Composition Effect of Tunneling and Charge Trap Layer for Enhanced Cycle Retention in VNAND Flash Memory

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***Abstract*— In this study, we present an optimized composition of the ONO (Tunneling Oxide-Charge Trap-Blocking Oxide) layer to enhance data retention layer to enhance data retention characteristics in three-dimension vertical NAND (3D VNAND) flash memory. To this end, a novel atomistic-based TCAD simulator integrated with density functional theory (DFT) was developed to evaluate reliability as a function of the nitrogen concentration profile within the tunneling oxide (TO) and charge trap (CT) layers. The analysis demonstrates that reliability is strongly influenced by the composition ratio of TO and CT, as well as the thickness of the mixed composition between the two layers. Based on these findings, an optimized composition and thickness of ONO layer is proposed. Compared to the reference composition, the proposed configuration achieves a 58% improvement in 1K endurance and enhancement of 104mV in 1K retention.**

Keywords*— *SiON composition, DFT, trap energy, trap concentration, cycle retention

I. INTRODUCTION

Three-dimension vertical VNAND (3D VNAND) flash memory has been implemented high storage density and low bit cost through scaling down of architecture [1]. However, such scaling introduces critical reliability concerns, as charge loss in memory cells that retain stored information tends to increase over time. To address these reliability issue, several studies have investigated the optimization of material composition in ONO layer of VNAND. Nonetheless, conventional TCAD simulators are designed for characteristics evaluation and optimization through structural analysis, making them unsuitable for evaluating the properties of material compositions. To overcome this limitation, we have developed the first atomistic-based TCAD device simulator integrated with density functional theory (DFT), enabling a comprehensive analysis environment for evaluating the impact of ONO layer material composition on device reliability. This simulator is equipped with a mathematical model capable of interpreting essential material properties—including band gap, dielectric constant and trap distributions (i.e., trap density and energy levels)—across the composition range from SiO2 to Si3N4 using DFT. Using this atomistic-based simulation framework, we proposed optimized material compositions for the tunneling oxide (TO) and charge trap (CT) layers, along with optimal thickness combinations for each layer. These design optimizations are targeted at improving retention characteristics under program/erase (P/E) cycling conditions ($\geqslant$ 1K cycles), thereby enhancing the overall reliability of 3D VNAND flash memory.

II. MODELING AND SIMULATION RESULT

A. Atomistic-based TCAD device simulator platform

To establish a correlation between the atomic composition of silicon (Si), oxygen (O), and nitrogen (N) in the amorphous ONO layer and key thermodynamic properties—including bulk bandgap (Eg), valence band maximum (Ev), conduction band minimum (Ec), permittivity (K), trap distributions—we performed DFT calculations on 77 SixOyN1-x-y composition samples within the range of $0 \leqslant x-1/2\ y-3/4\ (1-x-y) \leqslant 0.12$ [2-4]. The resulting data were fitted using third-order polynomial and Gaussian functions, which were subsequently integrated into a TCAD device simulator. Fig. 1 shows the integrated simulation framework that facilitates automated evaluation of ONO composition effects on device reliability.

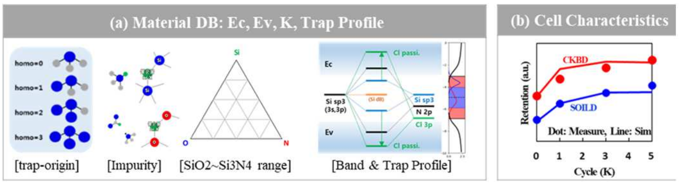


Fig. 1. Atomistic-based TCAD simulator platform: (a) applied material property (b) accuracy for cycle retention characteristics

B. Impact of CT layer composition charges on retentions

To evaluate the reliability characteristics, we considered not only the thermodynamic properties but also the VNAND structure parameters summarized in Table 1. In addition, we implemented physical models for trap-to-band (T2B), trap-to-trap (T2T), and thermal emission mechanisms, as shown in Fig. 2. These models were utilized to evaluate the retention characteristics across various CT compositions.

