Spin injection and magnetoresistance in MoS$_2$-based tunnel junctions using Fe$_3$Si Heusler alloy electrodes

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Recently magnetic tunnel junctions using two-dimensional MoS$_2$ as nonmagnetic spacer have been fabricated, although their magnetoresistance has been reported to be quite low. This may be attributed to the use of permalloy electrodes, injecting current with a relatively small spin polarization. Here we evaluate the performance of MoS$_2$-based tunnel junctions using Fe$_3$Si Heusler alloy electrodes. Density functional theory and the non-equilibrium Green’s function method are used to investigate the spin injection efficiency (SIE) and the magnetoresistance (MR) ratio as a function of the MoS$_2$ thickness. We find a maximum MR of ~300% with a SIE of about 80% for spacers comprising between 3 and 5 MoS$_2$ monolayers. Most importantly, both the SIE and the MR remain robust at finite bias, namely MR > 100% and SIE > 50% at 0.7 V. Our proposed materials stack thus demonstrates the possibility of developing a new generation of performing magnetic tunnel junctions with layered two-dimensional compounds as spacers.
In the search for an alternative ferromagnetic electrode to combine with MoS$_2$ we propose here Fe$_3$Si. This is a Heusler alloy with a lower Gilbert damping parameter, $\alpha$, and a higher saturation magnetization, $M_S$, than those of both of Py ($\alpha = 0.0149$, $M_S = 53522$ emu/cm$^3$) and Fe$_3$O$_4$ ($\alpha = 0.0370$, $M_S = 47124$ emu/cm$^3$). A small Gilbert damping parameter leads to a potentially low critical current density for spin-transfer torque switching. Moreover, the Curie temperature of Fe$_3$Si is large, above 800 K, and the spin-polarization at low temperature (~45%) compares favorably with that of Fe (~44%), Co (~34%) and Ni (~11%). These combined materials properties make Fe$_3$Si an attractive material for fabricating spin-valves and several experimental attempts have been made. MTJs based on Fe$_3$Si include Fe$_3$Si/AlO$_x$/Co$_{60}$Fe$_{40}$, Fe$_3$Si/CaF$_2$/Fe$_3$Si, Fe$_3$Si/Fe$_2$Si/Fe$_3$Si, Fe$_3$Si/Ge/Fe$_3$Si and Fe$_3$Si/GaAs/Fe$_3$Si junctions. Previous theoretical study predicted the high TMR ratio of ~5000% for an epitaxial Fe$_3$Si/MgO/Fe$_3$Si junction, which however is rather sensitive to the Fe$_3$Si structure and decreases rapidly with bias.

In this work, we focus on the spin transport properties of Fe$_3$Si/MoS$_2$/Fe$_3$Si MTJs. An illustration of the structure of a 3-monolayer MoS$_2$ junction is presented in Fig. 1(a). We first investigate the electronic properties of the interface between Fe$_3$Si and MoS$_2$ by using density functional theory (DFT). Then, by combining DFT with the non-equilibrium Green's function (NEGF) method for transport, we are able to analyze the dependence of the transmission coefficient on the MoS$_2$ thickness at zero bias. The spin-injection efficiency (SIE), $\eta$, and the magnetoresistance (MR) ratio for different MoS$_2$ layer thicknesses are then calculated. We obtain a maximum MR ratio of ~300% with a SIE of ~80% for a junction comprising only three MoS$_2$ monolayers. The details of the electronic transport are explained thoroughly by looking closely at the $k$-resolved transmission coefficients at the Fermi level, $E_F$. Finally, we further investigated the SIE and the MR ratio as a function of the bias voltage.

