Search for alternative magnetic tunnel junctions based on all-Heusler stacks

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I. INTRODUCTION

Spin valves displaying large tunnel magneto-resistance (TMR) have undoubtedly revolutionized the electronics industry and now form the central component of many technologies, the most successful device being the read heads in hard-disk drives [1]. Importantly, spin valves are set to become the central component of many devices of the future, such as magnetic random access memories and spin-torque oscillators. The major breakthrough was the fabrication of CoFeB/MgO/CoFeB spin valves requiring the growth of rather large effort in both industry and academia [6], no junction alternative to CoFeB/MgO/CoFeB has been adopted by the community. This is a significant deficiency, since little room is left for tuning the materials properties necessary for the development of new applications of the technology. It is therefore imperative to explore alternative materials combinations which offer more freedom to engineer the device properties.

Heusler alloys are a large class of binary (X3Z), ternary (X2YZ), and quaternary (XXX′YZ) compounds with more than 1500 known members and an impressively wide range of properties [7]. Many elements can be incorporated into the Heusler structure, making it rich and tunable, and as such ideal for developing new technologies.

One key example for the switching of tunnel junctions is the Gilbert damping, which is strong in the FeCoB system [8], restricting the maximum operational frequency. Many Heuslers including Fe3Si [9], Co2FeSi [10], and Co2FeAl [11] all show a significantly lower Gilbert damping in comparison to FeCoB. Unfortunately, to the best of our knowledge, the Gilbert damping of Fe3Al, our most promising alternative material, has not been measured.

Several attempts have been made to substitute the magnetic electrodes of the FeCoB/MgO/FeCoB stack with Heusler magnets, and successes have been obtained by replacing one or both the electrodes with Co2MnSi, which displays a TMR ratio of 1.995% at 4 K [15]. In this system, however, the magnetoresistance is sensitive to temperature with the TMR reducing to 354% at room temperature [15]. Such temperature sensitivity suggests interfacial magnetic defects or secondary phases, which disrupt the coherent tunneling. Co and Mn can directly substitute into the rock-salt MgO structure with formation energies of −3.0 eV and −4.0 eV, respectively [16], making substitutional Mn in the MgO lattice a likely culprit.

A second approach has been to construct all Heuslers giant magneto-resistance (GMR) stacks, where the spacer between the magnetic electrodes is a metal. The relevant literature is summarized in Table II. Although a MR has been demonstrated, its small for all the known experiments, so that further work is needed to explain these negative results in view of the large MR predicted by ab initio calculations [33].

The question that we answer in this paper is the following: Given the wide variety of properties available in the Heusler class, is it possible to create an all-Heusler TMR junction with...
materials alternative to the Fe/MgO system? In this work we will use simple design concepts and screen candidates based on the symmetry filtering mechanism, which has been so successful for the Fe/MgO junction. Our screening the materials alternative to the Fe/MgO system? In this work we will use simple design concepts and screen candidates based on the symmetry filtering mechanism, which has been so successful for the Fe/MgO junction. Our analysis returns the Fe2Al/BiF3 system as a promising stack for large magnetoresistance with a strong TMR retention at high bias. The paper is organized as follows. We open our II. SCREENING THE MATERIALS

A. The tunnel barrier

In order to propose a new junction we must satisfy a number of constraints, which we will use to screen candidate materials combinations. First, the barrier material must be a robust insulator and therefore must have a large band gap, $E_g$. If we use a cutoff band gap of 2.5 eV, we will reduce the number of the candidate Heusler materials from over 300 000 (these include those reported in literature and the hypothetical ones contained in the AFLOW.org database) [16] to just 26. Notably, only four of these have been grown experimentally before; the remaining 22 are only predicted from ab initio calculations [16]. The 26 barrier candidates are shown in Table III. Note that the band gaps reported here are computed by density functional theory (DFT) in the generalized gradient approximation (GGA), therefore they are expected to be significantly smaller than the true quasiparticle band gap. As such our $E_g \geq 2.5$ eV criterion effectively selects insulators with a band gap, which is likely to be significantly larger than 2.5 eV.