Structure	Value
Hole CD	12xnm
Lg	2xnm
Ls	1xnm
Tunneling Oxide	5.Xnm
Charge trap	5.Xnm
Blocking Oxide	6.Xnm
Ch. Poly	5.xnm

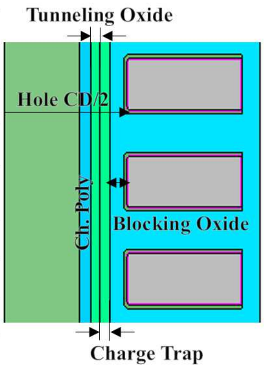


Table 1. Structure parameters

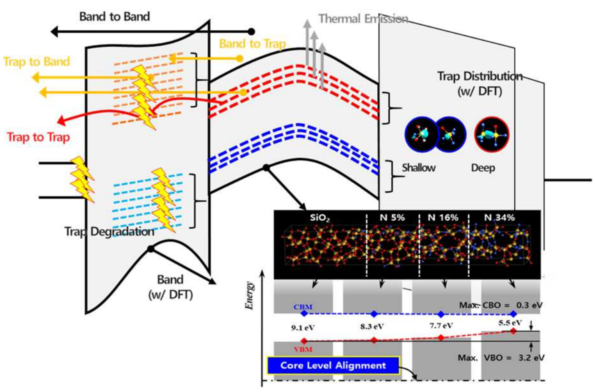


Fig. 2. Schematic diagram of the charge loss mechanism in our TCAD device simulator

To validate the accuracy of material analysis in an atomistic-based TCAD simulator, we evaluated the 0K retention characteristics for the various compositions, as shown Fig. 3. The simulation results exhibited high correlation with experiment data, demonstrating an accuracy of 92%. Based on this data, we investigated the impact of increasing the N/Si ratio from 1 to 1.26 on retention characteristic. As the N/Si ratio increased, the electron trap energy level becomes deeper, while the hole trap level becomes shallower. This led to an increase in vertical charge loss by Δ41mV, electron spreading decrease by Δ240mV, and an increase in hole spreading by Δ327mV. Consequently, the optimal retention characteristics were observed at an N/Si ratio of 1.12.

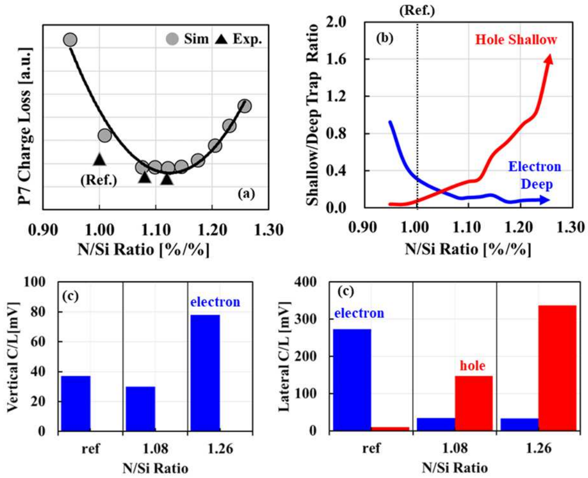
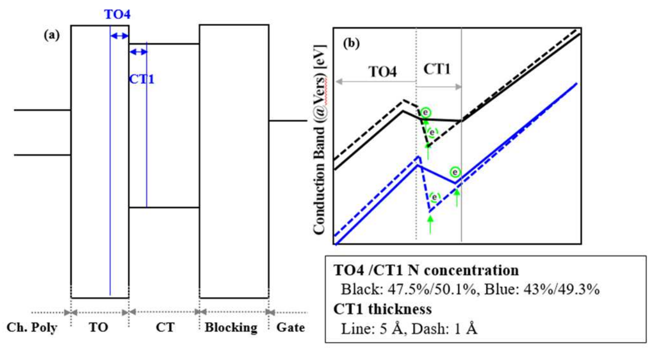


Fig. 3. (a) 0K retention (85℃ 10hr) by N/Si ration in CT layer (b) change of trap energy shift by N/Si ratio (c-d) Segmentation of major components causing retention

