Magnetic properties of phase-change films hidden in the structures

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Abstract

Since the discovery of phase-change switching in chalcogenides, phase-change memory (PCM) has been irrelevant and insensitive to magnetic field. Actually, in the development of digital versatile disc (DVD) using a red laser, optical PCM had fought with magneto-optical memories. However, the fundamental concept is removed completely by the emergence of interfacial phase-change memory (iPCM), which is designed to reduce entropic energy loss as small as possible using a growth-oriented superlattice structure. We report that iPCM show a giant magneto-resistivity > 2,000% at more than 400K under a magnetic field of 0.1T, and surprisingly can discriminate the external magnetic field direction optically. These magnetic properties of iPCM may open a new era to the PCM world associated with spintronics.

I. Introduction

Phase-change memory (PCM) is considered to be the leading candidate for nonvolatile memory (NVM). PCM has several advantages over other type NVMs such as magnetoresistive (MRAM), metal oxide resistive (RRAM) and FLASH because of its scalability, understandable and hence predictable switching mechanism, and large resistance differences between set and reset states. Although PCM operation typically has required large power for switching, especially for the reset process, this drawback has been mitigated significantly by replacing the typically used monolithic GeSbTe film by an "interfacial phase-change memory, iPCM" structure [1]. Due to a significant reduction in entropic losses associated with both set and reset states, the required input energy has been reduced by around 90% compared to conventional PCM devices. The energy saving property of iPCM devices is a consequence of the one dimensional motion of Ge atoms normal to the GeTe/Sb_2Te_3 interfaces. High quality interfaces and crystallographic alignment along the growth direction of each GeTe and Sb_2Te_3 sub-layer is required.

Recently, topological insulators, (TI) have attracted much attention in graphene as well as several crystals including heavier elements [2]. Very recently, the bulk crystalline phase of $Ge_2Sb_2Te_5$ has been predicated to be a TI using first-principles computer simulations [3] as well as the Sb_2Te_3 trigonal phase [4]. If both predictions of TI behavior are true, iPCM films and devices may become some of the most suitable materials to confirm the existence of topological insulating properties of phase-change materials.

In this paper, we report on the results of first-principles computer simulations of iPCM structures including a spin-orbit coupling (SOC), that confirm iPCM is a suitable candidate to exhibit topological insulating behavior and related properties.

II. First principle simulation including spin-orbit coupling

To investigate the topological characteristics of iPCM structures theoretically, inclusion of spin-orbit coupling (SOC) is required. SOC is a relativistic effect and is an additional term to the total hamiltonian $\hat{H}$ because inner electrons in a heavy element move faster than outer shell electrons and the velocity v_e is proportional to atomic number Z: $v_e \propto Z/n$, where n is the principal quantum number. When relativistic effects are important, it is necessary to solve the Dirac equation to solve for the electron band structure. The total hamiltonian $\hat{H}$ including the SOC term thus becomes [5],

$$\hat{H} = \hat{H}_0 + \hat{H}_{so} = -(\hbar^2/2m)\nabla^2 + (\hbar/4m^2c^2)\,\sigma\cdot(\nabla \boldsymbol{V(r)} \times \boldsymbol{p}) \qquad (1).$$

Where, σ is the spin operator. If eq.(1) is invariant under spatial inversion, the SOC energy $\hat{H}_{so}$ becomes zero because of symmetry. However, if spatial inversion symmetry is broken (for example, V(r) has a gradient), $\hat{H}_{so}$ assumes a non-zero value, resulting in spin-splitting because the $\nabla V(r) \times p$ term operates on spin-electrons in the same manner as a magnetic field. If $\nabla V(r) = (0, 0, E_z)$ is applied normal to a 2-dimensional surface and electrons move on the surface with a momentum p **(or k)**, the spin directions are confined to the plane and quantized. As a result, the energy of free electrons in the plane splits,

$$E(k) = (\hbar^2/2m)k^2 \pm (\hbar/4m^2c^2)\, E_z\, k = E_{non\text{-}so}(k) \pm \alpha_R k \qquad (2).$$

Where, α_R is called Rashba parameter, which provides an estimate of the strength of the SOC.