Next we consider the transport properties of the tunnel barrier. In epitaxial spin valves the magnitude of the TMR is determined by the symmetry matching between the evanescent wave functions in the insulating barrier and the Bloch wave functions for majority and minority spins in the magnetic electrodes. In particular the TMR will be large if such wave-function symmetry match occurs for only one of the two spin species, i.e., if only one of the two spin species is transmitted with large probability [4,5].

In order to further screen these candidate barrier materials we have performed electronic structure calculations using self-interaction-corrected [36,37] DFT as implemented in the atomic-orbital-based code SIESTA[38]. In general the inclusion
of self-interaction corrections drastically improve the band gap of a broad range of insulators, and here it brings the calculated gap of the chosen Heusler barriers within 10\% from the experimental one. Core electrons are treated with norm-conserving relativistic Troullier-Martin pseudopotentials [39], while multi-$\zeta$ numerical atomic orbitals are used to represent the electron density and all the operators. Total energies are computed on a uniform real-space grid with an equivalent cutoff of 600 Ry, while the primitive unit cells are sampled for each direction, as calculated in this work. We report the symmetry of the slowest decaying state along the [001] direction, as calculated in this work.

For each of the insulators we determine the symmetry of the slowest decaying state along the [001] direction, and we restrict ourselves to the experimentally verified insulating Heusler alloys, namely, BiF$_3$, LiMgN, LiMgP, and TaIrGe. Our results are presented in Table IV, where we list the experimental structural parameters and quasiparticle band gap, together with the symmetry of the evanescent wave function with the slowest decay across the barrier. Notably, while for BiF$_3$ there is only one low-lining complex band crossing the barrier, this is not the case for the other three alloys. In fact, for LiMgN, LiMgP, and TaIrGe the symmetry of the valence band maximum (VBM) and conduction band minimum (CBM) is different. This means that there is not a single complex band bridging the band gap, since the one starting at the VBM (CBM) does not end at the CBM (VBM). As such, the symmetry of the slowest decaying state across the barrier depends upon the exact position of the Fermi level in the hypothetical junction, namely, on the band alignment. This situation is not desirable in a tunneling junction [49]. When all these features are brought together, BiF$_3$ appears as our best candidate. Its band structure is illustrated in Fig. 1(d).

BiF$_3$ is the naturally occurring mineral gananite, which has been reported to have a D0$_3$ structure and a lattice parameter of 5.861 Å [43]. The $F$ atoms occupy the 4$a$, 4$b$, and 4$c$ Wyckoff positions, while $Bi$ is accommodated in the 4$d$. Gananite is a wide band-gap insulator with an experimentally observed optical gap of $\sim$5.10 eV [44]. Theoretical band gaps of 3.81 and 3.94 eV were calculated with the LDA (at the LDA lattice constant of $a_0^{\text{LDA}} = 5.865$ Å) [50] and the GGA (at the GGA lattice constant of $a_0^{\text{GGA}} = 5.860$ Å) [51,52], respectively. In this work the atomic self-interaction correction (ASIC) scheme built on top of the LDA returns a value of 5.25 eV ($a_0^{\text{ASIC}} = 5.836$ Å).

### Table IV. Insulating Heusler materials with a band gap $E_g \geq 2.5$ eV.

| Material | SB      | $a_{\text{exp}}$ (Å) | $E_g$ (eV) | Symmetry               |
|----------|---------|-----------------------|------------|------------------------|
| BiF$_3$  | D0$_3$  | 5.861 [43]            | 5.10 [44]  | $\Delta_{\text{CB-VB}}$ |
| LiMgN    | C1$_f$  | 4.955 [45]            | 3.20 [45]  | $\Delta_{\text{CB}}, \Delta_{\text{VB}}$ |
| LiMgP    | C1$_f$  | 6.005 [46]            | 2.43 [46]  | $\Delta_{\text{CB}}, \Delta_{\text{VB}}$ |
| TaIrGe   | C1$_{4f}$ | 5.967 [48]          | 3.36 [48]  | $\Delta_{\text{1}}^{\text{CB}}, \Delta_{\text{2}}^{\text{VB}}$ |

FIG. 1. Electronic structure of Fe$_3$Al and BiF$_3$ along the device stack direction, [001]. Panels (a), (b), and (c) are the majority band structure, the density of states, and the minority band structure for D0$_3$-Fe$_3$Al, respectively. The bold lines represent the $\Delta_{\text{1}}$ bands. Panel (d) displays the complex band structure of the bulk BiF$_3$.