C. Impact of TO & CT layer composition on cycle retention

Cycle retention degradation is primarily attributed to increased vertical charge loss via T2B and T2T mechanisms. This phenomenon is caused by the generation of traps within the TO, which results from anode hole injection (AHI) [5] occurring during the application of erase voltage among P/E cycle. To address this issue, it is essential to enhance the band offset at the interface between the TO and CT layers and to suppress electron tunneling from the CT to the TO during the erase operation. To this end, we investigated the nitrogen concentration of TO4 (43% and 47.5%) and CT1 (49.3% and 50.1%), along with inter-mixed layer thickness ranging from 0 to 0.5nm. This inter-mixed (TO4, CT1) layer between the TO and CT layers was analyzed by incorporating the AHI model, which is the primary mechanism responsible for the generation of interface and bulk traps in the TO layer, as illustrated in Fig. 4(a). Fig. 4(b), (c) show that, depending on the composition of TO4/CT1, there exists an optimal CT1 thickness that effectively suppresses electron tunneling, which is the source of AHI. When the nitrogen concentration are 43%/49.3% and 47.5%/49.3%, the optimal Ct1 thickness is 0.5nm. In contrast, for concentrations of 43%/50.1% and 47.5%/50.1%, the optimal thicknesses are reduced to 0.25nm and 0.1nm, respectively. Consequently, increasing the band offset difference between TO4 and CT1, while maintaining the CT1 thickness above a certain threshold, is expected to mitigate trap generation induced during P/E cycle.



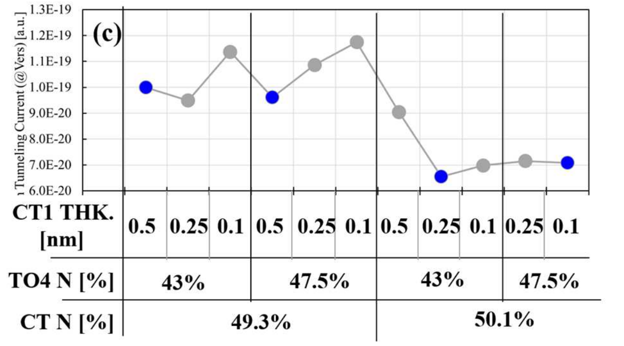


Fig. 4. (a) Schematic diagram of the structure (b) Band diagram and the position of electrons (c) electron tunneling current inducing AHI during erase operation

To determine the optimal composition and thickness for cycle retention, we extended our evaluation to TO4 nitrogen concentrations ranging from 43% to 48.5% and CT1 thickness from 0 to 1.25nm, with CT nitrogen concentration fixed at 49.3% and 50.1%. The retention characteristics were assessed using both the SOLID pattern, which evaluates vertical charge loss, and the CKBD pattern, which reflects lateral charge spreading. The results showed that the best retention values were 227mV/429mV (SOLID/CKBD, 85°C 10hr). At lower temperature conditions, the optimal values were 264mV/353mV (SOLID/CKBD, 25°C 4day), as shown in Fig. 5.

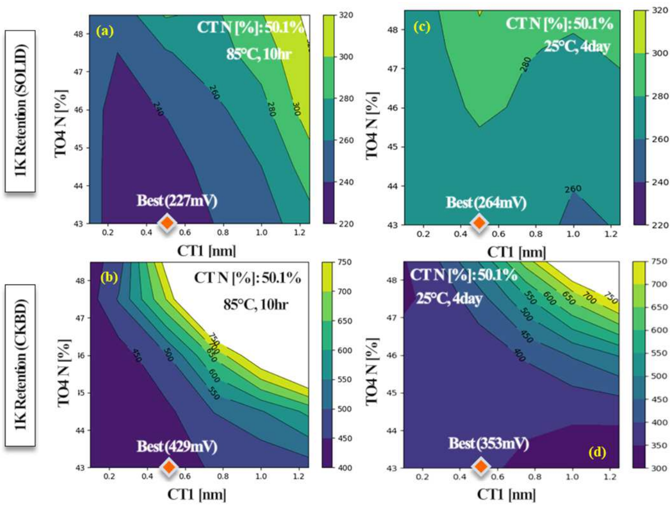


Fig. 5. 1K Cycle Retention according CT1 thickness and TO4 nitrogen concentration (left) 85°C, 10hr (right) 25°C, 4day

Ultimately, it was determined that within the CT nitrogen concentration range of 49.3% to 50.1%, the optimal CT1 thickness for achieving the best cycle retention characteristics is 0.5nm when the TO4 nitrogen concentration is below 46%, 0.25nm when the TO4 concentration is between 46% and 48%, and 0.1nm when the TO4 concentration exceeds 48%, as shown in Fig. 6.

