

Spin-storage mechanism in interfacial phase-change memory (iPCM)

J. Tominaga, A. V. Kolobov, P. Fons, X. Wang, J. Richter, Y. Saito, and T. Nakano
National Institute of Advanced industrial Science and Technology (AIST),
Tsukuba Central 4, 1-1-1 Higashi, Tsukuba 305-8562, Japan

S. Murakami

Department of Physics, Tokyo Institute of Technology, 2-12-1 Ookayama, Meguro-ku, Tokyo 152-8551, Japan

ABSTRACT

Interfacial phase change memory (iPCM) is magnetic sensitive at room temperature while the alloy with same composition is not. The unique property has been thought to be related to the topological insulating property. We discuss the magnetic properties on the point of view of the spatial inversion symmetry of iPCM structures and ferroelectricity of GeTe layers sandwiched by topological insulating layers.

Key words: iPCM, topological insulator, magnetic property.

Introduction

Since EPCOS2007 Zermatt in Switzerland, we have proposed and designed GeTe/Sb₂Te₃ superlattice structures in crystal state to reduce the switching energy based on the second law of thermodynamics [1]. In a conventional phase change memory (PCM), the switching between SET and RESET states depends on a thermodynamical cycle through an adjacent heat reservoir (heater element). When a Joule heat is injected to a phase-change film through the reservoir, a portion in the film is melted or crystallized, depending on the current and the pulse time. However, it is noted that any thermodynamical system to make a work to the outside requires to remove the heat left to the outside, which is usually surrounded at room temperature, after the work is done. Otherwise the system cannot do a work. The heat energy has only a small part used for a work, while the others must be wasted out of the system. In addition, it is noted that the energy unused for the work must be removed out of the system. Due to the reason, a heat-accumulation structure typically equipped in PCM devices may not be a suitable cell design. The energy loss, which is not used for a work, is called entropy energy loss, which is estimated from a statistical calculation using the Boltzmann equation related to a geometrical coordination number of atoms or molecules included in a thermodynamical system [2]. Therefore, if the total coordination number in the vicinity of a phase transition is small, the entropy loss becomes small. In the GeTe/Sb₂Te₃ superlattice structures, which is called interfacial phase-change memory (iPCM), it was designed to reduce the number as small as possible forcing a single dimensional motion before and after the phase transition. based on a flip-flop transition of a Ge atom located in a Te -fcc sub-lattice, which was proposed by Kolobov et al [3]. Since the first demonstration of a low energy switching in 2011, we have succeeded in further reducing energy loss by ~1/100, compared with that of a PCM using the same composition alloy film on the same platform device. In addition, the RESET and RESET cycle was elongated by >10⁹ times, holding two orders of magnitude in the resistance change [4]. In EPCOS2011 and 2012, we reported that iPCM films exhibit magnetic properties at room temperature in both electrical and optical measurement without any magnetic dopant [5,6]. The properties are highly unusual because it was already reported that typical GST alloys are nonmagnetic [7]. The origin of the magnetization in iPCM films however has not been cleared.

In EPCOS2013, we first time propose and discuss the magnetization model of iPCM using *ab-initio* computer simulations.

Structure of iPCM

iPCM is a crystalline superlattice built up from fcc-GeTe layers and A7-Sb₂Te₃ quintuple layers: [(GeTe)_l(Sb₂Te₃)_m]_n block, where *l*, *m* and *n* are integers. For example, a [(GeTe)₂(Sb₂Te₃)_m]_n block has the same composition as Ge₂Sb₂Te₅. The former has the atomic layer structure, while the latter has a NaCl-type fcc lattice with a random occupation of Ge or Sb at cation sites. Sb₂Te₃ has a feature to grow the crystal phase on a Si wafer orientating the [111] axis normal to the surface at a high temperature [8]. On the other hand, fcc-GeTe has a feature to grow the crystal phase orientating the [111] axis normal to the Sb₂Te₃ (111) surface at 200~250°C [4]. Therefore, a highly

