Electronic Structures of Ge$_2$Sb$_2$Te$_5$/Co$_2$FeX (X: Al, Si) Interfaces for Phase Change Spintronics

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Supporting Information

ABSTRACT: Phase change materials (PCMs), such as Ge$_2$Sb$_2$Te$_5$, are highly attractive in modern electronics and photonics. However, their spintronic applications remain largely unexplored. Here, we propose a tentative modality of phase change spintronic devices based on the ferromagnet/PCM/ferromagnet structure. The electrically tunable properties of a PCM interlayer give rise to new possibilities of manipulating spin transport through phase change, adding new functionalities and modes of operation to the spintronic devices. As the first step toward realizing such phase change spintronic devices, we calculate the electronic structures of the interfaces of c-Ge$_2$Sb$_2$Te$_5$ and half-metallic ferromagnetic Co$_2$FeX (X: Al, Si). The interfaces are found not to be genuine half-metallic, indicating room for improvement. The band alignments are largely determined by the termination of c-Ge$_2$Sb$_2$Te$_5$. Two types of band alignments are found for c-Ge$_2$Sb$_2$Te$_5$/Co$_2$FeX interfaces. Considering c-Ge$_2$Sb$_2$Te$_5$ as heavily p-type-doped, interfaces with Te termination are generally suitable such that they offer low contact resistance for hole injection from Co$_2$FeX to c-Ge$_2$Sb$_2$Te$_5$ in the majority spin channel; at the same time, they naturally form tunneling barriers, alleviating the degradation of spin injection efficiency because of occasional hole injection in the minority spin channel. This work provides important insights into this proposed phase change spintronic framework.

1. INTRODUCTION

Chalcogenide-based phase change materials (PCMs) such as Ge$_2$Sb$_2$Te$_5$ have revolutionized the frontier of data storage industries. The initial applications of PCMs in the rewritable optical disk exploit the reversible change of their optical properties. In the past decade, extensive studies on the reversible change of the electrical conductivity of PCMs have been carried out to develop the nonvolatile phase change random access memories (PCRAMs) as a strong contender to c-Ge$_2$Sb$_2$Te$_5$ in the majority spin channel; at the same time, they naturally form tunneling barriers, alleviating the degradation of spin injection efficiency because of occasional hole injection in the minority spin channel. This work provides important insights into this proposed phase change spintronic framework.

All of these applications capitalize on either the large optical or electrical contrast of PCMs between the crystalline and amorphous phases. Despite the prevalence of PCMs in both optics and electronics, the studies of PCMs for spintronic applications are scarce. The attempt of introducing spin degree of freedom into PCMs was initiated by Song et al. Ge$_2$Sb$_2$Te$_5$ was doped with a small amount of iron atoms and phase-dependent ferromagnetism appeared at low temperature. A potential application of doped ferromagnetic PCM is the fast manipulation of magnetic properties by the phase change mechanism. By using Mn as an alternative doping element, Adam et al. also reported phase-dependent ferromagnetism at low temperature. In fact, doping semiconductors with transition metals has been a main way to realize ferromagnetism in otherwise nonmagnetic semiconductors. However, experimental demonstration of materials with high Curie temperature remains a major challenge to magnetic semiconductor research. To this end, the electronic properties of transition-metal-doped PCMs have been investigated theoretically. Cr has been predicted to be the most promising doping element for magnetic PCMs with high Curie temperature up to 239 K which is, however, still too low for real applications. Moreover, these studies have suggested that suitable transition-metal dopants for magnetic PCMs are very limited. Recently, Sc dopants are found to assist ultrafast crystallization of PCMs, but, unfortunately, they do not induce any ferromagnetism. Therefore, identifying alternative routes toward phase change spintronics other than doping PCMs is still essential.

