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Possibility of MONOS Type Memory for Long Lifespan Archive Memory

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1. Introduction

There is an increased demand for digital technology in archival storage infrastructure. For example, Motion picture industry, Library of Congress, Healthcare industry and the others have been archiving their contents as a digital data since late years. Nowadays, digital contents increase at the ratio of 50% per year, and its data size is estimated to become 72ZByte ($Z=10^{21}$) by 2020 year [1]. However, digital data has a serious issue of lifespan as storage devices. Typical lifespan of storage devices is only about 20 years, but it is required longer than 50 to 100 years [2] in terms of reliability of long-term access to digital contents. Therefore, a long lifespan archive memory with high-density integration is inevitable.

In this study, we discuss the possibly of the MONOS (Metal-Oxide-Nitride-Oxide-Semiconductor) type charge trap memory with high density integration for a long lifespan archive memory, on the basis of *ab initio* calculations. It is known that such memories show two types of structural changes in general as shown in Fig. 1 [3]; (a) reversible structural change and (b) irreversible and large structural change. The reversible structural change is suitable for the devices with high Program/Erase (P/E) cycles endurance (Fig. 1(a)). On the other hand, the irreversible structural one is suitable for a long lifespan archive memory (Fig. 1(b)), because it prevents the programmed state changing to the initial state. Moreover, a long lifespan archive memory is essentially read-only-memory (ROM), which does not require the high Program/Erase (P/E) cycles endurance. In this sense, the guiding principles for a long lifespan ROM is much different from the well-known memories such as flash memories and charge trap memories which require high P/E cycles endurance. We focus our attention on this point, and our present calculations clearly show that MONOS-type memories with O related defects reveal large and irreversible structural change upon carrier injection, indicating that MONOS is one of the most promising future high density archive memories.

2. Methods and Models

Total-energy electronic-structure calculations were performed on the basis of density-functional theory (DFT) with Perdew–Burke-Enzerhof generalized gradient approximation implemented in the ultra-soft pseudo-potential codes of Tokyo Ab-initio Program Package (TAPP) [4,5]. The cutoff energy of the plane-wave basis set was 36 Ry. The number of irreducible k-point samplings in the Brillouin zone was two. We found that the calculation error was less than 0.03 eV for typical relaxation energies. We used the constraint-minimization method [6] and force-inversion method [7] to estimate activation barrier of structural changes.

In MONOS type memories, it has been reported that many O atoms are incorporated and electron occupied defects are confirmed near SiO_2/SiN interfaces (Fig.2) [8]. We prepared 84-atoms super cell of β-Si_3N_4 (Fig.3(a)). To describe the O related defect in SiN layer near SiN/SiO_2 interfaces, we substitute two N atoms for two O atoms as shown in Fig.3(b), considering the experimental finding of O incorporation. Figure 4 shows the calculation procedures of P/E operation.

3. Atomistic Characteristics of MONOS type Memory

First, we mention the important atomistic characteristics of MONOS type memories. It has been reported that MONOS type memory has also two types of structural changes (reversible and irreversible structural changes) during P/E cycles as discussed in the introduction (Fig. 1) [3]. One is related to N vacancy defects in Silicon Nitride. Most stable structure of one-N-vacancy-model with neutral charged state has an isosceles triangle structure formed by three Si atoms as shown Fig.5. This asymmetric structure originates from the Jahn-Teller effect, in which a symmetry breaking structural transformation stabilizes the electron energy by splitting degenerate energy levels. This structural change is reversible which takes a system back to the original structure after the P/E operation (Fig.1(a)), since this structural change is Jahn-Teller type symmetry breaking changes without rearrangement of the covalent bond networks. Thus, N vacancy defects has high P/E endurance. However, it is not suitable for a long lifespan archive memory since it is not accompanied with large structural change. The other one is related to excess O defects in SiN layers. Fig.6(a) shows the most stable structure (initial) in which two O atoms substitute two N atoms in SiN layers. As shown, all O and Si atoms are two-fold-coordinated and four-fold-coordinated, respectively. Also, Fig.6(b) is shown meta-stable-I structure. After carrier-injection (programmed), large structural change occurs as shown in Fig.6(c). All O atoms become three-fold-coordinated by forming strong Si-O bond. It is noted that, the programmed structure does not change back to initial or meta-stable-I structures even after erase operation (carrier removal). As shown in Fig. 6(d), the obtained structure after P/E operation is much different from initial and meta-stable-II structures, but it is similar to the programmed structure. This indicates that two O substituted defects reveal irreversible structural changes by carrier injection with a large rearrangement of the bond-networks. As discuss above, O related defects are suitable for a long lifespan archive memory, indicating the possibility of MONOS-type memory for future high density archive memories.

