Switching mechanism in GeSbTe phase change memory superlattices

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Abstract
The switching process in GeSbTe superlattice phase change memory is modeled as a vertical displacement of a Ge atomic layer plus a lateral shift of this layer.

1. Introduction
Phase change materials based on Ge, Sb and Te (GST) are candidates for non-volatile random-access memories due to scalability, endurance, retention and fast switching speed [1]. Recently, a low power variant the ‘interfacial phase change memory’ (iPCM) or ‘chalcogenide superlattice’ (CSL) was proposed [2,3]. The CSLs consist of hexagonal (GeTe)_n(Sb_2Te_3)_m layer units along a (111) direction of the original cubic cell. The transition is now between two crystalline structures, and constrains switching to 1D instead of 3D, to consume less energy [3].

Despite various experimental demonstrations of CSL memory [3-7], the mechanism is not fully agreed at an atomic level, for the low resistance state (LRS) and high resistance states (HRS) between two groups. Two models were proposed, based on high-resolution electron microscope images. In model 1, the transition is from a ‘Ferro’ LRS to an ‘Inverted-Petrov’ structure HRS [4,5]. In model 2, the transition is from a ‘Petrov’ LRS to an ‘Inverted-Petrov’ HRS [6-9]. As the external electrical field is applied normal to the layers, both models have focused on the vertical movement of Ge atoms through a Te atom layer. However, considering the atomic structures of the stable phases, a second additional lateral movement is also required which is calculated here.

2. Method
We perform simulations using the plane wave, density function theory CASTEP code using the generalized gradient approximation (GGA) with a van der Waals correction using the Grimme scheme [10]. For the energy barrier calculation, we use the transition state search algorithm.

3. Results and Discussion
The simplest CSL supercell consists of hexagonal (GeTe)_n(Sb_2Te_3)_m units (n=2, m=1). This unit can adopt four different basic structures in which the primary bonds in different layers are aligned (Fig. 1); the Kooi (K), the Ferro (F), the Petrov (P) and the Inverted Petrov (IP), according to the ordering of the Ge, Sb and Te layers. The stability of these four structures depends on temperature, which we calculated from the phonon spectrum. The Kooi structure has the lowest enthalpy at 0 K [4]. However, this phase is unfavorable for switching. Raising the temperature by 200 K increases the enthalpy of the Kooi, and the Ferro becomes the more stable phase.

Now, a simple vertical displacement of Ge planes from the Ferro state or Petrov state does not give the basic Inverted-Petrov state, but a variant of it. We thus consider related F, P, and IP stackings with different intra-layer order. Using IP as an example, there are three different structures, IP_0, the original IP structure, plus IP_1 and IP_2. Similar, from F_0 we can generate F_1, F_2 and F_3, and from P_0 we can generate P_1 and P_2.

The variant structures are fully relaxed at 0 K and the total energies calculated. The F_0 is set to 0 eV, as reference. The four (original) structures with the aligned bonds have the lower total energy than the new structures.

We now consider the full switching transition for both model 1 and model 2. The IP_0 structure is the HRS for both models, and the LRS is either F_0 or P_0, with reached through vertical atomic displacement. The completed SET and RESET cycle for each model is, Fig. 3(a,b).

Model 1:
RESET: F_0 → IP_1 → IP_0  SET: IP_0 → F_2 → F_0

Model 2:
RESET: P_0 → IP_2 → IP_0; SET: IP_0 → P_2 → P_0

Note that lateral motion occurs for both SET and REST.

We calculate the energy barriers for each case. As the vertical flip has the Ge and Te layers cross each other, the highest energy point on the transition is where the Ge and Te atoms are in the same layer. In this case, the distance between atoms is lowest and the energy barrier is high, between 2.58 eV and 3.10 eV, Fig 3(c).

The lateral movement is more complicated than the vertical one. The Ge and Te atoms in their sublayers can exchange positions with their nearest bonded atoms by lateral motion. A typical sublayer viewed from [001] direction is plotted in Fig. 4(a). The primitive cell was expanded to a 2×2 supercell along x and y directions. In the initial structure, the Ge atoms are on site A while Te atoms are on site B. After the movement, the Ge atoms move to site B and Te atoms are on site A.

There are two possibilities. First, an atom can roll over the top of an adjacent atom, which compresses the surrounding Sb_2Te_3 and GeTe layers and only one bond is conserved, Fig 4(b). Or, the atoms move in plane, an atom breaks one bond, but conserves two other bonds, in a snake-like motion. Once reaching the next low energy site, the atom rebonds with its new neighbor. As two bonds per atom are conserved in choice 2, this motion has a lower energy barrier of ~0.44 eV, ~0.5 eV less than the 0.92 eV for the overhead rolling motion. The overall energy barrier for the whole transition varies from 2.56eV to 3.10eV,
which is close to the experiment value of 2.3 eV [6]. As the vertical flip motion has the larger energy barrier, this will dominate the switching process. In model 1, only one GeTe sublayer is involved in the lateral movement. However, for model 2, both two GeTe sublayers must move. Interestingly, the energy barrier is similar in both cases. We also found the barrier for lateral motion of Ge vacancies to be 0.44 eV. Thus, lateral motion may occur by snake-like motion of GeTe sublayers, or Ge vacancy diffusion.

In summary, the switching transition in CSL materials occurs as a 2-step process, a vertical flip of Ge sublayers through Te sublayers driven by the applied field, followed by a low energy lateral motion of the GeTe sublayers back to their more stable configurations. The energy barrier for the vertical atomic flip of Ge layers is 2.56 to 3.1 eV, followed by a lateral snake-like motion of GeTe sublayers with barriers of 0.44 eV.

The authors thank K Shiraishi and J Tominaga for discussions and to EC project Pastry colleagues for support.