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Physics in Charge Injection Induced On-Off Switching Mechanism of Oxide-Based Resistive Random Access Memory (ReRAM) and Superlattice $GeTe/Sb_2Te_3$ Phase Change Memory (PCM)

K. Shiraishi[*1,2], M.Y. Yang[1], S.Kato[1], M. Araidai[3], K. Kamiya[1], T. Yamamoto[1], T. Ohyanagi[4], N. Takaura[4], M. Niwa[5], B. Magyari-Kope[6], and Y. Nishi[6]

[1]Graduate School of Pure and Applied Science, Univ. of Tsukuba, 305-8571, Japan, [2]Graduate School of Engineering, Nagoya Univ., Furo-cho, Chikusa, Nagoya, 464-8603, Japan, [3]Center for Computational Sciences, Univ. of Tsukuba, Tsukuba, 305-8577, Japan, [4]Low-power Electronics Association & Project, Onogawa, Tsukuba, 305-8569, Japan, [5]Center for Innovative Integrated Electronic Systems, Tohoku Univ. Aoba, Sendai, 980-8579, Japan, [6]Department of Electrical Engineering, Stanford University, Stanford, CA 94305, USA
Phone&FAX: +81-52-789-3715, E-mail: shiraishi@cse.nagoya-u.ac.jp

Abstract

We propose a new on-off switching mechanism for oxide based resistive random access memory (ReRAM) and superlattice $GeTe/Sb_2Te_3$ (GST) 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 carriers into oxide-based ReRAM and superlattice GST-PCM. This charge injection mechanism drastically accelerates the structural change between HRS and LRS and is also suitable for high program/erase (P/E) cycles endurance.

1. Introduction

In recent years, emerging non-volatile memories such as resistive random access memory (ReRAM), phase change memory (PCM) attracted significant attention as next generation non-volatile memories. However, the physical understandings of ON-OFF switching mechanism of such emerging memories are still insufficient especially from atomistic and electronic viewpoint.

In case of ReRAM, it is well-known that the formation and disruption of O vacancy filament is relevant to ON-OFF switching [1] (Fig.1). In case of superlattice $GeTe/Sb_2Te_3$ (GST) PCM, on the other hand, it has been proposed that displacement of Ge atom in GST is the crucial mechanism for resistive switching [2] (Fig.2). However, the triggers of the above structural changes have not been clarified yet.

In this paper, we perform quantum mechanical discussions on ON-OFF switching mechanism of oxide-based ReRAM and superlattice GST-PCM by using ab initio calculations. We have found that charge injection/removal can play crucial roles on structural change from high-resistivity-state (HRS) to low-resistivity-state (LRS) for both ReRAM [3-6] and superlattice GST-PCM [7,8].

2. Calculation Method and Calculation Models

Calculation method

We calculated atomic and electronic structures based on density functional theory including LDA+U with Vienna Ab-initio Simulation Package [9].

Calculation models

In oxide-based ReRAM calculations, atomistic structures of the ON (LRS) and OFF (HRS) states in ReRAMs are constructed by introducing V_O into rutile TiO_2, cubic HfO_2, and α-state Al_2O_3 (Fig.3) [3,4]. In case of superlattice GST-PCM, we prepare hexagonal structures of $GeTe/Sb_2Te_3$ (Fig. 4). This model consists of hexagonal Sb_2Te_3 layers and cubic structure GeTe layers with [111] direction. GeTe layers ordering Te-Ge-Ge-Te and Ge-Te-Te-Ge correspond to HRS and LRS, respectively [7].

3. Result and Discussion

First, we discuss the charge injection effects into oxide based ReRAM. As shown in Fig. 5, the most stable charged state of isolated V_O is doubly positive in almost all range of Fermi level in TiO_2, HfO_2 and Al_2O_3. Moreover, isolated V_O is structurally more favorable than filament states when V_O is doubly positive. After injecting electrons, however, the situation changes drastically. As described in Fig. 6, filament structure becomes more favorable when V_O becomes singly positive and neutral after electron injection. This drastic structural change upon electron injection is schematically described in Fig. 7. The existence of electrons enables the formation of bonding states between V_Os, which promotes the filament formation. As a result, carrier injection/removal induces cohesion-isolation phase transition in oxide based ReRAM, which results in the ON-OFF switching and improve P/E cycles endurance [3-6].