#### B. The magnetic electrodes

We now move to select the magnetic materials to be used as electrodes. A crude screening criterion is that the magnetic electrodes must be made of materials having a magnetic ordering temperature significantly higher than room temperature. Here we have chosen the cutoff to be 700 K, a value that should be sufficient to ensure little magnetization degradation for temperatures around room temperature. Such a cutoff temperature reduces the number of candidates to the 20 alloys listed in Table V.

Second, there should be a good lattice match between the magnetic electrodes and the insulator. This is a necessary condition to ensure the epitaxial grow of the stack, which in turn is necessary for the spin filtering. We set the tolerance for the lattice match to less than 1.5\%. Such match can be achieved either by having a one-to-one match between the insulator and the magnet (the two share the same crystallographic axes) or by rotating one of them by 45° in the plane of the stack [here we consider only the (100) growth direction]. Table VI presents all the possible electrode (barrier) combinations having a lattice mismatch smaller than 1.5\%, with the 45°-rotated epitaxial structures being in gray.

From the table it is easy to note that there are only eight magnets presenting a lattice mismatch smaller than 1.5\% with our chosen insulator, BiF$_3$. Two of these, Mn$_2$CoGa and Mn$_2$VAl, are Mn$_2$-based Heusler alloys, which we exclude from further analysis. The reason for such exclusion is that...
TABLE V. Magnetic Heusler materials with a $T_C$ greater than 700 K considered as potential electrode. We report the Strukturbericht (SB) symbols, the experimental lattice constant ($a_{\text{exp}}$ [Å]), the Curie temperature ($T_C$ [K]), and the magnetic order, FM = ferromagnetic, HMF = half-metal. Here “ferri” means that the magnetic order is ferrimagnetic, although the electronic structure is that of a half-metal.

| Material       | SB     | $a_{\text{exp}}$ | $T_C$ | Magnetic ground state | Ref. |
|----------------|--------|------------------|-------|-----------------------|------|
| Co$_2$FeSi     | D0$_3$ | 5.793            | 713   | FM                    | [53] |
| Fe$_2$Si       | D0$_3$ | 5.553            | 840   | FM                    | [53] |
| Co$_2$CoGe     | D0$_3$ | 5.780            | 925   | FM                    | [54] |
| Fe$_2$CoSi     | D0$_3$ | 5.645            | 1105  | FM                    | [55] |
| Fe$_2$CuAl     | A$_2$  | 5.830            | 975   | FM                    | [56] |
| Fe$_2$NiAl     | L$_2$  | 5.778            | 965   | FM                    | [56] |
| Fe$_2$NiSi     | D0$_3$ | 5.671            | 755   | FM                    | [56] |
| Co$_2$MnAl     | B2     | 5.671            | 710   | HMF                   | [57] |
| Co$_2$MnSi     | L$_2$  | 5.655            | 985   | HMF                   | [58] |
| Co$_2$MnGe     | L$_2$  | 5.749            | 905   | HMF                   | [59] |
| Co$_2$MnSn     | L$_2$  | 6.000            | 829   | HMF                   | [60,61] |
| Co$_2$FeSi     | L$_2$  | 5.640            | 1100  | HMF                   | [62–64] |
| Co$_2$CoAl     | B2     | 5.737            | 1000  | HMF                   | [64–66] |
| Co$_2$FeGa     | L$_2$  | 5.751            | 1100  | HMF                   | [60,64] |
| Co$_2$FeGe     | L$_2$  | 5.743            | 981   | HMF                   | [64,67] |
| Co$_2$CrSi     | L$_2$  | 5.647            | 747   | HMF                   | [68] |
| NiMnSb         | Cl$_6$ | 5.903            | 730   | HMF                   | [69] |
| Mn$_2$VAl      | L$_2$  | 5.920            | 760   | HMF (ferri)           | [70] |
| Mn$_2$CoGa     | L$_2$  | 5.873            | 740   | HMF (ferri)           | [71] |