Results and Discussion

The details of the relaxed structure at the interface are presented in Fig. 1(c). In the D0$_3$ structure (Fm3m) the A, B and C sites of Fe$_3$Si are occupied by Fe ions, while Si is placed at the remaining octahedral-coordinated D site. By comparing the binding energy, $E_B$, we can conclude that it is more energetically favorable to terminate the Fe$_3$Si surface with A and C sites. In this case $E_B = -1.13$ eV per surface atom, indicating covalent bonding with MoS$_2$. The shortest S-Fe bond length is found to be 2.09 Å, while the average separation between the top layer of Fe$_3$Si and the bottom Mo layer is 3.49 Å [this is taken from the Mo plane - see Fig. 1(c)]. The equilibrium distance between the Fe and the S closest planes is 1.90 Å, while the MoS$_2$ inter-layer distance is 6.15 Å.

We start our analysis by looking at the spin-resolved transmission coefficients, $T(\sigma)(E)$ ($\sigma = \uparrow, \downarrow$), for all the systems studied in the parallel (P) and anti-parallel (AP) configuration. For the 1L-MoS$_2$ junction the transmission of the P configuration shows a metallic-like behaviour for both spin channels [see Fig. 2(a)]. This is due to the strong hybridization between the Fe(A,C) and the S atoms at the interface, resulting in the metallization of the MoS$_2$ monolayer. Metallization of thin MoS$_2$ barriers is confirmed by the projected density of states (PDOS) presented in Fig. 3(a), where one can clearly see that the PDOS of the Mo atoms at the surface is different from that of bulk MoS$_2$ and displays a small spin polarization. Such result is consistent with previous studies using Fe electrodes. As presented in Fig. 3(c), one can see that the minority-spin PDOS of the interface Fe(A,C) atoms increases significantly around the Fermi energy, as compared to those in the bulk-like region. This means that...
the impact of the Fe-S chemical bonding at the interface on the minority spin tunneling is much larger than that on the majority. It is, therefore, reasonable to assume that the strong hybridization between Fe and S will result in a change of the transport mechanism from tunneling to metallic as the MoS₂ thickness is reduced. As a result of

Figure 2. Spin-resolved transmission coefficients $T(E)$ as a function of energy for (a,b) 1L-MoS₂ junction in both the parallel and anti-parallel configurations and (c,d) 3L-, 5L-, 7L- and 9L-MoS₂ junctions in both the parallel and anti-parallel configurations.

Figure 3. Projected density of states (PDOS) on (a) the Mo atoms at the interface of the 1L-MoS₂ junction as compared to bulk MoS₂; (b) the Mo atoms located in the middle layer and at the interface for 3L-MoS₂ junction; (c,d) the Fe(A,C) and Fe(B) atoms at the interface as compared to those in a bulk-like region.
the metallization the spin-down transmission at the Fermi level of the 1L-MoS 2 junction, \( T_{\downarrow} \) \( (E_F) \), is significantly larger than that of the up spins [see Fig. 2(a)], reflecting the spin polarization in the DOS of Fe 3Si [see Fig. 3(c)]. Finally in the AP configuration shown in Fig. 2(b), the transmission is identical for both spins owing to the symmetrical geometry of the junction.

Increasing the MoS 2 thickness reduces the transmission of both the P and AP configurations for all the spin channels, as shown in Fig. 2(c,d). As the spacer thickness is increased to 3 monolayers [see Fig. 3(b)], the PDOS of the Mo atoms located in the middle of the junction becomes almost identical to that of bulk MoS 2, indicating that the metallization extends only to the layers adjacent to the electrodes. Remarkably, \( T_{\downarrow} \) \( (E_F) \) decreases faster than \( T_{\uparrow} \) \( (E_F) \), as it will be discussed in more detail later. When compared to the 1L-MoS 2 junction, \( T_{\downarrow} \) \( (E_F) \) for the 3L-, 5L-, 7L- and 9L-MoS 2 junction is reduced by about two, four, six and seven orders of magnitude, respectively. This demonstrates the tunneling transport regime. Notably the drop in transmission is much more evident in the energy region [−0.3 eV] than in the DFT local spin-density approximation bandgap of bulk MoS 2 (−1.8 eV), indicating that the electrodes screening plays a dramatic role in determining the bandgap of the spacer in the junction. A similar behaviour has been already observed for transition metals electrodes 16,18. The zero-bias transport properties of Fe 3Si/MoS 2/Fe 3Si junctions with different tunnel barrier thicknesses are summarized in Table 1.