Nanodevices generally require the integration of different materials, such as dielectric and electrode material, into heterostructures. An example is the metal/PCM/metal sandwich structure for PCRAMs, in which the metal electrodes provide suitable electrical contact with the PCM interlayer which actively tailors the electrical conductivity of the device through the phase change mechanism. Recently, the use of the phase change mechanism to tune the electronic properties of graphene as the electrode(s) has been proposed. A second example is the ITO/PCM/ITO structure for phase change optoelectronics, as proposed by Hosseini et al. Indium tin oxide (ITO) is a special type of electrode, both metallic and...
transparent to visible light, making electrically switchable color pixels possible. PCMs actively tailor the optical reflectivity/refractivity of this structure through the phase change mechanism. Ferromagnet/nonferromagnet/ferromagnet structure is the basis of modern spintronic devices, including magnetic random access memories (MRAMs) and spin valves. The ferromagnet serves as both metallic electrode and spin polarizer. The magnetization orientations of the two ferromagnetic electrodes, parallel or antiparallel, determine the device resistance and can be modified magnetically or electrically. The nonferromagnet interlayer serves as a tunneling barrier which is normally magnetically and electrically inactive. The use of metallic, insulating, and semiconducting interlayers has been reported. This work follows that of Tsafack et al. In the hexagonal representation, the unit cell has 30 atomic layers including electronic structures of c-Ge$_2$Sb$_2$Te$_5$/Co$_2$FeAl and c-Ge$_2$Sb$_2$Te$_5$/Co$_2$FeSi. We perform first-principles calculations have reported values to date. First-principles calculations have reported even smaller GGA band gaps for cubic Ge$_2$Sb$_2$Te$_5$ than range from 0.1 to 0.37 eV. For Co$_2$FeAl and Co$_2$FeSi, they crystallize in the L$_2$$_1$ structure. We relax these two unit cell structures by GGA functional and obtain lattice constants of 5.64 and 5.55 Å for Co$_2$FeAl and Co$_2$FeSi, respectively, close to the experimental values. It has been reported that GGA functional fails to give the correct magnetic moment of Co$_2$FeSi. This is partially due to the nearly closed GGA band gap in the minority spin channel and the Fermi level lies in the conduction band. We perform spin-unconstrained GGA + U calculation on the electronic structures of Co$_2$FeAl and Co$_2$FeSi and follow Khoshravizadeh et al. to use medium-effective $U$ parameter $U_{Co} = 2.5$ eV and $U_{Fe} = 2.5$ eV. It opens the band gaps in the minority spin channels to about 0.75 eV for both Heusler alloys. The magnetic moment of a Co$_2$FeSi unit cell is also greatly improved from 5.0 $\mu_B$ by GGA to 5.8 $\mu_B$ by GGA + $U$, close to the integer experimental value of 6 $\mu_B$. The Fermi level now lies around the threshold of the conduction band in the minority spin channel, comparable to the previous GGA + $U$ results. It is reported that the hybrid functional can further increase the band gap so that the Fermi level unambiguously lies within the band gap. Nevertheless, minor deviation of the Fermi level around the band edge should not affect the schematic energy band alignment across the c-Ge$_2$Sb$_2$Te$_5$/Heusler-alloy interface. For Co$_2$FeAl, the Fermi level lies around the valence band edge and the unit cell has an integer magnetic moment of 5 $\mu_B$. It should be emphasized that all GGA + $U$ calculations are performed on GGA-relaxed structures. To justify the reliability of this approach, we also relax the Co$_2$FeSi structures by GGA + $U$ and find that the resulting lattice constants are close to those obtained by GGA. In particular, the GGA + $U$ and GGA lattice constants of Co$_2$FeSi (Co$_2$FeAl) are 0.40 nm (0.41 nm) and 0.39 nm (0.40 nm), respectively.

