Carrier Injection Induced Switching of Supper-lattice GeTe/Sb$_2$Te$_3$ Phase Change Memories

S. Kato$^1$, M. Araidaii$^1$, K. Kamiya$^1$, T. Yamamoto$^1$, T. Ohyanagi$^2$, N. Takaura$^2$ and K. Shiraishi$^1$

$^1$ Univ. of Tsukuba, Graduate School of Pure and Applied Sciences
1-1-1, Tennodai, Tsukuba, Ibaraki 305-8571, Japan
Phone: +81-29-853-5600-8233 E-mail: kato@comas.frs.tsukuba.ac.jp
$^2$ Low-power Electronics Association & Project
Onagawa, Tsukuba, Ibaraki 305-8569, Japan

Abstract

We propose a new on-off switching mechanism for super-lattice GeTe/Sb$_2$Te$_3$ phase change memories (PCM) from the atomistic level. Relative energy stability between high resistivity state (HRS) and low resistivity state (LRS) can be controlled by injecting carrier into super-lattice GeTe/Sb$_2$Te$_3$ PCM, which drastically accelerates the structural change between HRS and LRS and is also suitable for high program/erase (P/E) cycles endurance.

1. Introduction

Super-lattice GeTe/Sb$_2$Te$_3$ PCM (Fig. 1) is intensively studied as a next generation non-volatile memory. It is theoretically reported that Ge coordination-number change between 4-fold and 6-fold caused by Ge short range displacement induces phase change between HRS and LRS [1]. It is also reported that Ge coordination-number change was driven by carrier injection (Fig. 2) [2]. According to this mechanism, super-lattice GeTe/Sb$_2$Te$_3$ expects to switch at lower power than conventional alloy GeSbTe (GST). However, the phase change mechanism of Ge displacement in super-lattice GeTe/Sb$_2$Te$_3$ has not been understood in detail. It is essential to clarify phase change mechanism at atomistic level in real memory structures. In this study, we theoretically investigate the atomistic origin of on-off switching mechanism of super-lattice GeTe/Sb$_2$Te$_3$ PCM by ab-inito calculations. We found that carrier injection by the applied voltage is essential for the on-off switching of the super-lattice GeTe/Sb$_2$Te$_3$ PCM (Fig. 3). Moreover, we found that carrier injection into super-lattice GeTe/Sb$_2$Te$_3$ PCM essentially attacked only Ge atoms and short range displacement of a small number of Ge atoms is sufficient to cause structural change between HRS and LRS. This strongly suggests that PCM with carrier injection induced on-off switching is likely to have high P/E cycles endurance.

2. Calculation Model and Method

We prepared hexagonal super-lattice GeTe/Sb$_2$Te$_3$ with [111] direction as they show Fig. 1. GeTe layers ordering Te-Ge-Ge-Te and Ge-Te-Ge correspond to HRS and LRS, respectively [1]

We calculated atomic and electronic structures based on density functional theory with Vienna Ab-initio Simulation Package [3]. In addition, we calculated steady electron currents based on non-equilibrium Green’s function method with Atomistix Tool Kid [4] (Fig. 4).

3. Result and Discussion

I-V characteristics of Super-lattice GeTe/Sb$_2$Te$_3$

We first investigated I-V characteristics of HRS and LRS with first principles calculation. Our calculation shows that HRS has 10 times higher resistance than LRS (Fig. 6 (a)). Actually, experimentally observed I-V characteristic reveals 100 times resistance ratio between HRS and LRS [3] (Fig. 6 (b)). The resistance difference is caused by local-DOS in GeTe layers (Fig. 7 (a)). Conduction channels of HRS GeTe layers are significantly disrupted (Fig. 7 (b)).