To understand the different MR ratios presented before, in Fig. 4(a) we show the zero-bias MR value. This needs to be compared with what found in MoS 2-based MTJs with Fe electrodes, for instance Fe 3O 4 junctions 20,21 and Co 19, Ni 20 and Py 15 electrodes and slightly larger than that for Fe 18. However, it should be noted that for 7L- and 9L-MoS 2 junctions, our results demonstrate that the MR values with Fe 3Si electrodes become less than that of previous studies 18, using Fe electrodes.

### Table 1. Calculated transport properties of Fe 3Si/MoS 2/Fe 3Si junctions with different spacer thicknesses. \( T_{\uparrow} \) and \( T_{\downarrow} \) are spin-up (down) transmission coefficients at the Fermi energy for parallel (antiparallel) configuration. \( G_{P/\text{AP}} \) is the quantum conductance (in the unit of \( e^2/h \)) for the P (AP) configuration. \( \eta_{P/\text{AP}} \) is the spin injection efficiency (SIE) for the P (AP) configuration. MR is the magnetoresistance ratio of the junctions.

| Spacings | 1L-MoS 2 | 3L-MoS 2 | 5L-MoS 2 | 7L-MoS 2 | 9L-MoS 2 |
|-----------|----------|----------|----------|----------|----------|
| \( T_{\uparrow} \) | 0.353    | 4.03 \times 10^{-7} | 1.53 \times 10^{-5} | 3.03 \times 10^{-5} | 7.62 \times 10^{-5} |
| \( T_{\downarrow} \) | 1.060    | 3.14 \times 10^{-7} | 1.77 \times 10^{-7} | 3.22 \times 10^{-7} | 1.28 \times 10^{-7} |
| \( \eta_{P} \) | 0.337    | 8.50 \times 10^{-6} | 2.14 \times 10^{-4} | 6.25 \times 10^{-6} | 1.91 \times 10^{-7} |
| \( \eta_{\text{AP}} \) | 0.340    | 9.10 \times 10^{-7} | 2.36 \times 10^{-4} | 6.92 \times 10^{-6} | 2.11 \times 10^{-7} |
| \( G_{P} \) | 1.420    | 7.16 \times 10^{-2} | 1.70 \times 10^{-2} | 3.35 \times 10^{-2} | 8.90 \times 10^{-2} |
| \( G_{\text{AP}} \) | 0.676    | 1.76 \times 10^{-2} | 4.50 \times 10^{-4} | 1.32 \times 10^{-4} | 4.02 \times 10^{-5} |
| MR (%) | 109.44  | 306.95 | 278.87 | 154.56 | 121.63 |
| \( \eta_{P} \) | −50.17 | 12.41 | 79.17 | 80.81 | 71.23 |
| \( \eta_{\text{AP}} \) | −0.39 | −3.47 | −4.88 | −5.12 | −4.95 |

The bias dependence of the SIE and the MR ratios both characterize the MTJs quality in practical applications. These are defined as their corresponding linear response quantities, with \( \eta(E) \) and \( G \) being replaced by the spin-polarized and the total current, respectively. Our results for voltages up to 0.7 V are presented in Fig. 4(b,d) for the 1L-, 3L- and 5L-MoS 2 junctions. Except for the 1L-MoS 2 case, the SIEs in the P configuration increase with increasing the applied bias, whereas the opposite is observed in the AP one. Note that at finite bias the junction symmetry is broken and the SIE for the AP case may differ from zero, but the actual sign depends on the bias polarity. Interestingly in the P configuration the SIE increases to a maximum at high voltage for the 3L-MoS 2 junction, whereas it remains roughly constant and then decreases for the 5L-MoS 2 one. Finally the SIE of the 1L-MoS 2 junction follows the behaviour of the 3L-MoS 2 one, but starts from a negative value at \( V = 0 \). A more detailed discussion of the spin-polarized \( I-V \) curves can be found in the Supplementary Information.

