Extended Abstracts of the 2016 International Conference on Solid State Devices and Materials, Tsukuba, 2016, pp725-726

PS-4-02

Modified Switching Mechanism for GeSbTe based Chalcogenide Superlattice Phase Change Memories

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Abstract

A modified switching process for GeSbTe superlattice phase-change memories is developed that allows chemically disordered layers and produces a band gap.

1. Introduction

GeSbTe-based phase change materials have been the basis of non-volatile phase-change random access memories (PRAM). GeSbTe-based superlattices were developed to try to lower the switching energy of these devices [1]. Efforts focused on the shortest periodicity superlattices. Their atomic structures were believed to be one of four canonical forms, as shown in Fig. 1. There were two proposals for switching based on high resolution TEM images. The first by Tominaga et al [2,3] was that switching was between a Ferro low resistance state (LRS) and an Inverted-Petrov high resistance state (HRS). The second, by Takaura et al [4], was that switching occurred between a LRS Petrov structure and am Inverted-Petrov HRS state. The actual atomic mechanism would need to involve a flipping of one or two GeTe atomic planes followed by lateral motion [5]. This mechanism gave activation energies near the experimental value.

However, subsequent high resolution STEM and EXAFS data [6,7] found the atomic structures to be less ordered than in Fig. 1. Momand [6] found that the originally chemically pure layers were in fact disordered and the GeSbTe blocks could vary in height and tended to have SbTe layers facing the van der Waals bonding gap.

Here we show how the block heights can vary by a stacking fault mechanism. We also consider chemical disorder. But the final problem is that HRS states do not have a band gap to be HRS.

2. Method

We perform simulations using the density function CASTEP code using the generalized gradient approximation (GGA) with van der Waals correction using the Grimme scheme.

3. Results and Discussion

The simplest CSL supercell consists of hexagonal $(GeTe)_2(Sb_2Te_3)$ 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.

Fig 2 shows a SbTe bilayer stacking fault varying the height of the GeSbTe blocks. The stacking fault moves from the lower to the upper block in the central area by means of a Te or Sb vacancy passing along the line.

Fig. 3(a) shows some chemically disordered GeSbTe blocks which simulate the observed structures. Disordering slightly lowers the total energy, Fig 3(b). The problem is that disordering removes the ability to two metastable states to switch between. TeSbTe blocks have a center of symmetry so no Peierls distortion. Thus, we must re-introduce some GeTe clusters to give this distortion, Fig 4(a). A cluster size of 3x3 is found to be the minimum, Fig 4(b).

Finally, all the four structures of Fig 1 have little band gap. Takaura [5] noted that the best switching material tended a have a Ge deficit. Shiraishi [8] proposed that the Ge_xTe layer became disordered and could then have a band gap. We propose a very simplified model in which the GeTe block is $GeTe_2$, so that the Ge sites become 4-fold sp^3, Fig 5(a). These then have a band gap, Fig 5(b). We made a supercell in which the SbTe blocks are hexagonal and square GeTe blocks are aligned together.

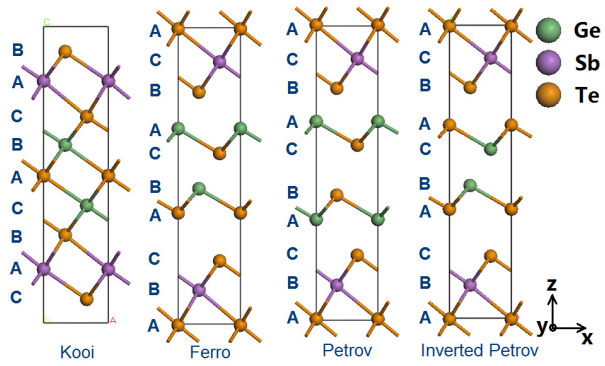

Fig 1. The four lowest energy configurations for the $(GeTe)_2$, (Sb_2Te_3) superlattice.

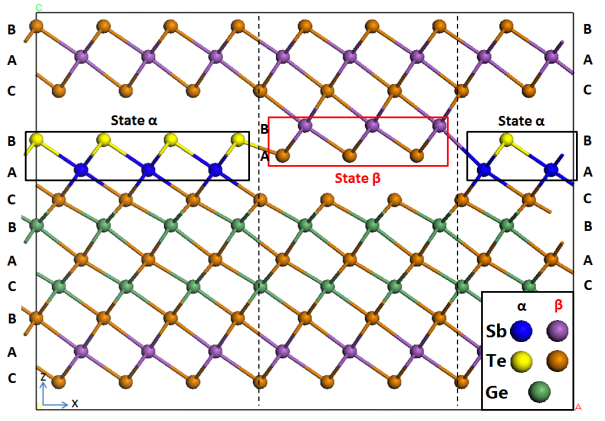

Fig 2. Two bonding blocks with SbTe bilayer stacking fault passing between them, allowing hieght variation.

