Theoretical and experimental research for $SiTe/Sb_2Te_3$ phase change superlattice

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ABSTRACT

In this study, the fundamental properties of $SiTe/Sb_2Te_3$ superlattices were investigated theoretically and experimentally. In the theoretical study, *ab-initio* density functional theory (DFT) codes were used. Several $(SiTe)_2(Sb_2Te_3)_x$ superlattice models were designed with different numbers of the Sb_2Te_3 blocks and the corresponding band structures were calculated with and without spin-orbit coupling (SOC). It was found that the band gap of a $(SiTe)_2(Sb_2Te_3)_1$ superlattice closes only at the Γ point. This is the most basic feature of a Dirac semimetal. Based on the simulations, the $SiTe/Sb_2Te_3$ superlattices were experimentally fabricated on a Si substrate by RF magnetron sputtering at various deposition temperatures. The deposition temperature dependence of the crystal growth and crystallinity of the $SiTe/Sb_2Te_3$ superlattices were studied by x-ray diffraction (XRD) analysis and transmission electron microscopy (TEM).

Key words: Phase change superlattice, iPCM, Topological insulator

1. INTRODUCTION

Recently, interfacial phase-change memory (iPCM) was reported using $GeTe/Sb_2Te_3$ superlattice structure and showed superior performance such as extremely low power switching with a much faster switching speed compared with a PCM using the conventional $Ge_2Sb_2Te_5$ alloy film [1]. In iPCM, coherently aligned Ge atoms are reversibly switched between octahedral and tetrahedral states based on the umbrella flip model proposed by Kolobov et al. [2], resulting in a sufficient resistance difference. Furthermore, besides such the excellent properties as memory application, it was reported that iPCM showed magnetic properties, which is speculated to a relation to topological insulators [3]. Although iPCM has been attracting considerable attention as both electrical non-volatile memory and magnetic device, the material research has not yet been carried out sufficiently. In this work, we report several properties of $SiTe/Sb_2Te_3$ superlattices as an alternative candidate.

2. EXPERIMENTS

In order to investigate the structural stability and corresponding band structure, two kinds of *ab-initio* density functional theory (DFT) codes, called *CASTEP* and *WIEN2K*, were carried out. In both calculations, a generalized gradient approximation (GGA) of Perdew-Burke-Ernzerhof (PBE) was used. In *WIEN2K* calculation, spin-orbit coupling (SOC) was included to introduce the relativistic effects. $[(SiTe)_x/(Sb_2Te_3)_y]_z$ (x, y and z are integer) superlattice films were prepared by RF-magnetron sputtering on a Si single crystal using SiTe and Sb_2Te_3 alloy targets. The film thickness of each layer and the number of cycles were controlled by opening and closing the shutters in front of each sputtering target. The deposition temperatures were controlled by a heater equipped under the substrate station in the sputter chamber. X-ray diffraction (XRD) analyzes were carried out using Cu-Kα as an x-ray source to investigate the crystal orientation of the superlattice films. Transmission electron microscope (TEM) was used to observe the cross-sectional microstructure of the superlattice films.

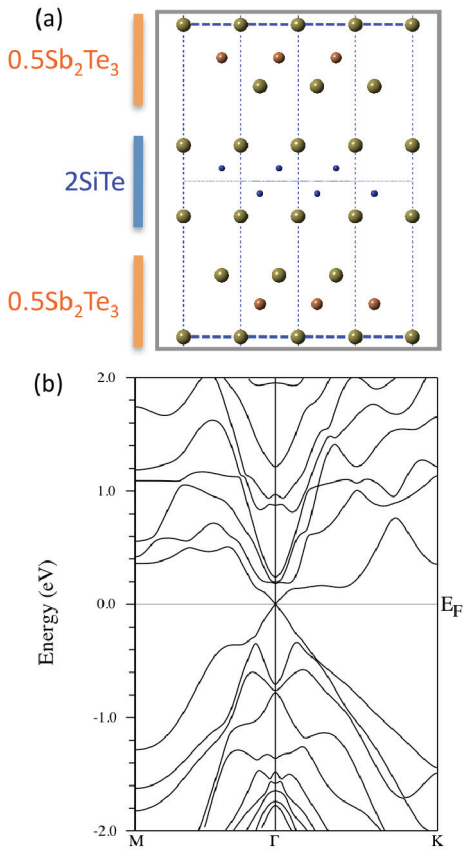

Fig. 1 (a) Structure of $(SiTe)_2(Sb_2Te_3)_1$ superlattice after structural stabilization. (b) Calculated band structure of $(SiTe)_2(Sb_2Te_3)_1$ superlattice.