often the ground state of Mn$_2$-type alloys presents a complex magnetic structure with ferrimagnetic order between the crystallographic inequivalent Mn ions (e.g., see Mn$_3$Ga)[72]. This is a situation which is not suitable for a spin valve. We also exclude the half-Heusler, NiMnSb, which has a half-metallic electronic structure, but it is prone to disorder that strongly modifies its magnetic properties [73]. The electronic structure of the remaining five electrode compounds has been calculated, the symmetry of the states at the Fermi-level has been analyzed, and it is summarized in Table VII. Given the symmetry of the relevant complex band in BiF$_3$, the electrodes must present bands with $\Delta_1$ symmetry at the Fermi level for only one spin channel along the [001] direction. All five remaining candidates meet this criterion.

When looking at the electronic structure of the five remaining Fe-containing magnetic Heusler alloys, we notice that all of them present bands at the Fermi level with both $\Delta_1$ and $\Delta_5$ symmetry in the majority (↑) channel, while the symmetry of the minority one (↓) differentiates them. In two cases, Fe$_2$CoGe and Fe$_2$CuAl, the minority Fermi surface is dominated by the $\Delta_5$ symmetry, while for other two, Fe$_2$NiAl and Fe$_2$NiGe, the minority Fermi surface is dominated by the $\Delta_1$ symmetry.

TABLE VI. Materials combinations presenting a lattice mismatch smaller than 1.5%. This can be obtained with the barrier and the magnet sharing the same crystallographic axes, or by rotating one of them by 45° (in gray).

| Material       | SB     | $a_{\text{exp}}$ | $T_C$ | Magnetic ground state | Ref. |
|----------------|--------|------------------|-------|-----------------------|------|
| BiF$_3$        | 1.3    | 1.1              | 1.0   | 0.9                   | 1.2  |
| TaIrGe         | 0.4    | 1.3              |       |                       |      |
| LiMgP          | 0.4    | 1.2              |       |                       |      |
| Cl$_2$KTI      | 0.5    | 1.2              |       |                       |      |
| Br$_2$KLi      | 0.6    | 1.1              |       |                       |      |
| ClHgK          | 0.9    | 1.4              |       |                       |      |
| Br$_2$KNa      | 0.9    | 1.1              |       |                       |      |
| BrHgK          | 0.9    | 1.1              |       |                       |      |
| Br$_2$KTI      | 0.9    | 1.4              |       |                       |      |

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TABLE VIII. Calculated formation energy [16,42].

| Atoms      | Lowest Heusler formation energy (eV/atom) | Lowest formation energy (eV/atom) |
|------------|------------------------------------------|----------------------------------|
| Bi, F      | BiF$_3$ −2.22                            | −                                |
| Al, F      | AlF$_3$ −2.11                            | −                                |
| Fe, F      | FeF$_3$ −1.33                            | FeF$_2$ −4.25                    |
| F, Al, Fe  | F$_2$AlFe −0.78                          | −                                |
| Fe, Al, F  | FeAlF$_2$ −0.62                          | −                                |
| Fe, Al     | Fe$_3$Al −0.22                           | −                                |

both $\Delta_2$ and $\Delta_2$ bands are present (in the case of Fe$_2$NiGe there is also a $\Delta_3$ one). Fe$_3$Al sets a case on its own, since there is a spin gap in the minority band. Note that this is not a complete spin gap, namely, Fe$_3$Al is not a half-metal, but it is present along the (100) direction. For this reason, among the different possibilities, we have then chosen Fe$_3$Al as electrode material. Fe$_3$Al has high $T_C$ (713 K) [53] and only a 1.2% lattice mismatch to BiF$_3$. It has a D$_0_1$ structure ($Fm\bar{3}m$), Fe(I) atoms occupy the Wyckoff positions 4$a$ (0,0,0) and 4$b$ (1/2, 1/2, 1/2), while Fe(II) and Al atoms occupy the 4$c$ (1/4, 1/4, 1/4) and 4$d$ (3/4, 3/4, 3/4) ones, respectively.

