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Atomistic Design of Guiding Principles for High Quality MONOS Memories -First Principles Study of H and O Incorporation Effects for N Vacancies in SiN Charge Trap Layers-

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Abstract

We have theoretically investigated the effect of O and H atom incorporation into a N vacancy in a SiN layer in MONOS memories from a view point of memory characteristics. We have found that a N vacancy maintains its high P/E endurance characteristics even when H and O atoms are incorporated, based on the first principles calculations. N vacancies are suitable defects for future MONOS memories, even considering realistic process conditions in which incorporation of H and O atoms is inevitable.

Introduction

MONOS memories have attracted a great attention for the aggressive scaling of non-volatile memories. One of merits of MONOS memories is that they can trap charges inside very small atomistic regions such as defect sites in charge-trap layers. Recently, we have pointed out that defects with reversible structural changes are suitable for charge trap memories (Fig. 1(a)) [1]. Whereas, defects with irreversible structural changes tend to cause degradation of memory characteristics (Fig. 1(b)) [1]. Moreover, we have also proposed that "pure N vacancies" which reveal reversible structural changes, are desirable atomistic defects for future MONOS memories, although defects with excess O atoms are not suitable for MONOS memories (Fig. 2) [1]. On the other hand, it has been experimentally reported that both H and O are incorporated in SiN charge trap layers after real processes (Fig. 3) [2,3]. Thus, to obtain realistic guiding principles for future MONOS memories, the effects of H and O atoms should be taken into account.

In this paper, we study N vacancies with H and O atoms in order to clarify the effects of H and O atom incorporation by using first principles calculations. Moreover, we also discuss atomistic guiding principles of suitable charge trap defects by considering the realistic process conditions.

Calculation Method

In this study, total-energy electronic-structure calculations were performed based on the density functional theory (DFT) [4]. We prepared two types of N vacancy with H atoms in an 84-atom supercell of Si_3N_4 to investigate structural change during P/E operations induced by charge injection and removal. In the calculation, we investigated two models. One is a N vacancy (Fig. 4(a)) and the other is a N vacancy with one substitutional O atom (Fig.4(b)). Relative stability of H-incorporated N vacancies was studied by considering the total energies of molecular hydrogen.

(a) Number of H atoms in N vacancies

First, we consider the number of H atoms in N vacancies. When two Si dangling bonds in a N vacancy are terminated, H-H distance becomes shorter than 0.5 Å, leading to the unstable nature of two-H-incorporated N vacancies (Fig. 5). Accordingly, two H atoms cannot be incorporated in N vacancies. The number of H atoms in a N vacancy should be zero or one.

(b) A N Vacancy Model

Next, we investigate the H effect to "a pure N vacancy model". In a one-H-incorporated N vacancy, the optimized structure is shown in Fig. 6. In this structure, three Si dangling bonds are stabilized by H termination and formation of a new Si-Si bond. It is also noted that calculated total energy of this N vacancy is more stable than that with "a pure N vacancy + ½ H_2 molecules". These results clearly indicate that "pure N vacancies" tend to incorporate one H atom, which is in good agreement with a recent report [2]. The stable charged states of this system are doubly positive (+2) , neutral (0), and doubly negative (–2). Moreover, a one-H-incorporated N vacancy reveals reversible structural changes during P/E cycles (Fig. 7) [5]. This clearly shows that H incorporation into a N vacancy does not degrade high P/E cycle endurance characteristics of N vacancy defects.

(c) A N Vacancy With One Substitutional O Atom

Finally, we investigate the H incorporation effect into a N vacancy with one substitutional O atom. The obtained one H-atom incorporated structures are shown in Fig. 8. H is located near the center of a Si-Si bond (Fig.8). Without H incorporation, on the other hand, Si dangling bonds are stabilized by the formation of two Si-Si bonds (Fig. 9). The stabilization mechanism is as follows. One additional electron is supplied from a neighboring O atom which enables the formation of two Si-Si bonds (Fig. 10). Moreover, it is noticeable that the calculated total energy of the one-H-incorporated structure is larger than that without H incorporation. Accordingly, a N vacancy with one substitutional O atom does not incorporate H atoms. The stable charged states of this N vacancy are doubly positive (+2), neutral (0), and doubly negative (–2). Moreover, this N vacancy reveals reversible structural changes during P/E cycles (Fig.11). This also indicates that neighboring O atoms to a N vacancy does not degrade high P/E cycle endurance characteristics of N vacancy defects.