anisotropic film is formed by controlling the formation temperature. Figure 1 shows the film structure of a typical GeSbTe superlattice $[(\text{GeTe})_2(\text{Sb}_2\text{Te}_3)_1]_n$ with $a=4.22$ Å and $c=18.71$ Å. It is recently noticed that the Sb_2Te_3 sub-layer (quintuple layer QL) is a 3D-topological insulator. On the other hand, the GeTe layer is known to be a ferroelectric material [9]. The models shown in Figure 1 are two of the atomic sequence orders in the GeTe sub-layer. Although the other sequence besides the models, Ge-Te-Te-Ge (Petrov) is possible, we found that the Petrov sequence is unstable at the film deposition temperature ($\sim 250^\circ\text{C}$) than the other two sequences using *ab-initio* molecular dynamics simulations. It is easily understood that phase transition between the two models in Figure 1 occurs by Ge-flip-flop transition through the Te plane in the GeTe sub-layers. In addition, the transition process breaks the spatial inversion symmetry of the Te-Ge-Ge-Te sequence.

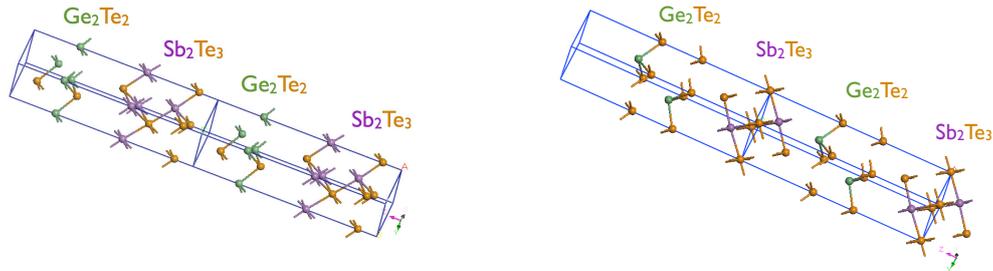


Figure 1 Basic cell models of iPCM with $[(\text{GeTe})_2(\text{Sb}_2\text{Te}_3)_1]_n$. Two Ge atoms are installed in the GeTe layer, and the Sb_2Te_3 layer is composed of a Te-Sb-Te-Sb-Te stacking sequence (QL). Te-Ge-Ge-Te sequence (left: RESET) and Ge-Te-Ge-Te sequence (right: SET).

It is noticed that Te-Ge-Ge-Te sub-layer is dielectric due to holding the spatial inversion symmetry (RESET state) while the Ge-Te-Ge-Te sub-layer is ferroelectric due to the break of the inversion symmetry (SET state). Each sub-layers are weakly bonded by *van der Waals* force. Due to the feature, Sb_2Te_3 QLs may play a role in a 3D-topological insulator independently in some extent. As increasing the QL blocks ($l \geq 1$) in the superlattice $[(\text{GeTe})_2(\text{Sb}_2\text{Te}_3)_m]_n$, the surface bands are generated at the top and bottom surfaces play independently. On the other hand, when the GeTe sublayer is thicker or thinner than a critical thickness, the iPCMs have a band gap, due to the hybridization of the bottom edgeless band and the top edgeless band in the adjacent Sb_2Te_3 sub-layers [10]. In the former case, the iPCM becomes a 3D-TI, while the latter becomes a bulk insulator. But, the top and bottom surfaces of the film holds the 2D-TI features if the number of the QL is ≥ 1 . It is noticed that a Dirac cone is formed in the bulk band structure when the hybridization is balanced. The structure of $[(\text{GeTe})_l(\text{Sb}_2\text{Te}_3)_m]_n$ iPCM films may take the critical condition, depending on each block thickness.