2. RESULTS AND DISCUSSION

2.1. Bulk c-Ge$_2$Sb$_2$Te$_5$, Co$_2$FeAl, and Co$_2$FeSi. The atomic structure of crystalline cubic Ge$_2$Sb$_2$Te$_5$ used in this work follows that of Tsafack et al. In the hexagonal representation, the unit cell has 30 atomic layers including layers of structural vacancy. The cubic phase of Ge$_2$Sb$_2$Te$_5$ is metastable and therefore allows fast phase transition in conventional phase change memory devices. Recently, a new interfacial phase change mechanism has been reported which differs from the conventional bulk phase change mechanism. In this interfacial structure, the stable hexagonal phase of Ge$_2$Sb$_2$Te$_5$ is found to be relevant. This makes sense because there is no bulk phase transformation and therefore the structure has to be stable. The unit cell structure is relaxed by generalized gradient approximation (GGA) functional in CASTEP. We employ ultrasoft pseudopotentials and 330 eV cutoff energy. The calculated band gap of c-Ge$_2$Sb$_2$Te$_5$ is 0.45 eV, slightly smaller than the hybrid functional result but close to the experimental value of 0.5 eV. We notice that several works have reported even smaller GGA band gaps for cubic Ge$_2$Sb$_2$Te$_5$ than range from 0.1 to 0.37 eV. For Co$_2$FeAl and Co$_2$FeSi, they crystallize in the L$_2$$_1$ structure. We relax these two unit cell structures by GGA functional and obtain lattice constants of 5.64 and 5.55 Å for Co$_2$FeAl and Co$_2$FeSi, respectively, close to the experimental values. It has been reported that GGA functional fails to give the correct magnetic moment of Co$_2$FeSi. This is partially due to the nearly closed GGA band gap in the minority spin channel and the Fermi level lies in the conduction band. We perform spin-unconstrained GGA + $U$ calculation on the electronic structures of Co$_2$FeAl and Co$_2$FeSi and follow Khoshravizadeh et al. to use medium-effective $U$ parameter $U_{Co} = 2.5$ eV and $U_{Fe} = 2.5$ eV. It opens the band gaps in the minority spin channels to about 0.75 eV for both Heusler alloys. The magnetic moment of a Co$_2$FeSi unit cell is also greatly improved from 5.0 $\mu_B$ by GGA to 5.8 $\mu_B$ by GGA + $U$, close to the integer experimental value of 6 $\mu_B$. The Fermi level now lies around the threshold of the conduction band in the minority spin channel, comparable to the previous GGA + $U$ results. It is reported that the hybrid functional can further increase the band gap so that the Fermi level unambiguously lies within the band gap. Nevertheless, minor deviation of the Fermi level around the band edge should not affect the schematic energy band alignment across the c-Ge$_2$Sb$_2$Te$_5$/Heusler-alloy interface. For Co$_2$FeAl, the Fermi level lies around the valence band edge and the unit cell has an integer magnetic moment of 5 $\mu_B$. It should be emphasized that all GGA + $U$ calculations are performed on GGA-relaxed structures. To justify the reliability of this approach, we also relax the Co$_2$FeSi structures by GGA + $U$ and find that the resulting lattice constants are close to those obtained by GGA. In particular, the GGA + $U$ and GGA lattice constants of Co$_2$FeSi (Co$_2$FeAl) are 0.40 nm (0.41 nm) and 0.39 nm (0.40 nm), respectively.

2.2. c-Ge$_2$Sb$_2$Te$_5$/Co$_2$FeAl interface. The in-plane lattice parameters of the (111) surface of Co$_2$FeSi (0.39 nm) and Co$_2$FeAl (0.40 nm) are comparable to those of the (0001) surface of c-Ge$_2$Sb$_2$Te$_5$ in the hexagonal representation (0.42 nm), and the sublattice of Co (or Fe/Si) bare resemblance to the rock-salt lattice of c-Ge$_2$Sb$_2$Te$_5$. We build supercell models for epitaxial interfaces of (0001) c-Ge$_2$Sb$_2$Te$_5$/(111)Heusler-alloy by fixing the in-plane lattice parameters to those of c-Ge$_2$Sb$_2$Te$_5$. This leads to 7.6% (5.0%) biaxial tensile strain on Co$_2$FeSi (Co$_2$FeAl). The lattice perpendicular to the interface is allowed to relax by GGA functional, thus mitigating the in-plane strain effect on the electronic structures. The total energy is converged to 0.0001 eV. There are various surface terminations for (0001) c-Ge$_2$Sb$_2$Te$_5$ and (111) Heusler-alloy. We first consider the c-Ge$_2$Sb$_2$Te$_5$/Co$_2$FeAl interfaces by all possible combinations of surface terminations (for Te termination, we only consider nonstoichiometric termination). To investigate the electronic and magnetic properties of the interface, we perform spin-unconstrained GGA + $U$ calculation. The partial density of states (PDOSs) of a central Te
atom in c-Ge$_2$Sb$_2$Te$_5$ and the interfacial and central Co, Fe, and Al atoms in Co$_2$FeAl are examined. Figures 1–4 show the representative interface structures and the corresponding PDOSs. Electron localization function (ELF) is used to