4. Potential of MONOS for Archive Memoreis

Now, we estimated the lifespan by calculating energy surface of two O substitution model during P/E cycle. We calculated energy barrier of structural change between initial and programmed structures with neutral charged state (Fig.7). We found that there are two metastable states along such structural change. The lowest energy barrier is seen between meta-stable-I and meta-stable-II (1.9 eV). Therefore, we can estimate a minimum lifespan of MONOS type memories with neutral charged state by using 1.9 eV energy barrier based on Arrhenius framework with $Y = 1/\nu \cdot exp(-\Delta E/k\mathrm{T})$, where Y, ν, ΔE, k, T, a correspond the lifespan, phonon frequency, Energy barrier, Boltzmann constant and temperature, respectively. We used $\nu = 1.6 \cdot 10^{14}$ Hz which is the Debye frequencies of β-Si_3N_4 [9]. In Fig.9, we show the estimated lifespan as a function of T. As shown, the lifespan of two O substitution defects is at least 1000 years at 100°C. On the other hand, we could obtain only one stable structure (Fig. 6(c)) with hole-trapping-state, indicating that this structure is very stable. Thus, hole-trapping-state is expected to have a long lifespan.

5. Conclusions

We investigated the possibility of MONOS type memories for a long lifespan archive memory based on *ab initio* calculations. Our calculations indicated that O related defects in MONOS type memory is one of the most promising future high density archive memories, since carrier injection induces very large structural change. It is similar to carving on the stone.

Refarences

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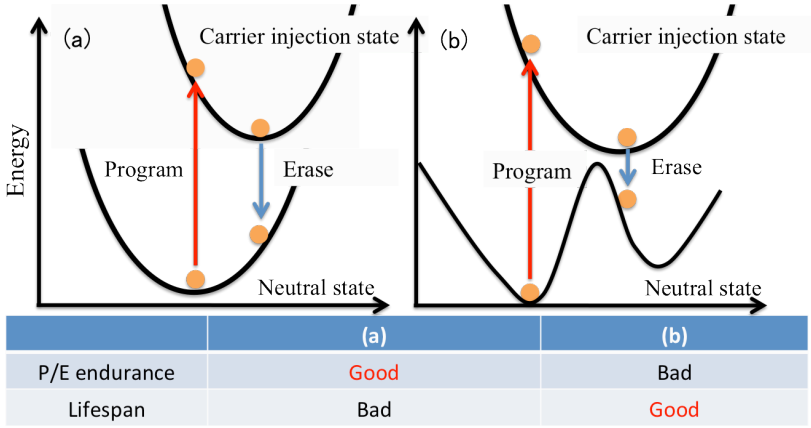

	(a)	(b)
P/E endurance	Good	Bad
Lifespan	Bad	Good

Fig 1. Schematic illustration of two types of structural change. (a) Reversible structural change during P/E cycles. (b) Irreversible structural change during P/E cycles.

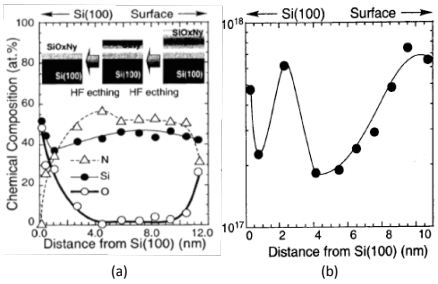

Fig 2. (a) Chemical composition (b) Electron occupied defects in MONOS structure. O inter-diffusion is observed at SiN/SiO2 interface. Lots of defects are located in O containing interfacial SiN regions. (Ref [8])