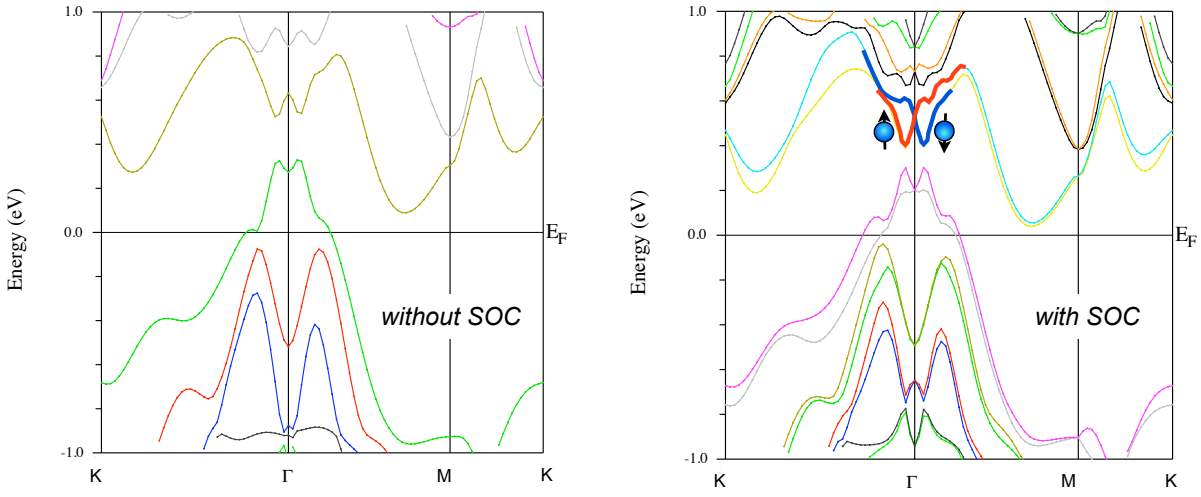

Figure 1 Band structures with (right) and without (left) SOC for the $[(GeTe)_2(Sb_2Te_3)_1]$ iPCM structure with tetrahedrally coordinated Ge atoms. Due to SOC, the spin degeneracy of each band is lifted.

Two density functional codes, *CASTEP* and *WIEN2K* were used to calculate the band structures of iPCM superlattice structures built from the unit block $[(GeTe)_2(Sb_2Te_3)_1]$. *WIEN2K* is an all electron code that includes relativistic wave-functions and includes spin-orbit coupling. In *CASTEP* calculations, the local spin density approximation (*LSDA)* was used, while in *WIEN2K* a linearized augmented plane waves (*LAPW*) was used in conjunction with the GGA for the exchange-correlation term. First, two models with tetrahedrally coordinated Ge atoms and trigonally coordinated Ge atoms were relaxed at 0 K under spin-polarized conditions using the *CASTEP* in order for the more computationally complex all-electron to convergence faster, and then the relaxed structures were moved to *WIEN2K*. **Figure 1** shows two band structures of $[(GeTe)_2(Sb_2Te_3)_1]$ with and without SOC. Without SOC, each energy band is spin-degenerate, while with SOC the degeneracy is lifted. In the vicinity of $k=0$ *(the* Γ *point)*, the band symmetry is preserved, however, the spin polarization is exchanged. It should be noticed that time reversal symmetry: $E(k, \uparrow) = E(-k, \downarrow)$ is invariant, while spatial inversion symmetry is not preserved; $E(k, \uparrow) \neq E(-k, \uparrow)$. At the Γ *point*, two valleys appear symmetrically for $k<0$ and in $k>0$ with a maximum energy difference around 0.2 eV. (see the red and blue lines at the bottom of the conduction bands). Each band has a different spin polarization, which is also depicted in **figure 1**. This is a very important criteria to be a candidate as a TI with a large Rashba effect. Up and down spin electrons lifting of the spin degeneracy of the bands are all aligned within the interfaces of the iPCM <111> structure, and application of an electrical field normal to the surface may induce a large Rashba effect similar to magnetic field of SOC. The iPCM structure can have magnetic sensitivity, which is completely absent in the identical composition alloy of $Ge_2Sb_2Te_5$! In our simulations, it was