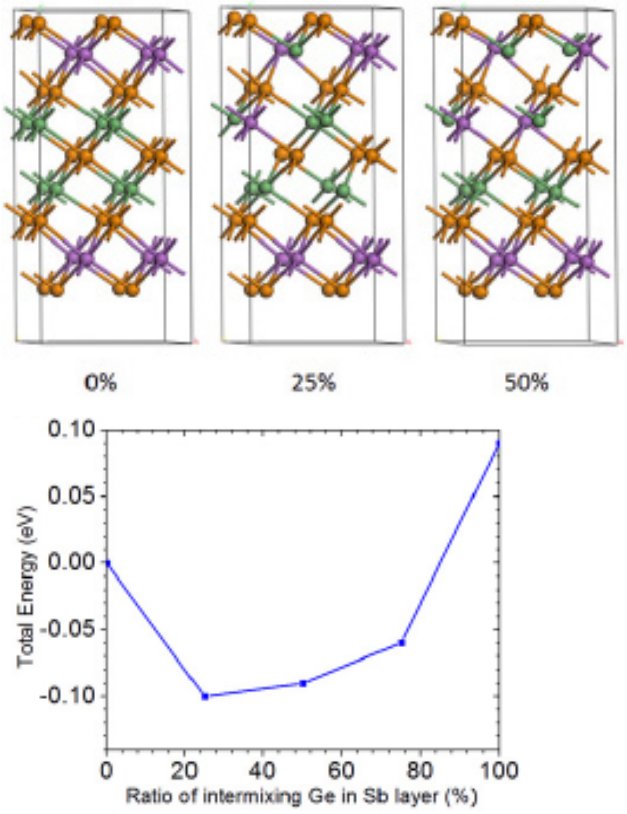

Fig. 3(a,b) Mixed CSL layers, showing smaller lowering of total energy.

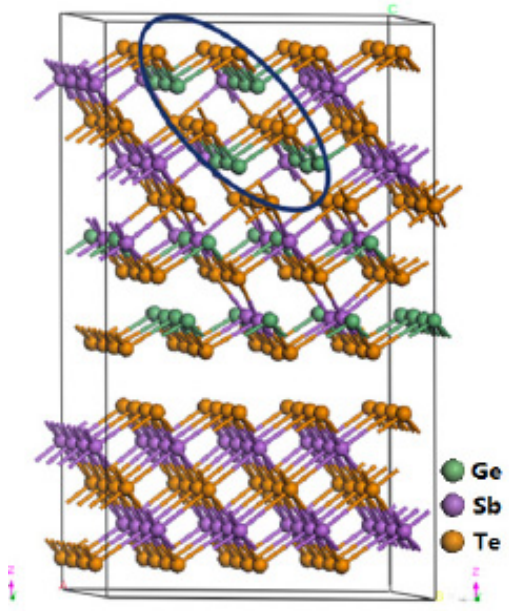

Fig. 4(a) Showing GeTe clusters that then allow the formation of metastable Peierls distorted states. Note that when a local Peierls distortion occurs, there is a bond on only one side of the Ge atom.

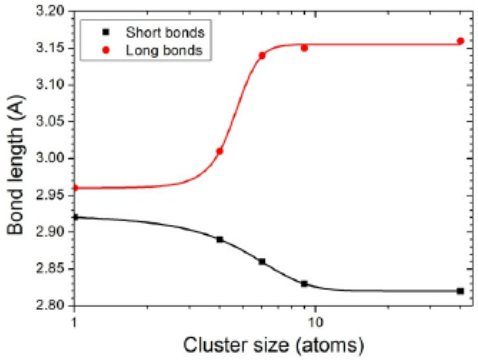

Fig 4(b). Showing the short and long bond lengths of Peierls distorted states as function of cluster size, and minimum cluster size.

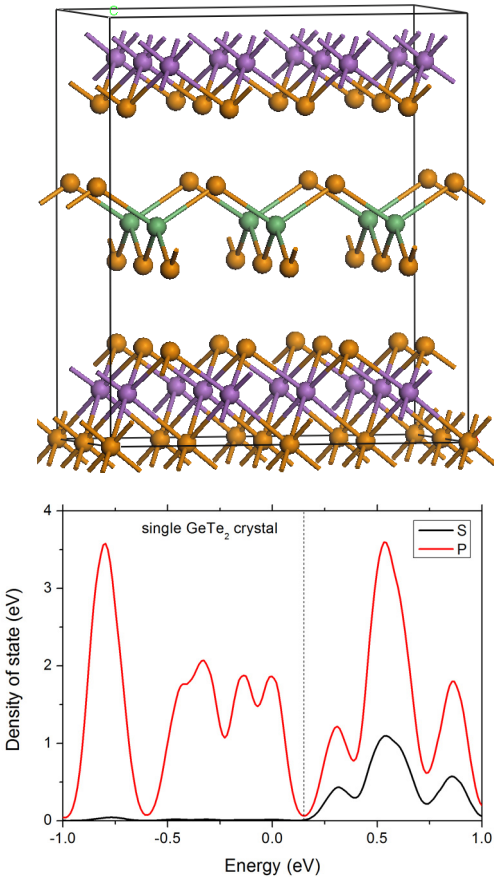

Fig. 5. Formation of hypothetical ordered $GeTe_2$ sulayer with sp3 Ge sites, giving a band gap for the HRS.

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

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