Carrier Injection Effect to Super-lattice GeTe/Sb$_2$Te$_3$ PCM

We investigated structural change between HRS and LRS caused by charge injection into super-lattice GeTe/Sb$_2$Te$_3$ PCM (Fig. 8). Our calculation clearly shows that electron injection stabilizes 4-fold HRS structures. Whereas, 6-fold LRS structures are preferable after hole injection. These structural changes between 4-fold and 6-fold Ge structures govern the on-off switching of super-lattice GeTe/Sb$_2$Te$_3$ PCM. These results originate from the intrinsic properties of bulk Ge itself. Electron removal causes structural transition from a well-known 4-fold diamond structure to a 6-fold cubic structure (Fig. 2). This result shows that only 3% removal of electron causes change of Ge coordination number, resulting in the metallization of Ge. Actually, electron number of LRS around Ge is 2% lower than that of HRS. Thus, we can conclude that super-lattice GeTe/Sb$_2$Te$_3$ on-off switching is governed by the intrinsic properties of Ge which has both metallic and semiconducting characteristics.

Electronic states of Ge atoms play an important role in super-lattice GeTe/Sb$_2$Te$_3$ PCM. Figure. 9 shows charge density change from neutral state to carrier injecting state. Hole injection into HRS weakens Ge-Ge bonds in GeTe layers by decreasing bond charge. Whereas, electron injection into LRS tends to increase Ge-Te bond charge, leading to strengthen Ge-Te bonds. These results show the detailed electronic feature that electron or hole injection accelerates phase change of super-lattice GeTe/Sb$_2$Te$_3$ PCM.

Moreover, carrier injection induced switching of PCM leads to a promising property of super-lattice GeTe/Sb$_2$Te$_3$ PCM as follows. The conventional switching mechanism of structural change between crystal and amorphous by thermal heating is irreversible since large number of atoms movement in GST is inevitable (Fig. 10 (a)), which is unsuitable for high P/E cycles endurance. However, the situation is quite different in carrier injection mechanism. Carrier injection into super-lattice GeTe/Sb$_2$Te$_3$ PCM induces only short range displacement of small number of Ge atoms (Fig. 10 (b)). This property causes reversible structural change between HRS and LRS, naturally leading to the high P/E cycles endurance.

4. Summary

We found that electron injection and removal accelerated phase change of super-lattice GeTe/Sb$_2$Te$_3$. GeTe layer contributes to resistance of HRS and LRS. These phase change mechanism of super-lattice GeTe/Sb$_2$Te$_3$ takes advantage of high P/E endurance.
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References

Fig. 1 Atomic structure of super-lattice GeTe/Sb$_2$Te$_3$. (a) HRS. (b) LRS.

Fig. 2 Energy diagram of structural transition induced by electron removal from intrinsic valence charge for bulk Ge.

Fig. 3 Schematic illustration of on-off switching mechanism for super-lattice GeTe/Sb$_2$Te$_3$ by carrier injection. Electron and hole injection induces Ge short range displacement and Ge coordination number change between 4-fold and 6-fold.

Fig. 4 First principles calculation method of electron conduction. Steady electric currents can be calculated selfconsistent.

Fig. 5 Obtained I-V characteristics. (a) First principles calculation. (b) Experimental observation normalized to two GeTe layers.

Fig. 6 Obtained density of states (DOS). (a) Local DOS of GeTe layers. (b) Schematic illustration of difference in conduction channels between HRS and LRS.

Fig. 7 Obtained density of states (DOS). (a) Local DOS of GeTe layers. (b) Schematic illustration of difference in conduction channels between HRS and LRS.

Fig. 8 Energy diagram of carriers injection into super-lattice GeTe/Sb$_2$Te$_3$. Electron injection stabilizes HRS and hole injection stabilizes LRS.

Fig. 9 Iso-surfaces of charge density change from intrinsic state to carriers injecting state. (a) Hole injection into HRS. (b) Charge injection into LRS.

Fig. 10 Schematic illustrations of PCM on-off switching. (a) Conventional GST PCM switching is irreversible structural change by thermal heating. (b) Super-lattice GeTe/Sb$_2$Te$_3$ PCM switching is reversible structural change by carrier injection into Ge atoms, which induces short range displacement of small number of Ge atoms.