

# Study of SiTe/Sb<sub>2</sub>Te<sub>3</sub> phase change superlattices

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## ABSTRACT

Interfacial phase change memory (iPCM) has been attracting considerable attention not only for new type of non-volatile memory but also for magnetic device application. In this study, we first report the bulk band structures of SiTe/Sb<sub>2</sub>Te<sub>3</sub> superlattices using *ab initio* computer simulation based on density functional theory. It is suggested that the newly developed SiTe/Sb<sub>2</sub>Te<sub>3</sub> superlattice is a Dirac semimetal.

**Key words:** Phase change memory, Superlattice, iPCM, Topological insulator

## 1. INTRODUCTION

Phase change memory (PCM) is one of the candidates for next-generation non-volatile memory. In PCM, Joule heating induced by electrical pulses generally achieves reversible phase change between amorphous and crystalline states. A Ge<sub>2</sub>Sb<sub>2</sub>Te<sub>5</sub> (GST) compound is most widely used as the material. However, since the amorphization process requires the large energy due to the high melting point ( $\sim 600^\circ\text{C}$ ), power reduction is one of the key technical issues in the PCM devices. It was reported by Tominaga *et al.* [1] that applied energy is largely wasted as entropic loss accompanied by large atomic movement through melting process. Based on this thermodynamic principle, Simpson *et al.* successfully fabricated interfacial phase change memory (iPCM) using GeTe/Sb<sub>2</sub>Te<sub>3</sub> superlattice structure, which forced Ge atoms to transit within a low dimension, resulting in an order of magnitude smaller energy consumption compared with that used in the conventional alloy device [2]. Furthermore, it was reported that the iPCM exhibits magnetic properties and the phenomena can be explained by the topological insulating property [3, 4]. Although the iPCM using phase change superlattice has been attracting attention not only for electrical non-volatile memory application but also for magnetic devices, the material has been almost limited to GeTe/Sb<sub>2</sub>Te<sub>3</sub> superlattice. In this work, we report SiTe/Sb<sub>2</sub>Te<sub>3</sub> phase change superlattice.

## 2. CALCULATIONS

To investigate the stable structure and the corresponding band structure, two kinds of *ab initio* codes, called *CASTEP* and *WIEN2K*, based on density functional theory (DFT) were carried out. In *CASTEP* calculations, a generalized gradient approximation (GGA) of Perdew-Burke-Ernzerhof (PBE) was used and in *WIEN2K* a linearized augmented plane wave (LAPW) was used. In this study, the superlattices of (SiTe)<sub>2</sub>(Sb<sub>2</sub>Te<sub>3</sub>)<sub>x</sub> (x: 1, 2 and 4) structure were investigated with different Sb<sub>2</sub>Te<sub>3</sub> blocks, which are called quintuple layer (QL).

## 3. RESULTS & DISCUSSIONS

Fig. 1(a) shows the calculated crystal structure of the 2QL structure after the geometry optimization. A bilayer of SiTe is sandwiched by the QLs. The space group of the structure is 164 (P-3m1) and the lattice constants are  $a = 4.18 \text{ \AA}$  and  $c = 31.31 \text{ \AA}$ , respectively. The calculated band structures of each model are shown in Fig. 1(b)-(d). Since the superlattices include heavy atoms such as Sb and Te, in which the relativistic effect is not negligible, spin-orbital

coupling (SOC) Hamiltonian was considered to calculate the band structures. It can be seen from Fig. 1(b) that the band gap of the 1QL structure closes at the  $\Gamma$  point and this is the most basic feature of a Dirac semimetal [5]. This result is similar to that of other topological insulating phase change materials such as  $\text{Sb}_2\text{Te}_3$  [6],  $\text{Ge}_2\text{Sb}_2\text{Te}_5$  [7] and  $\text{GeTe}/\text{Sb}_2\text{Te}_3$  superlattice [8]. The band structures of the (c) 2QL and (d) 4QL, however, have a band gap between the top valence and bottom conduction bands, which increases with increasing the number of QL.

The QL number dependences on band gap ( $E_g$ ) are summarized in Table 1. The calculations were carried out both with and without SOC. The results of  $\text{GeTe}/\text{Sb}_2\text{Te}_3$  superlattices are also shown in the same table for comparison. It is obvious that the band gap increases with increasing the QL number and has a smaller value when SOC is considered for the calculation. The reason of opening the band gap in 2QL and 4QL is presumably thought to be due to the hybridization of the interface bands of QLs across the  $\text{SiTe}$  layers. Further discussion will be done in the poster presentation. It was found that unlike  $\text{GeTe}/\text{Sb}_2\text{Te}_3$  superlattices, the  $\text{SiTe}/\text{Sb}_2\text{Te}_3$  superlattice is sensitive to the number of QLs.