The most interesting feature of Fig. 4(d) is that the MR ratios gradually decrease under the application of a bias voltage. Already at 0.1 V the MR is reduced by approximately 25%, 10% and 18% for the 1L-MoS 2, 3L-MoS 2 and 5L-MoS 2 junctions, respectively. Note that such percentage changes are calculated as the decrease from the zero-bias MR value. This needs to be compared with what found in MoS 2-based MTJs with Fe electrodes, for which the MR drop is of the order of ~80% 18,19. In order to understand the different MR ratios presented before, in Fig. 5(a) we show the \( k_F \)-resolved transmission coefficients at \( E_F \) for the 1L-MoS 2 and 5L-MoS 2 junctions. In general in the P configuration the transmission profile in the 2D Brillouin zone orthogonal to the transport direction follows somehow closely the
distribution of open channels in the electrodes [see Fig. 5(c)]. This is much more evident for the 1L-MoS₂ junction, confirming that in case of MoS₂ metallization the MR is entirely dominated by the electronic structure of the electrodes. As expected for the AP configuration the transmission profile is a sort of convolution of that of the two spin channels in the P one.

Moving our attention to the 5L-MoS₂ junction the situation becomes somehow more complex. The most striking feature is the appearance of regions of low transmission in the Brillouin zone, which are present for both spin channels regardless of the electrodes configuration. In particular such regions are concentrated around the $k_z = 0$, and $k_y = \pm \pi/2$ axes. This behaviour can be explained by looking at Fig. 5(d), where we show the smallest MoS₂ complex wave-vector, $\kappa$, in the direction of the transport for any given transverse $k$. Note that $\kappa$ is essentially the wave-function decay coefficient across the barrier, so that the highest transmission is expected for the smallest $\kappa$. From the figure one can clearly see that the regions of small transmission identified in Fig. 5(b) correspond to those where $\kappa$ is large, and that the transmission is maximized at the edge of the Brillouin zone in the $k_x$ direction.

Importantly, from the transmission plots it emerges that in the regions of high transmission both spin channels are present, so that a clear spin filtering is not in action in this material system. Thus, increasing the barrier thickness has the sole effect of changing the distribution of the $k$ wave-vectors contributing to the conductance. This in general changes the MR. However, since both spin channels are transmitted across the $k$ regions filtered by the barrier, the MR does not increase significantly with the layer thickness.

Certainly our theoretical predictions now need to be passed to the experimental scrutiny. On the one hand we are confident that, should epitaxial junctions be made, the MR and SIE will be large. On the other hand, it might be the case that the fabrication process produces interdiffusion at the Fe₃Si/MoS₂ interface, which will

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**Figure 4.** Spin injection efficiency (SIE) and magnetoresistance (MR) as a function of (a,c) the thickness and (b,d) the applied bias. Only the bias dependence of the MR for the 1L-, 3L-, 5L- MoS₂ junctions is shown.

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**Table 2.** Literature review of magnetic tunnel junctions using MoS₂ as spacer. The magnetoresistance (MR ratio) is reported for DFT predictions and experimental studies (Exp.) at low temperatures.

| Electrodes | Calculated MR (%) | Exp. | Max. MR (%) |
|------------|------------------|------|-------------|
| Fe¹⁰       | 70               | 225  | 250         |
| Co²¹       | 52.8             | 55   | 56          |
| Ni²²       | 5.3              | 13.8 | 1.1         |
| NiFe (Py)²³ | 9                |      | 0.73        |
| Fe₃O₄      |                  |      | 0.20        |
| Fe₃Si (This work) | 109.44 | 306.95 | 278.87 |

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affect the magnetization as well as the MR ratio of the MTJs. Intriguingly, previous experiments exploring the room-temperature structure ordering of Fe$_3$Si films on Ge(111) have revealed an improvement of the degree of the D0$_3$ ordering with increasing the film thickness. This leads us to believe that structural robust junctions with good epitaxy may be fabricated.