Figure 1. (a) Atomic structure and projected ELF isosurface of the c-Ge$_2$Sb$_2$Te$_5$/Co$_2$FeAl interface of the combination of Te–Fe terminations. The balls in green, orange, violet, blue, gray, and pink represent Ge, Te, Sb, Co, Fe, and Al, respectively. The terminated atoms are labeled by arrows. (b) GGA + U PDOSs of central Te in a c-Ge$_2$Sb$_2$Te$_5$ slab and interfacial Co and central Co, Fe, and Al in a Co$_2$FeAl slab. The thick and thin lines are for majority and minority spin channels, respectively. The Fermi level is set to zero. The band edges of c-Ge$_2$Sb$_2$Te$_5$ and Co$_2$FeAl in the minority spin channel are indicated by short vertical lines. (c) Band alignment diagram drew from the PDOSs, considering c-Ge$_2$Sb$_2$Te$_5$ as heavily p-type-doped. The empty arrow indicates the direction of hole injection. The large and small empty balls represent holes in the majority and minority spin channels, respectively.

Figure 2. (a) Atomic structure and projected ELF isosurface of the c-Ge$_2$Sb$_2$Te$_5$/Co$_2$FeAl interface of the combination of Ge–Fe terminations. (b) Corresponding GGA + U PDOSs. (c) Corresponding band alignment diagram.

Figure 3. (a) Atomic structure and projected ELF isosurface of the c-Ge$_2$Sb$_2$Te$_5$/Co$_2$FeSi interface of the combination of Te–Fe terminations. (b) Corresponding GGA + U PDOSs. (c) Corresponding band alignment diagram. The full arrow indicates the direction of electron injection. The small full ball represents an electron in the minority spin channel.
According to the simple Schottky calculated trend of band alignments with surface termination, the valence band maximum (VBM) of c-Ge₂Sb₂Te₅ lines up with the VBM of Co₂FeAl in the minority spin channel, and therefore, the Fermi level lies around the CBM of c-Ge₂Sb₂Te₅. This is consistent with the Fermi energy of c-Ge₂Sb₂Te₅ to be below the VBM, indicating c-Ge₂Sb₂Te₅ to be a degenerate p-type semiconductor. Tong et al. measured the Fermi energy of c-Ge₂Sb₂Te₅ to be below the VBM, indicating c-Ge₂Sb₂Te₅ to be a degenerate p-type semiconductor. For its application in spintronic devices, hole injection is therefore more relevant. As we have seen, c-Ge₂Sb₂Te₅/Co₂FeAl with Te termination has a large p-type Schottky barrier height (p-SBH) for the majority spin channel. Given the heavy hole doping in c-Ge₂Sb₂Te₅, however, the Schottky barrier can be thin enough to become a tunneling barrier so that the contact becomes practically Ohmic, as shown in Figure 1c. Moreover, this natural tunneling barrier obviates the need for a discrete layer like MgO to alleviate the conductivity mismatch which impedes high spin injection efficiency. Therefore, the problem of occasional hole injection in the minority spin channel can be mitigated. For the

Figure 4. (a) Atomic structure and projected ELF isosurface of the c-Ge₂Sb₂Te₅/Co₂FeAl interface of the combination of Ge−Fe terminations. (b) Corresponding GGA + U PDOSs. (c) Corresponding band alignment diagram.
interface with Ge/Sb termination, the p-SBH for the majority spin channel is nearly zero which provides low resistivity. However, the valence band offset (VBO) for the minority spin channel is also small such that minority spin injection cannot be blocked, as shown in Figure 2c. Occasional minority spin injection occurs as a result of, for example, non-quasi-particle state-induced gap states and the minority gap reduction which may vanish the half-metallicity.\textsuperscript{35,66} Co\textsubscript{2}FeAl has its Fermi level near the VBM of the minority spin channel which is susceptible to these thermal instabilities.