confirmed that other iPCM structures with plural blocks of Sb_2Te_3, $[(GeTe)_2(Sb_2Te_3)_n]$ show similar TI feature to the iPCM with $[(GeTe)_2(Sb_2Te_3)_1]$.

III. Experimental verification of IT property and the Rashba effect in iPCM structures

As explained above, an electrical field applied normal to the <111> surface of an iPCM structure makes electrons on the surface or interfaces spin-polarize with Rashba effect because the external electrical field plays the role of generating an internal magnetic field via the $\sigma\cdot(\nabla V(r) \times p)$. In addition, it is hard for the spin-currents to penetrate normal to the iPCM film. Interestingly, by the Rashba effect as shown in eqs. (1) and (2), except for $k=0$, spin electrons feel a different energy depending upon the spin state around the Γ *point*. On the other hand, applying an external magnetic field in the plane make the spins states tighten up because the magnetic field plays a similar role to the $\sigma\cdot(\nabla V(r) \times p)$ in eq.(1). Therefore, by illuminating circular polarized electromagnetic light onto the iPCM film, one of the spin currents will be more induced than the other spin current. An optical response, such as reflectivity change, will be observed. The expected behavior, however, is clearly different from magneto-optical Kerr effect which shows a reduction in strength with wavelength. **Figure 2** shows optical reflectivity under ~0.2 T magnetic field, which was applied in plane along the edge of an iPCM structure $[(GeTe)_2(Sb_2Te_3)_2]_{12}$ on a Si wafer. It is found that the iPCM structure can be to identify the polarity of the magnetic field.

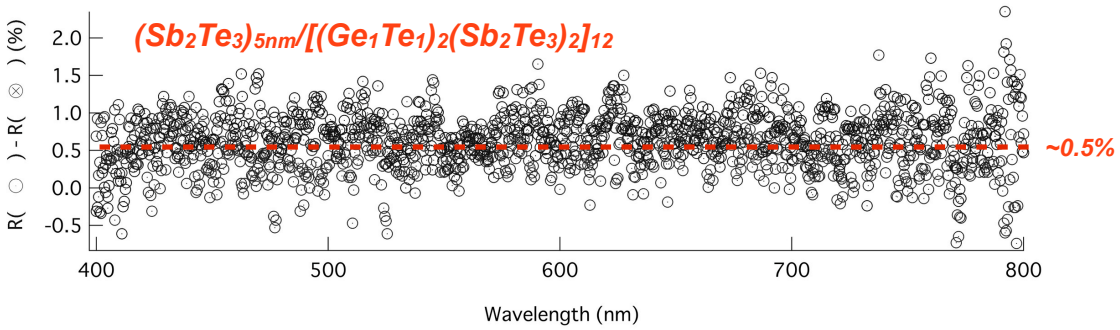

Figure 2. Optical reflectivity change induced by application of an external magnetic field (an average of 0.2 T) applied in plane along the edge of an iPCM structure $[(GeTe)_2(Sb_2Te_3)_2]_{12}$ on a Si wafer. The different magnetic polarity shows different reflectivity. This means that the iPCM film can be used to identify the magnetic field direction. Circular polarized light was used. It is confirmed that this was not a magneto-optical effect (Kerr or Faraday) by use of a polarizer.

IV. Conclusion

Magneto-reflection of an iPCM structure of GeSbTe was first observed under magnetic field. The film was sensitive to application of an external magnetic field, and the magnetic field direction could be identified. Due to the first principle computer simulations including SOC effect, iPCM structures are TI with a large Rashba effect.

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