Conclusion

In conclusion we have demonstrated that magnetic tunnel junctions based on Fe$_3$Si Heusler alloy electrodes and MoS$_2$ spacers may present advantages over the most conventional choices based on transition metals permalloy. In particular we have shown that the junctions, comprising only three MoS$_2$ monolayers, display a spin injection efficiency of the order of 80% and a MR ratio of 300%. These are both robust as the bias potential is increased, so that our proposed junctions can sustain a large current with significant spin polarization. Thus magnetic tunnel junctions constructed with 2D barriers appear promising for realizing current-operated spin devices.

Methods

MoS$_2$ is sandwiched in between the Fe$_3$Si electrodes, so that its cleavage plane binds to the (100) surface of Fe$_3$Si. Commensurability is obtained by aligning the Fe$_3$Si cubic cell with the planar $2 \times \sqrt{3}$ cell of MoS$_2$ and requires a uniform stretch of the Fe$_3$Si in plane lattice constants by about 5% (Fe$_3$Si becomes slightly orthorhombic). We have tested that such small strain on Fe$_3$Si does not affect its electronic structures significantly (see the Supplementary Information). The final cell describing the scattering region comprises a variable number of MoS$_2$ monolayers and two cells of Fe$_3$Si at each side. Note that 3 atomic layers of Fe$_3$Si (1.5 cells) are enough to screen out the perturbation of MoS$_2$ at the interface. As a matter of notation we denote as $nL$-MoS$_2$ junction in which the MoS$_2$ spacer is $n$ monolayers thick. Each cell is then fully relaxed by using the DFT code SIESTA, with basis set, exchange-correlation functional, real-space mesh cutoff and $k$-point grid identical to those used for the transport calculations. Note that Siesta is the DFT engine of Smeagol. The relaxation is performed by conjugate gradient until the residual forces on each atom are below 0.01 eV/Å, while the in-plane lattice parameters are kept to those of MoS$_2$.

The quantum transport calculations have been performed by employing a combination of the non-equilibrium Green’s function technique (NEGF) based on density functional theory (DFT) as implemented in the SMEAGOL package. For all calculations we have used the local spin density approximation (LSDA) to the exchange-correlation functional. The valence electrons are described by using a local double-$\zeta$ plus polarization basis set. The atomic core electrons are modelled with norm-conserving relativistic Troullier-Martín...
pseudopotentials. We have determined that convergence is achieved by using a real-space integration with a mesh cutoff of 300 Ry and a k-space grid of $8 \times 10 \times 1$ points. The transmission spectra and the current are then computed over a $80 \times 10 \times 1$ grid (see the Supplementary Information).

The fundamental quantities that characterize spintronics devices are the MR ratio and the SIE. The low-bias MR ratio is defined as $MR = \frac{G_{DP} - G_{AP}}{G_{AP}} \times 100\%$, where $G_{DP}$ and $G_{AP}$ are the total conductance respectively for the parallel (P) and antiparallel (AP) configuration of the electrodes. The SIE is instead defined as $\eta = \frac{T^+ - T^-}{T^+ + T^-} \times 100\%$ where $T^+$ and $T^-$ denote the transmission coefficients for the spin-up and spin-down channel, respectively.

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**Author Contributions**

J.P. designed the study. W.R. performed calculations. W.R. and J.P. analyzed the data and wrote the manuscript. W.P., T.A. and S.S. reviewed and commented on the manuscript.

**Additional Information**

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