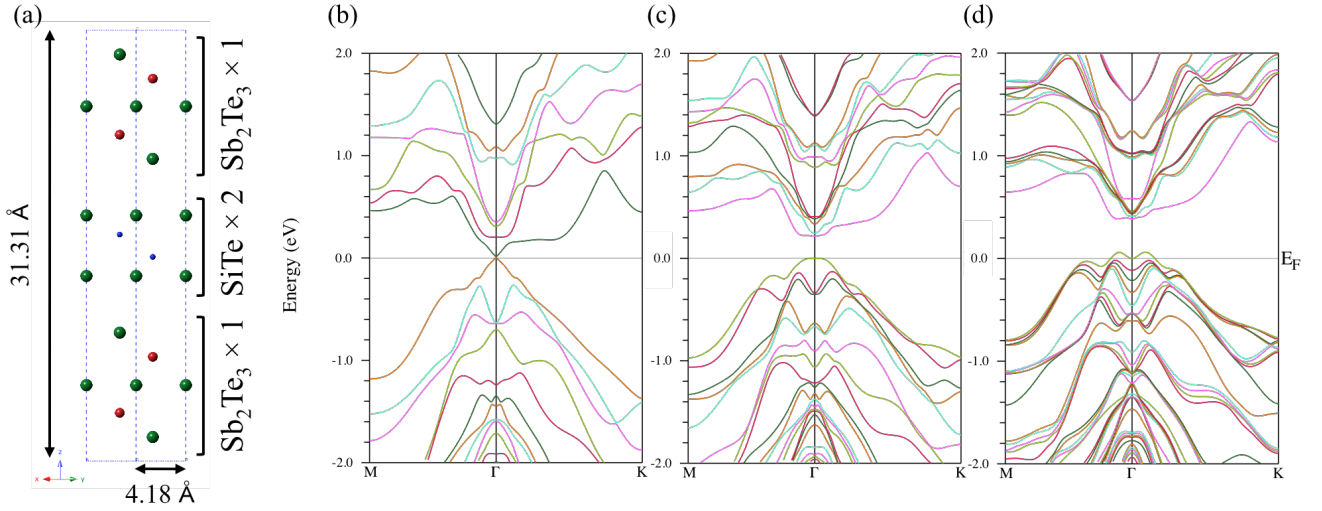


Fig. 1 (a) The crystal structure of the  $(\text{SiTe})_2(\text{Sb}_2\text{Te}_3)_2$  structure (2QL) (Si : blue, Sb : red and Te : green). The calculated band structure with SOC for (b) 1QL, (c) 2QL and (d) 4QL, respectively. Fermi energy was set to be 0 eV.

Table 1. The QL number dependence on energy band gap ( $E_g$ ) of  $(\text{SiTe})_2(\text{Sb}_2\text{Te}_3)_x$  superlattices calculated with and without SOC. The results of  $\text{GeTe}/\text{Sb}_2\text{Te}_3$  superlattice are also shown in comparison.

$E_g$ (eV)		1QL	2QL	4QL
$\text{SiTe}/\text{Sb}_2\text{Te}_3$	without SOC	0.05	0.27	0.39
	with SOC	$\approx 0$	0.21	0.32
$\text{GeTe}/\text{Sb}_2\text{Te}_3$	with SOC	$\approx 0$	$\approx 0$	$\approx 0$

#### 4. CONCLUSION

In this study, we first reported the band structures of  $\text{SiTe}/\text{Sb}_2\text{Te}_3$  superlattices using *ab initio* computer simulation based on DFT. The band gap of the superlattices depended on the number of  $\text{Sb}_2\text{Te}_3$  layers. The superlattice of  $(\text{SiTe})_2(\text{Sb}_2\text{Te}_3)_1$  showed the gapless state at the  $\Gamma$  point. Therefore, it is suggested that the newly developed  $\text{SiTe}/\text{Sb}_2\text{Te}_3$  superlattice has a potential as a new Dirac semimetal.

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## Biographies

Yuta Saito was born in 1985 in Japan. He received his B.S. and M.S. degrees from Tohoku University, Japan, in 2008 and 2010, respectively. He received his Ph.D. degree from Tohoku University in 2013 and the title of his doctoral thesis was "Phase Change Behavior of Ge-Te-X (X: Si, Cu) Thin Films for Non-Volatile Memory". After he got his Ph.D. degree, he moved to National Institute of Advanced Industrial Science and Technology (AIST) in Japan as a postdoctoral researcher. His research topic includes the development of phase change superlattice and the first principle simulation.