2.3. c-Ge\textsubscript{2}Sb\textsubscript{2}Te\textsubscript{5}/Co\textsubscript{2}FeSi Interface. Finally, we study the c-Ge\textsubscript{2}Sb\textsubscript{2}Te\textsubscript{5}/Co\textsubscript{2}FeSi interfaces. Similar to their Co\textsubscript{2}FeAl counterparts, none of the combinations of surface terminations lead to genuine half-metallic interface. Only in the central region of Co\textsubscript{2}FeSi do the PDOSs restore the bulk properties that we use to analyze band alignments. The substitution of Al by Si increases the number of valence electrons which can be seen as electron doping, in consistency with the upward shift of the Fermi level from near VBM in Co\textsubscript{2}FeAl to near CBM in Co\textsubscript{2}FeSi. For all interfaces with Te termination, except for the combination of Te−Si termination, the VBM of c-Ge\textsubscript{2}Sb\textsubscript{2}Te\textsubscript{5} lines up with the VBM of Co\textsubscript{2}FeSi in the minority spin channel, as shown in Figure 3b. The Fermi level lies near the CBM of c-Ge\textsubscript{2}Sb\textsubscript{2}Te\textsubscript{5} which is the same as in c-Ge\textsubscript{2}Sb\textsubscript{2}Te\textsubscript{5}/Co\textsubscript{2}FeAl interfaces of Te termination. The majority spin channel has large p-SBH at the interface, but the heavy hole doping of c-Ge\textsubscript{2}Sb\textsubscript{2}Te\textsubscript{5} may still make the barrier thin enough for Ohmic contact in practice, as mentioned above. The minority spin channel forms a heavily doped p–n junction (tunneling diode), and during hole injection from Co\textsubscript{2}FeSi to c-Ge\textsubscript{2}Sb\textsubscript{2}Te\textsubscript{5}, it is reverse-biased. This triggers band-to-band tunneling (BTBT) of electrons in the minority spin channel from the valence band of c-Ge\textsubscript{2}Sb\textsubscript{2}Te\textsubscript{5} to the conduction band of Co\textsubscript{2}FeSi, equivalent to hole injection in the minority spin channel from Co\textsubscript{2}FeSi to c-Ge\textsubscript{2}Sb\textsubscript{2}Te\textsubscript{5} as shown in Figure 3c. The tunneling barrier, however, is itself a remedy for the degradation of spin polarization due to these thermal instabilities, as mentioned above. For interfaces with Ge/Sb termination, the VBM of c-Ge\textsubscript{2}Sb\textsubscript{2}Te\textsubscript{5} lines up with the CBM of Co\textsubscript{2}FeSi in the minority spin channel, as shown in Figure 4b. The Fermi level lies near the VBM of c-Ge\textsubscript{2}Sb\textsubscript{2}Te\textsubscript{5} which is also the same as in c-Ge\textsubscript{2}Sb\textsubscript{2}Te\textsubscript{5}/Co\textsubscript{2}FeAl interfaces of Ge/Sb termination. For majority spin injection, the contact is Ohmic with nearly zero p-SBH. The minority spin channel forms a type II broken gap p–n junction, and during hole injection from Co\textsubscript{2}FeSi to c-Ge\textsubscript{2}Sb\textsubscript{2}Te\textsubscript{5}, it is reverse-biased, resulting in immediate injection of electrons from c-Ge\textsubscript{2}Sb\textsubscript{2}Te\textsubscript{5} to Co\textsubscript{2}FeSi, equivalent to hole injection in the minority spin channel from Co\textsubscript{2}FeSi to c-Ge\textsubscript{2}Sb\textsubscript{2}Te\textsubscript{5} as shown in Figure 4c. This decreases the spin injection efficiency. A type II staggered gap interface has been found for GaAs/Co\textsubscript{2}FeSi in the minority spin channel by first-principles calculations,\textsuperscript{45} which may also suffer from BTBT in the minority spin channel when p-type GaAs is used. Now, we return to see the c-Ge\textsubscript{2}Sb\textsubscript{2}Te\textsubscript{5}/Co\textsubscript{2}FeAl interface with the combination of Te termination and Si termination. The band alignment of this interface is similar to those of its Ge/Sb termination counterparts. This may be due to the fact that Si is more electronegative than Fe and Co and the polarity of interfacial bonding changes dramatically from Fe/Co−Te to Te−Si. Al does not have the problem because it has electronegativity comparable to those of Fe and Co. As mentioned before, taking the polarity of interfacial bonding explicitly into account is useful to understand the nature of band line-up in this case. Actually, we model the Te-terminated c-Ge\textsubscript{2}Sb\textsubscript{2}Te\textsubscript{5} surface with a surface Si adatom which is equivalent to the substitution of topmost Ge by Si in the Ge-terminated surface. The EA of such surface is 0.9 eV smaller than that of the pristine Te-terminated surface but still a bit larger than that of the Ge-/Sb-terminated one. This is the reason of close resemblance of the band alignment to its Ge/Sb termination counterparts. The interfaces with Ge/Sb termination are less sensitive to Co\textsubscript{2}FeSi terminations because they form nonpolar interface bonding.