As discussed above, N vacancy defects reveals reversible structural changes regardless of the existence of H and O atoms, which leads to a high P/E endurance characteristics. Thus, N vacancy defects are suitable and feasible defects for future MONOS memories by considering realistic process conditions, in which incorporation of H and O atoms is inevitable.

Conclusion

We have investigated the effect of O- and H-incorporation into N vacancies in SiN charge trap layers from view points of MONOS memory characteristics. We have found that N vacancies maintain high P/E cycle endurance characteristics regardless of the existence H and O atoms. Our calculated results clearly show that N vacancies are desirable and feasible defects for future MONOS memories, even considering realistic process conditions.

References

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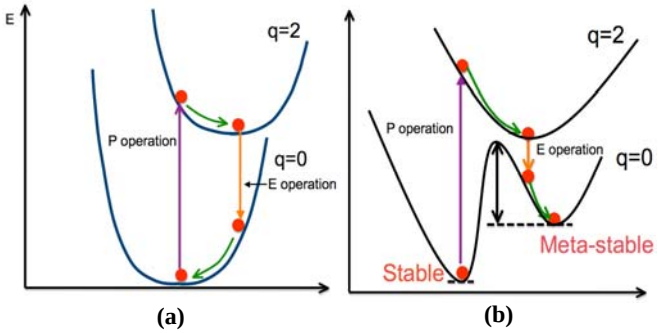

Fig. 1: Schematic illustration of two types of structural changes. (a) Reversible structural change during P/E cycles. (b) Irreversible structural change during P/E cycles. By program and erase operations, the most stable original structure changes into different meta-stable one [Ref 1].

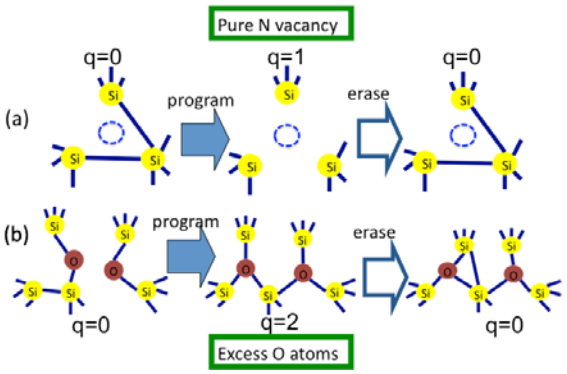

Fig. 2:Examples of reversible and irreversible structural changes during P/E cycles (a) Pure N vacancy reveals reversible change.(b) Defects with two substitutional O atoms at N sites structure has irreversible structural change (Not good for memory properties).

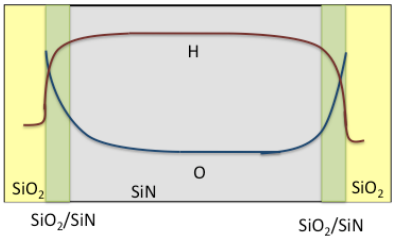

Fig. 3: H and O profiles in MONOS structures. A lot of H atoms are observed in SiN layer [Ref.2] and many O atoms are located at SiN/SiO_2 interfaces [Ref.3].

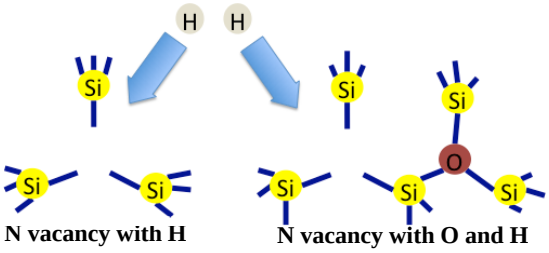

Fig. 4: Atomistic structures of our studied defect models. (Left) A pure N vacancy. (Right) A N vacancy with one substitutional O atom at a N site. We investigated H atom incorporation effect in each N vacancy model.

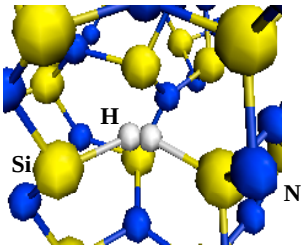

Fig. 5: N vacancy structure with two H incorporation. In this case, H-H distance is shorter than 0.5↗ .

