# Computational Study on Interfacial Phase Change Memory by Topological Superlattices

H. Nakamura*[1,2], I. Rungger[3], A. Narayan[3], S. Sanvito[3], Y. Asai [1,2], and J. Tominaga[1,2]

[1] National Institute of Advanced Industrial Science and Technology (AIST), Umezono 1-1-1, Tsukuba, 305-8568, Japan

[2] CREST-JST, 7 Gobancho, Chiyoda-ku, Tokyo 102-0076, Japan

[3] School of Physics, MBER and CRANN, Trinity College, Dublin 2, Dublin, Ireland

e-mail: hs-nakamura@aist.go.jp

### ABSTRACT

We performed first principles simulation of interfacial phase change memory device, which consists of GeTe-$Sb_2Te_3$ superlattice (GTS) and W(111) electrodes. On the contrary of standard phase change memory, SET/REST switch is possible only by phase change of the interface GeTe layer, i.e., crystalline-crystalline transition.[1] To argue the high/low resistance states (HRS/LRS), we examined three model device structures, i.e., inverted-Petrov, Petrov, and Ferro-GeTe phase, respectively, and carried out first-principles nonequilibrium Green's function theory (NEGF)[2,3]. We present the mechanism of resistive switch and importance of spin-orbit interaction. In addition, we discuss application of 3D homologous topological insulator to functional device.

### INTRODUCTION

The phase change memory (PCM) is one of most promising nonvolatile information storage technologies. Recently, the GTS structure is proposed as PCM and is called interfacial PCM (iPCM). SET and RESET states are realized only by the flip-flop transition of Ge atoms in crystal phase. Furthermore, the $Sb_2Te_3$ is topological insulator, and it is blocked by GeTe normal insulator; thus it is expected that the topological states is found on each GeTe/$Sb_2Te_3$ interface in GTS[4] although GTS is embedded in the electrodes as the device cell. In the present study, we identify HRS/LRS states and topological property *in device cell* by calculating Green's functions. Then we discuss relation of device function and Dirac cone (and/or semi-metallic behavior) dispersion, which is feature of topological insulator.

### CALCULATION OF IPCM DEVICE PROPERTIES

We adopted the model device structure analyzed $W/(QL)_2(Ge_2Te_2)(QL)_2/W$, where QL represents the quintiple layer, i,e, $Sb_2Te_2$ unit. As possible GeTe structures, we took three phases, inverted-Petrov, Ferro-GeTe, and Petrov, namely, as shown in Figure 1. The Petrov phase is considered as HRS while the last two phases are candidates of LRS. In Figure 2, our first-principles calculations of *IV* are presented for the above three phases. As shown in Fig. 2, Petrov phase provides better agreement of the resistive ratio of HRS/LRS with the experiments than that of Ferro-GeTe phase. Spin-orbit effect is important to ON/OFF current ratio as shown in Figure 3. Since spin-orbit effect to IV characteristic is large only for HRS, we calculated quasiparticle spectra, which is defined as the pole of Green's function on the QL/GeTe interface, as a function of energy and momentum (*k* parallel to the interface). The result is presented in Figure 4, and Dirac semi-metallic dispersion is observed.

### CONCLUSION

Our simulation confirms that distinct resistive switch is possible by only GeTe layer phase change. Spin-orbit effect changes resistance of inverted Petrov phase largely, which relates to HRS; thus NEGF with spin-orbit coupling is required to evaluate SET/RESET resistance qualitatively. GTS of inverted-Petrov phase *in device cell* has characteristic quasiparticle dispersion at each interfacial 2D edge of topological material like Dirac semi-metal.

### REFERENCES

[1] R. E. Simpson et al., Nat. Nanotech. **6**, 501 (2011)
[2] H. Nakamura et al., Phys. Rev. B **78**, 235420 (2008)
[3] A. R. Rocha et.al, Phys. Rev. B **73**, 085414 (2006)
[4] B. Sa, et al., Phys. Rev. Lett. **109**, 096802 (2012)

ISBN 978-0-692-50554-0 

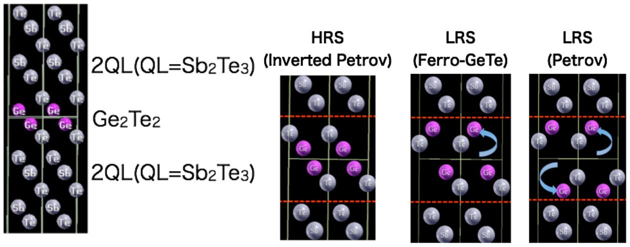


**Figure 1.** The models of GTS structures of the iPCM device. The left pannel is schematic view of GTS. The right panel consist of inverted-Petrov, Ferro-GeTe, and Petrov Phase, respectively. The thick grey, thin grey, and purple circles represent Sb, Te, and Ge atom, respectively. The device cell consists of W(111) electrode layers.

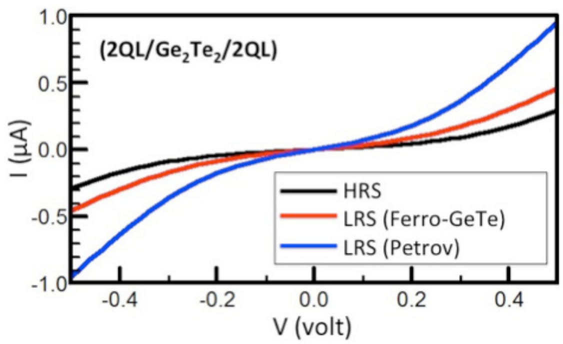


**Figure 2.** First principles *IV* characteristics of GTS iPCM device for the three GeTe phases. HRS is inverted-Petrov structure. Spin-orbit interactions are included in the transport calculations.

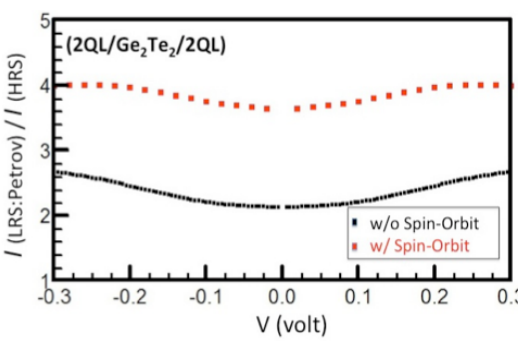


**Figure 3.** The plot of ON/OFF current as a function of bias voltage. On current is LRS of Petrov phase, and OFF current is obtained by HRS (inverted-Petrov). The red dot line is the result calculated by including spin-orbit interaction while the black dot line is obtained by omitting spin-orbit interaction.

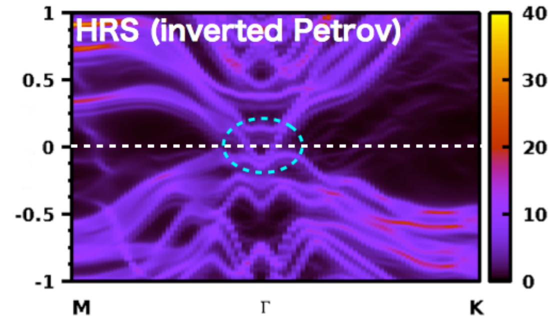


**Figure 4.** The contour plot of quasiparticle energy dispersion, which relates to the 2D band dispersion at $Sb_2Te_3$/GeTe interface of inverted-Petrov phase. The Fermi level of W electrode is set to zero. The right blue dot line circle is eye guide to figure out Dirac cone-like structure.