Next, we investigate the carrier injection effects for superlattice GST-PCM. We have found structural change between HRS and LRS caused by charge injection into superlattice GST-PCM (Fig. 8). Our calculation clearly shows that electron injection stabilizes 4-fold HRS structure. Whereas, 6-fold LRS structure becomes preferable after hole injection. These structural changes between 4-fold and 6-fold Ge structure govern the operation of superlattice GST-PCM. Thus, it is also concluded that carrier injection/removal surely causes structural transition between LRS and HRS in superlattice GST-PCM as well as oxide based ReRAM [7,8]. Moreover, following conclusion should be derived. Since carrier injection effects mainly govern the PCM operation instead of the conventional phase transition triggered by thermal effects, superlattice GST-PCM should have high P/E endurance. This is because structural changes triggered by electrons are essentially more reversible than those triggered by thermal effects [7,8].

Carrier injection/removal effect for oxide-based ReRAM and superlattice GST-PCM are schematically summarized in Fig. 9. Carrier injection/removal generally changes the relative stability between HRS and LRS, by changing atomistic and electronic structures of memory devices themselves.

4. Summary

We found that carrier injection/removal induces structural change between HRS and LRS of oxide based ReRAM and superlattice $GeTe/Sb_2Te_3$ PCM. In general, carrier injection essentially plays crucial roles on device operation through inducing atomistic and electronic structure changes of memory devices.

Acknowledgements

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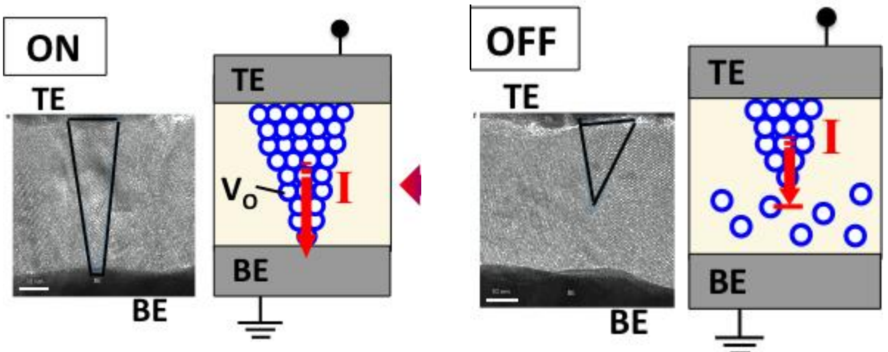

Fig. 1: ON-OFF switching of oxide based ReRAM. O vacancy filament is surly formed in case of ON state by TEM analysis. However, it is disrupted in case of OFF states. [Ref.1]

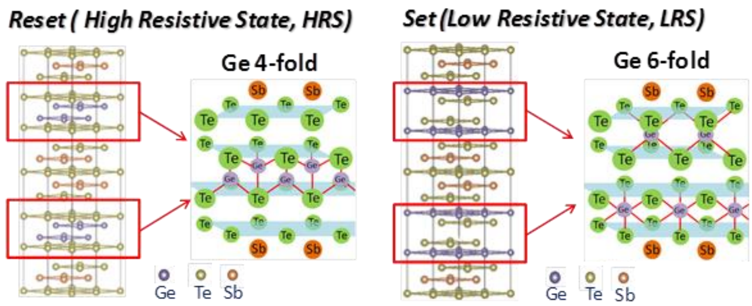

Fig.2: Schematic illustration of on-off switching mechanism for superlattice GeTe/Sb_2Te_3 PCM. Ge short range displacement and Ge coordination number change between 4-fold and 6-fold induce ON-OFF switching between HRS and LRS. [Ref. 7]