Magnetization of iPCM

Figure 2 shows the bulk band structure of $[(\text{GeTe})_2(\text{Sb}_2\text{Te}_3)_2]$ iPCM film. It is found that band gap is negligibly small and p_z -orbitals in Ge, Sb and Te invade into the conduction bottom band. A material with such a special condition is called *Dirac semimetal*. In the model (left) in Figure 1, the band structures of the spin-up and spin-down are degenerated, while the degeneration is lifted into split bands corresponding to each spin-state in the model (right). When an external electrical field is applied, there may generate a difference in between the spin densities of the state. This is called *Rashba* effect. Recently, it was reported that GeTe has a large *Rashba* effect [9]. If the iPCMs are Dirac semimetals, a band gap may easily open when a voltage is applied to an iPCM device, resulting in a *non-ohmic* resistance change. In addition, in an external magnetic field, the spin-density of the state may be no longer equal in between spin-up and spin-down electrons, resulting in an electrical-field-induced magnetization.

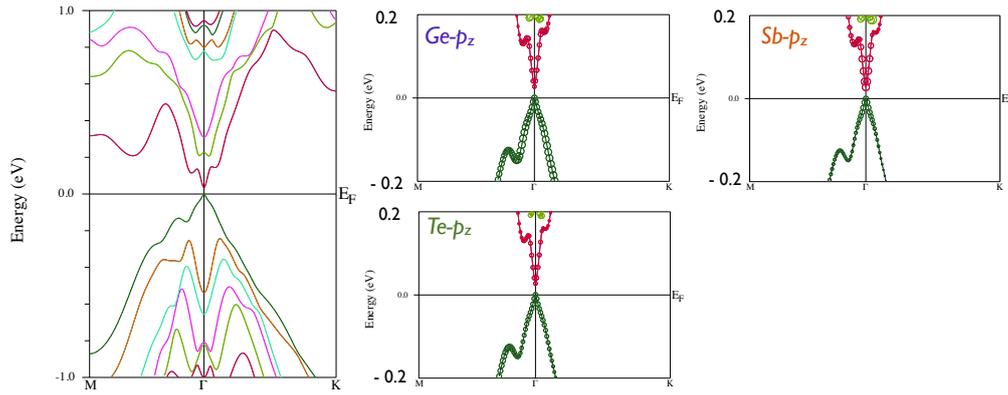


Figure 2 Bulk band structure of [(GeTe)₂(Sb₂Te₃)₂] iPCM (left). Three zoom images are of *Ge-p_z*, *Sb-p_z* and *Te-p_z* contributions (the size of the circles on the lines). The *p_z* orbitals in Ge, Sb and Te invade from the valence top to the conduction bottom.

Summaries

Electrical-field-induced magnetic properties in iPCMs may be generated by the break of the Dirac cone in the bulk state due to the combination between the ferroelectric & antiferroelectric GeTe layers and the topological insulating Sb₂Te₃ layers. IPCM is the first engineering material to probe topological insulating properties.

Acknowledgement

A part of the work was supported by FIRST program initiated by the Council for Science and Technology Policy (CSTP). We wish to thank Ms. Reiko Kondou for her assistance in the fabrication of iPCMs.

References:

1. J. Tominaga *et al.* EPCOS2007, Zermatt, Switzerland, 2007.
2. J. Tominaga *et al.* Phys. Status Solidi **B** 249, 1932 (2012).
3. A. Kolobov *et al.* Nature Matter, 3, 703 (2004).
4. R. Simpson *et al.* Nature Nano. **6**, 501 (2011).
5. J. Tominaga *et al.* EPCOS2011, Zurich, Switzerland, 2011.
6. J. Tominaga *et al.* EPCOS2012, Tampere, Finland, 2012.
7. J. Tominaga *et al.* Appl. Phys. Lett. **99**, 152105 (2011).
8. R. Simpson *et al.* Appl. Phys. Lett. **100**, 021911 (2012).
9. D. D. Sante *et al.* Adv. Mater. **25**, 509 (2013).
10. R. Takahashi and S. Murakami, Phys. Rev. Lett. **107**, 166805 (2011).

Biographies

Junji Tominaga is a prime senior scientist in Nanoelectronics Research Institute of AIST.