

Understanding resistive switching mechanism of interfacial phase change memory by topological superlattice and topological phase of interface states

H Nakamura

National Institute of Advanced Industrial Science and Technology (AIST), Japan

We performed first principles electric transport simulation of nano-scale interfacial phase change memory (iPCM) device, which consists of Ge, Sb and Te super-lattice (GST-SL) as resistive switching layer (RSL). GST-SL consists of the ordered layers of Sb₂Te₃ quintuple layers (QLs) and GeTe layers. Since phase change of iPCM is crystalline-crystalline transition, loss of enthalpy is quite small during SET/RESET processes. However, the High and Low Resistance State (HRS/LRS) is still under debates. To argue the HRS/LRS, we examined first-principles nonequilibrium Green's function theory (NEGF). In the present study, we adopted the device model of W/[(QL)_m(GeTe)_n]/(QL)₂//W, where (m,n) is (2,2) and /is set to 3 and 9 to check device-scale dependence of resistance. Though strong interlayer mixing is reported in some of recent studies, it is convinced that structural transition is within GeTe layer for iPCM when m and n is sufficiently small. We took three phases, inverted-Petrov, Ferro-GeTe, and Petrov, respectively, as shown in Figure 1. By analyzing calculated IV characteristics, we found that spin-orbit interaction is important to the ratio of high and low resistances in low bias regime, in particular, if resistive switch is triggered by field-driven bipolar mode.

It is also known that GST-SL is 3D strong topological insulator (TI). Furthermore, GST-SL is multilayer of TI (=QL) and normal insulator (=GeTe) layers: thus the 2D interface state confined in the RSL can be also topologically non-trivial. We construct simple effective Hamiltonian and calculates topological phase diagram of RSL as shown in Fig. 2. Comparing with our first-principles data, we discuss an alternative new device function using topological phase transition, not structure transition.

Figure 1. The detail structures of GST-SL of each structural phase.



Figure 2. The phase diagram of the topological phase of 3D TI/NI multilayer model as a functions of the scaled transfer integral between the nearest neighboring TI and NI layers.



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