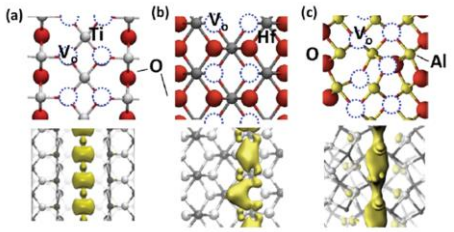

Fig.3: Model structures and partial charge density for V_O-chain in (a) TiO_2, (b) HfO_2, and (c) Al_2O_3. Conduction paths are formed in all of three oxides [Ref. 4]

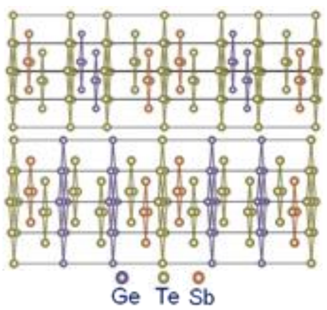

Fig. 4: Atomic structure of superlattice GeTe/Sb_2Te_3. (upper) HRS. (lower) LRS. [Ref. 8]

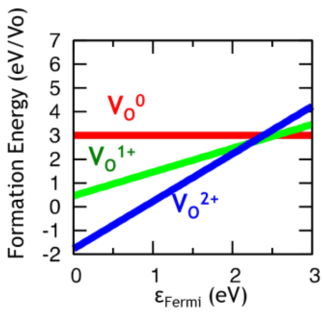

Fig.5: Formation energy diagram for an isolated V_O. Doubly positive V_O^{2+} is the most stable charge state [Ref. 3].

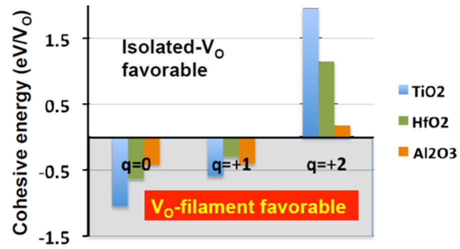

Fig.6: Cohesive energies of TiO_2, HfO_2, and Al_2O_3. All of three materials likely form V_O-filament in q=0 and q=+1 charge states after electron injection.

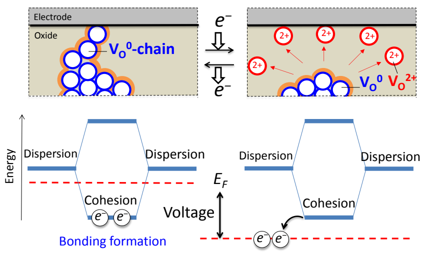

Fig.7: Schematic picture of the formation of bonding and anti-bonding levels in the V_O-filament. The bonding states are occupied after electron injection, leading to the large amount of electron energy gain. This promotes the V_O-filament formation.

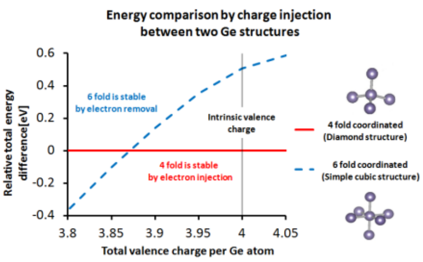

Fig. 8: Energy diagram of structural transition induced by electron injection from LRS (6-fold) to HRS (4-fold) for bulk Ge. Electron (hole) injection stabilizes HRS (LRS) in superlattice GST-PCM. [Ref. 7]

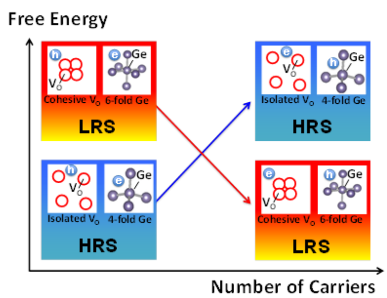

Fig. 9: Schematic illustration of structural transition in ReRAM and PCM induced by relative stability change between LRS and HRS by electron (hole) injection/removal. This change can be controlled by applying voltage.