3. RESULTS AND DISCUSSION

Fig. 1(a) shows the stabilized $(SiTe)_2(Sb_2Te_3)_1$ superlattice structure by *ab-initio* calculation. The structure has the same atomic layered structure as that of the $GeTe/Sb_2Te_3$ superlattice reported by Sa et al [4]. The calculated lattice constants are a = 0.4111 nm and c = 1.9447 nm, respectively, which are similar to that corresponding $GeTe/Sb_2Te_3$ superlattice (a = 0.4206 nm and c = 1.9357 nm). The bulk band structure including SOC in the $(SiTe)_2(Sb_2Te_3)_1$ superlattice is plotted in Fig. 1(b). It can be seen that the band gap closes only at the Γ point. This is the most basic feature of a Dirac semimetal.

Fig. 2 shows the XRD patterns of the $[(SiTe)_2(Sb_2Te_3)_1]_{20}$ superlattices deposited at 200, 250 and 280°C. XRD indicates that the $[(SiTe)_2(Sb_2Te_3)_1]_{20}$ film has highly oriented of to the 001 plane of Sb_2Te_3 normal to the substrate. The peaks, which are speculated to result in the superlattice structure, can be seen at the deposition temperature of above 250°C.

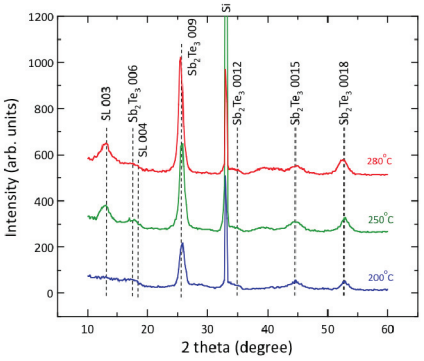

Fig. 2 XRD patterns of $(SiTe)_2(Sb_2Te_3)_1$ superlattice deposited at 200, 250 and 280°C.

A cross-sectional TEM image of a $[(SiTe)_2(Sb_2Te_3)_4]_8$ superlattice deposited at 250°C is shown in Fig. 3. The TEM also revealed that obtained superlattice film had a highly oriented structure characterized with the lattice fringes parallel to the Si substrate.

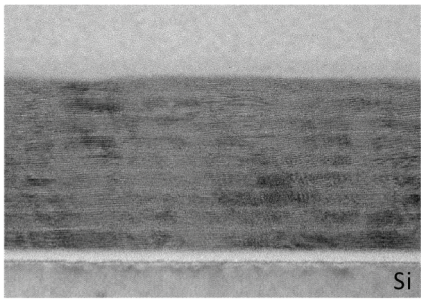

Fig. 3 Cross-sectional TEM image of $[(SiTe)_2(Sb_2Te_3)_4]_8$ superlattice deposited at 250°C.

4. CONCLUSION

We investigated the fundamental properties of $SiTe/Sb_2Te_3$ superlattices theoretically and experimentally. *Ab-initio* first principle calculation revealed that the $(SiTe)_2(Sb_2Te_3)_n$ (n: 1, 2, 4 and 6) structures could stably exist. The band structures of each superlattice structure were calculated with SOC. The $(SiTe)_2(Sb_2Te_3)_1$ superlattice showed a Dirac semimetal-like band structure. Based on the theoretical calculation, we successfully fabricated the $(SiTe)_2(Sb_2Te_3)_{1,4}$ film on a Si single crystal by RF-magnetron sputtering. The XRD and TEM indicated that the obtained superlattice films had highly oriented to the 001 plane of Sb_2Te_3 normal to the substrate.

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