width, n , in (Fe/MoS₂(n)/Fe).