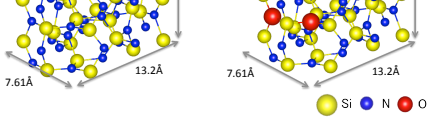

Fig 3. Calculation model used in this study. (a) 84 atoms super cell of SiN. (b) Two O substitution model

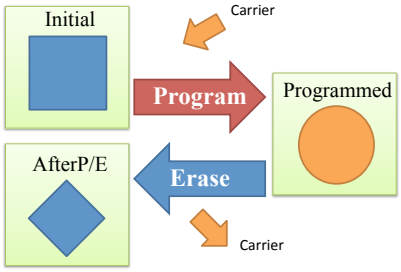

Fig 4. The calculation procedures of P/E operation. Atomic and electronic structure changes are investigated after charge injection.

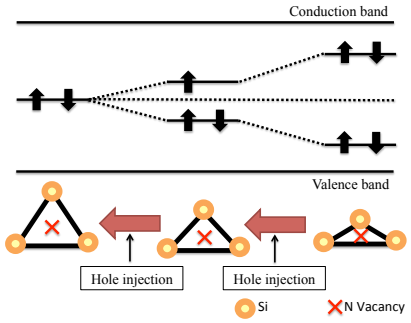

Fig 5. Schematic illustration of Jahn-Teller effect of N vacancies in SiN. Degenerated energy levels split due to symmetry breaking distortion, and an electron occupies a lower level with the energy gain ΔE.

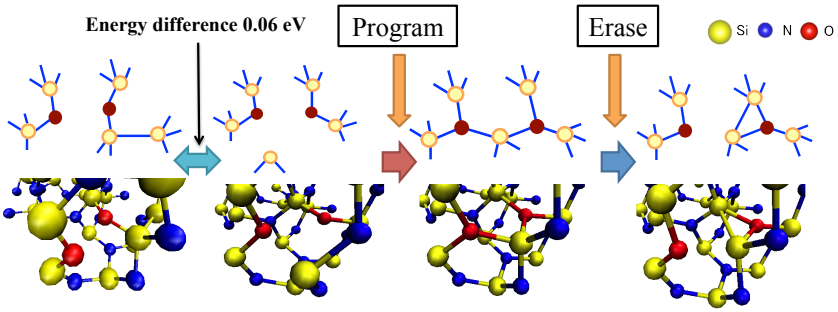

Fig 6. Optimized structure of two O substitution model. (a) Most stable neutral state structure (initial). (b) Meta stable neutral state structure (meta-stable-I). (c) Structure after hole injection (program). (d) Structure after hole injection and removal (meta-stable-II).

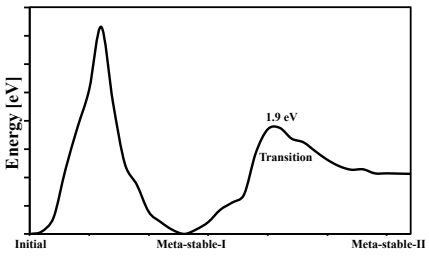

Fig 7. Schematic illustration of calculated potential energy surface of neutral two O substitution model between initial and meta-stable-II states. Activation barrier is at least 1.9 eV.

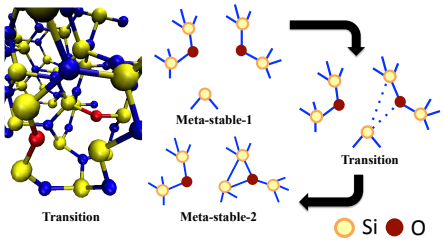

Fig 8. Transition state structure and it is schematic illustration with reaction coordinate.

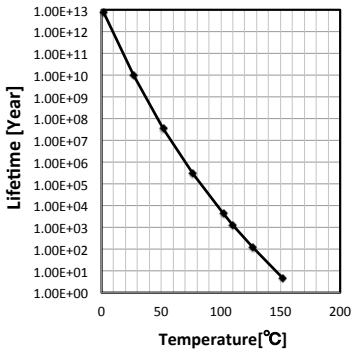

Fig 9. Estimated lifespan of MONOS type memory as a function of temperature