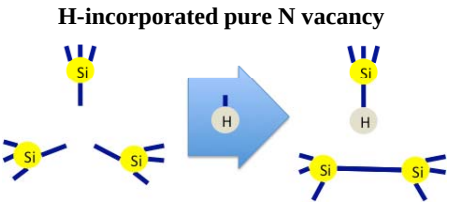

Fig. 6: H-incorporated pure N vacancy model. One dangling bond is terminated by a H atom, and other two dangling bond form a new Si-Si bond.

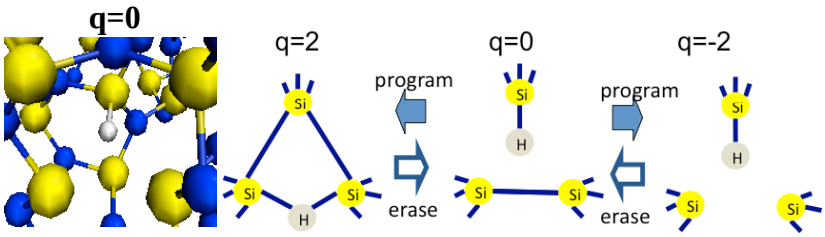

Fig. 7: (Left) Atomistic structures of a H-incorporated pure N vacancy. (Right) Atomistic structure change during P/E cycles (Injection and removal of electron and holes). Structural change is reversible, and high P/E cycle endurance of a N vacancy is maintained.

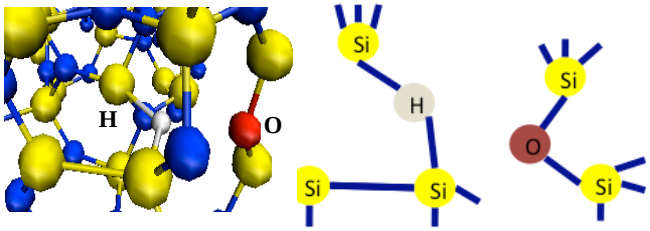

Fig. 8: Atomistic structures of a H-incorporated N vacancy with O atom. Schematic illusturaion is also shown

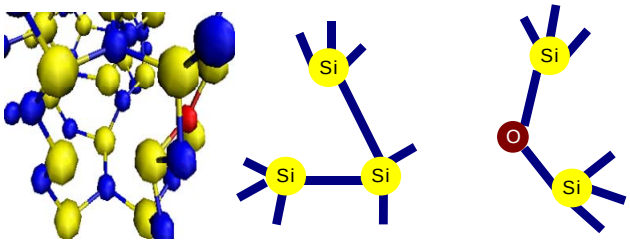

Fig. 9: Atomistic structure of a N vacancy with an O atom without H incorporation. Schematic illustration is also shown.

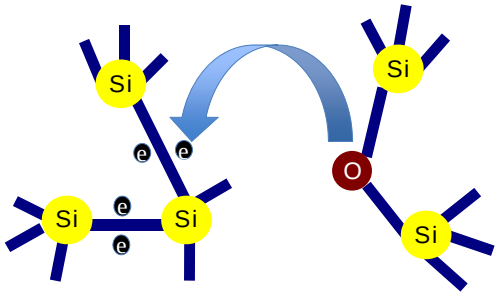

Fig. 10: Schematic view of stabilization mechanism of a N vacancy with an O atom without H incorporation. One electron is supplied from O to form a new Si-Si bond.

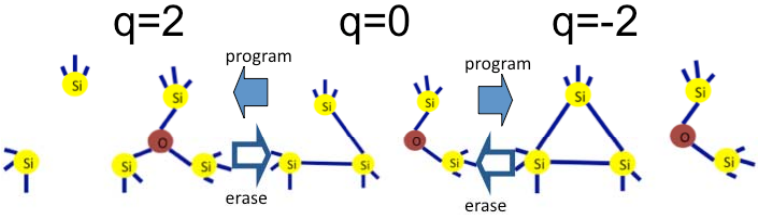

Fig. 11: The atomistic structural change of a N vacancy with one substitutional O atom during P/E cycles (Injection and removal of electron and holes). Structural change is reversible. This N vacancy also has high P/E cycle endurance