In Figs. 1(a) and 1(c) we present the band structure for majority and minority spins along [001] (the proposed stack orientation). As we have seen, BiF$_3$ filters states with $\Delta_1$ symmetry, which are present in Fe$_3$Al only for the majority band. In fact, along the [001] direction ($\Gamma \rightarrow X$ in k-space) at $E_F$ there is a wide $\Delta_1$ band originating from the Al 3$s$ and Fe 4$s$ states in the majority spin channel [Fig. 1(a)], and a band gap in the minority one [Fig. 1(c)]. The first $\Delta_1$ contributions for the minority spin appear at $\pm 1.5$ eV from $E_F$, providing a 3 V window in which the device is expected to show a large TMR. Note that, as already mentioned, the material is not half-metal as the gap in the minority channel is only along the specific $\Gamma \rightarrow X$ direction, as shown in Fig. 1(b).

C. Secondary phases

We now turn our attention to discuss the possibility of creating secondary phases or interfacial defects at the Fe$_3$Al/BiF$_3$ interface. Our criterion for phase separation is that the two materials in the stack, namely, Fe$_3$Al and BiF$_3$, should be thermodynamically well separated from any other phase containing the same elements. If we assume that an epitaxial growth can be maintained, we have to verify their thermodynamic stability against other competing Heusler structures. In Table VIII we present the calculated formation energy of likely Heusler phases created with Fe, Al, Bi, and F. Here we have investigated all the possible site occupancies and distortions within the Heusler structure. We observe that the lowest energy of formation is for BiF$_3$. Therefore, if the growth can be maintained in the Heusler structure, we would expect a clean junction to form. Importantly, there is no F-rich structure that also contains Fe with an energy of formation within 1 eV/atom from that of BiF$_3$, so Fe diffusion into the barrier is not likely reducing the probability that paramagnetic defects will be present to scatter the spin. However, if the growth quality is low, growth of non-Heusler phases becomes possible and FeF$_2$ is likely to form.

III. THE ALL-HEUSLER Fe$_3$Al/BiF$_3$/Fe$_3$Al SPIN VALVE

A. Zero-bias properties

The all-Heusler Fe$_3$Al/BiF$_3$/Fe$_3$Al spin valve is constructed by stacking Fe$_3$Al(001) on BiF$_3$(001), as shown in Fig. 2. Its transport properties are now systematically investigated. For our transport calculations the in-plane lattice constant is fixed at $a_0 = 5.836$ Å, equivalent to the theoretical cubic lattice constant of bulk BiF$_3$. Fixing the in-plane lattice constant induces a small tetragonal distortion in the semi-infinite Fe$_3$Al(001) leads with $c/a_0 = 1.124$ (the cell is relaxed to a forces tolerance of 10 meV/Å). Such a distortion has negligible effects on the electronic structure of the electrodes. The interface energy, corrected for basis set superposition error, is found to be 3.78 J/m$^2$. To put this in context, the computed Fe/MgO interface energy is reported to be 2.52 J/m$^2$ [74], namely, the Fe$_3$Al/BiF$_3$ interface seems to be stronger than the Fe/MgO one. The Fermi level of the junction is found to lie approximately in the middle of the BiF$_3$ band gap, with a valence band offset of 3.06 eV, as shown in Fig. 1(d).