We have calculated the c-Ge\textsubscript{2}Sb\textsubscript{2}Te\textsubscript{5}/Co\textsubscript{2}FeAl and c-Ge\textsubscript{2}Sb\textsubscript{2}Te\textsubscript{5}/Co\textsubscript{2}FeSi interfaces of different combinations of terminations. The Te termination (except for c-Ge\textsubscript{2}Sb\textsubscript{2}Te\textsubscript{5}/Co\textsubscript{2}FeSi interface of Te−Si termination) of both classes of interfaces is preferred from our band alignment analysis. In addition, first-principles calculations by Deringer and Dronskowski showed that for hexagonal Ge\textsubscript{6}Sb\textsubscript{4}Te\textsubscript{10}, Te termination is stable over the range of permissible chemical potentials.\textsuperscript{67} On the other hand, the flexible electronic structures of Heusler alloys offer the toolbox for realizing functionalities as desired.

We show here that the electronic structures of c-Ge\textsubscript{2}Sb\textsubscript{2}Te\textsubscript{5}/Co\textsubscript{2}FeX interfaces are tunable by the substitution of main group element X. Fecher and Felseret studied the composition-dependent electronic structures of Co\textsubscript{2}FeAl\textsubscript{1−x}Si\textsubscript{x} and found that the Fermi levels of Co\textsubscript{2}FeAl and Co\textsubscript{2}FeSi can be shifted away from band edges,\textsuperscript{48} as required by the temperature stability of bulk half-metallicity. It is also critical to find a guide rule for the selection of Heusler alloys for specific spacer materials to realize genuine half-metallic interfaces and suitable band alignments to for spin functionalities.

3. CONCLUSIONS

To summarize, we propose a tentative modality of phase change spintronic devices, namely, a ferromagnet/PCM/ferrimagnet structure. Using PCM as the semiconducting interlayer gives rise to a new possibility of manipulating spin transport through phase change, adding new functionalities and modes of operation to the device. The electronic structures of c-Ge\textsubscript{2}Sb\textsubscript{2}Te\textsubscript{5}/Co\textsubscript{2}FeX (X: Al, Si) interfaces of all combinations of terminations are studied by GGA + U method. None of them is genuine half-metallic, indicating that there is enough room for improvement. The interface band alignments are studied and preferable combinations of terminations as demanded by high spin injection efficiency are found. This work provides useful insights for follow-up experiments.

ASSOCIATED CONTENT

Supporting Information

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Atomic structures and electrostatic potentials of Te- and Ge-terminated surfaces of c-Ge\textsubscript{2}Sb\textsubscript{2}Te\textsubscript{5} (PDF)

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