Electronic transport is calculated for three junctions with different BiF$_3$ thicknesses, respectively, of 13.10, 18.94, and 24.77 Å. The zero-bias transmission coefficients as a function of energy, $T(E)$, are shown in Fig. 3 and clearly demonstrate that there is an exponential reduction of the transmission with the barrier thickness, confirming that the transport mechanism is indeed tunneling with little contribution from possible interface states.
The various transmission coefficients for the [001] direction calculated at the Fermi level are plotted in Fig. 4 as a function of the $k$-vector in the two-dimensional Brillouin zone orthogonal to the transport direction. For the parallel configuration the transmission is dominated by the majority spins and a $k$-region around the Γ-point, while for the minority band and for the antiparallel configuration the transmission is small and originates from narrow pockets of $k$-vectors away from Γ. This further confirms that the transport is dominated by the $\Delta_1$ symmetry, present only for the majority spins. Importantly, the relative contribution to the total current of the majority spin channel relatively to the minority one in the parallel configuration will exponentially grow as the barrier thickness increases, meaning that for barriers thick enough the Fe$_3$Al contributes to the total current of the majority spin channel present only for the majority spins. Importantly, the relative contribution to the total current of the majority spin channel to the minority one in the parallel configuration will exponentially grow as the barrier thickness increases, meaning that for barriers thick enough the Fe$_3$Al system behaves as a half-metal, exactly as Fe/MgO.

B. Finite-bias properties

For the 18.94 Å-thick junction we have calculated the current and the TMR as a function of bias (see Fig. 5). Calculations are performed on a $24 \times 1 \times 1$ $k$-point mesh (closed symbols at voltages $V = 0, 0.1, 0.5$ V) and have been verified against a $100 \times 100 \times 1$ mesh for a self-consistent calculation at a few selected biases (0, 0.1, and 0.5 V). We find that the $I$-$V$ characteristic of the parallel configuration is approximately linear at low bias and then saturates at about 0.2 V to a value of 0.25 mA/μm$^2$. Since the same curve for the antiparallel configuration is flat and the current is small, the TMR as a function of bias decays from the $V \sim 0$ value of 25 000% to about 5000% at $|V| > 0.2$ V [see below for $T(E; V)$]. This is indeed a very encouraging result since an extremely large TMR can be reached for a 2 nm thick barrier, and larger values can be obtained by making the barrier thicker. We must note that the theoretical TMR is for the perfect junction and demonstrates that symmetry filtering is the dominant mechanism. The actual TMR of any junction will depend on secondary phases or defects at the interface, so the values observed here should be considered an upper limit.

The transmission of the Fe$_3$Al/BiF$_3$/Fe$_3$Al junction has been self-consistently calculated at 0, 0.1, and 0.5 V. In Fig. 6 we present the transmission coefficient for each bias step, $T(E; V)$. The behavior of the junction can be understood by considering the $\Delta_1$ filtering of BiF$_3$ and the band structure of the Fe$_3$Al electrodes. We see that when the magnetizations of the electrodes are parallel, $T(E; V)$ for the majority spins is a smooth function of the energy, since the transmission originates from $\Delta_1$ band. At the same time there is no minority spin bands at the Fermi level along the [001] direction, resulting in a strongly suppressed minority transition around $E_{\text{F}}$. As the bias voltage increases, bands with $\Delta_3$, $\Delta_2$, and $\Delta_2'$ symmetry became available for transport. However, these are filtered by symmetry by the BiF$_3$ barrier, and the transmission remains generally small. $T(E; V)$ for the antiparallel configuration is essentially a convolution of those for the majority and minority spins in the parallel one, i.e., it traces closely the minority spin transmission.
IV. CONCLUSION

In conclusion, we have identified from all known and predicted Heusler alloys a materials combination which can act as an alternative to the FeCoB/MgO/FeCoB heterostructure. In particular we have looked at the Fe$_3$Al/BiFe$_3$/Fe$_3$Al stack and demonstrated that this junction operates with the same symmetry spin-filtering mechanism of FeCoB/MgO and as such can display extremely high TMR values. Interestingly, the extended $\Delta_1$ spin gap along the (100) direction of Fe$_3$Al gives us a large energy window where to expect a significant TMR. As such for this proposed junction we expect a strong TMR retention at high voltage.

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