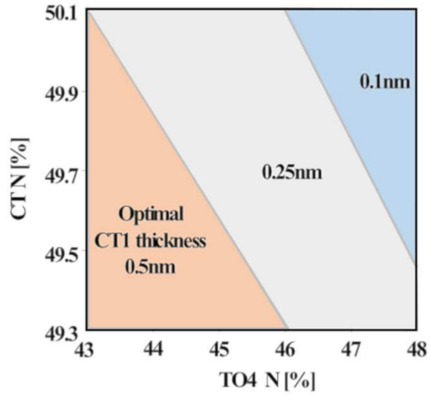


Fig. 6. Optimal CT1 thickness for the best 1K retention characteristics in combinations of TO4 N [%] and CT N [%]

III. Result and Discussion

To implement the proposed nitrogen concentration and thickness conditions, the simulation structure was configured by dividing the TO layer into four sub-layers (TO1-TO4) and the CT layer into three sub-layers (CT1-CT3), thereby enabling precise optimization of the nitrogen profile across the TO-CT layer. In cases where the nitrogen concentration in TO4 was reduced, the nitrogen content in TO2 was correspondingly increased to maintain an erase speed equivalent to that of the reference composition. This adjustment compensates for the extended hole tunneling path induced by the overall reduction in nitrogen concentration within the TO layer during erase operations. The nitrogen concentrations in TO4 and CT were set 43% and 50.1%, respectively, with the CT1 thickness fixed at 0.5 nm, forming a continuous nitrogen gradient profile consistent, as illustrated in Fig. 7.

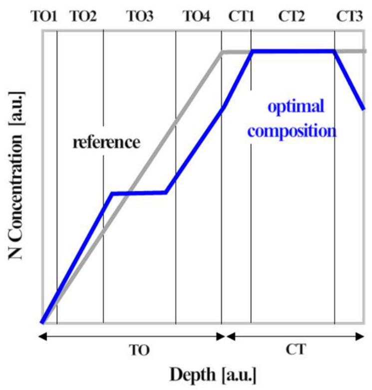


Fig. 7. Simulation evaluation conditions: (gray) reference, (blue) optimal nitrogen profile proposed in this paper

The evaluation results confirmed that the erase speed remained comparable to the reference composition. However, a degradation in 0K retention was observed, with an increase of Δ 29 mV/ Δ 30 mV for SOLID and CKBD patterns, respectively (25 ℃, 4 day). Component-wise retention analysis revealed that the primary factor contributing to this degradation was electron spreading, which deteriorated by Δ24 mV. This degradation is attributed to the shallower electron trap levels caused by the reduced nitrogen concentration in the CT layer compared to the reference, as shown in Fig. 8.

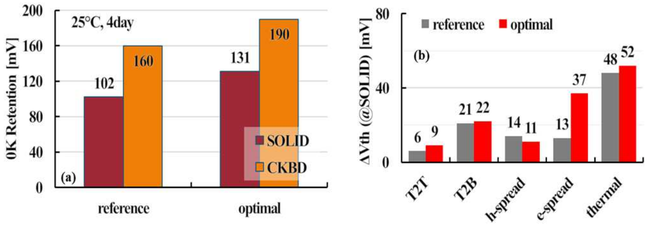


Fig. 8. 0K retention characteristics (SOLID/CKBD, 25 °C, 4 day) (b) component-wise 0K retention analysis

Since this condition was evaluated for post-cycling improvement, the 1K retention results demonstrated that, compared to the reference, the increased band offset and extended electron tunneling path during cycling led to a 58 % reduction in AHI-related components in the 1K endurance characteristics. This reduction in AHI contribution indicates a suppression of trap generation within the TO layer, thereby enhancing the T2B and T2T components, which are dominant in low-temperature retention. The computed results showed an improvement of Δ104 mV in the SOLID pattern. While this condition effectively suppresses vertical charge loss, the applied CT1 thickness leads to a bowl-shaped CT layer profile, which tends to trap both electron and holes. This results in a degradation of Δ 97mV in hole spreading and Δ61 mV in electron spreading, as shown in Fig. 9.

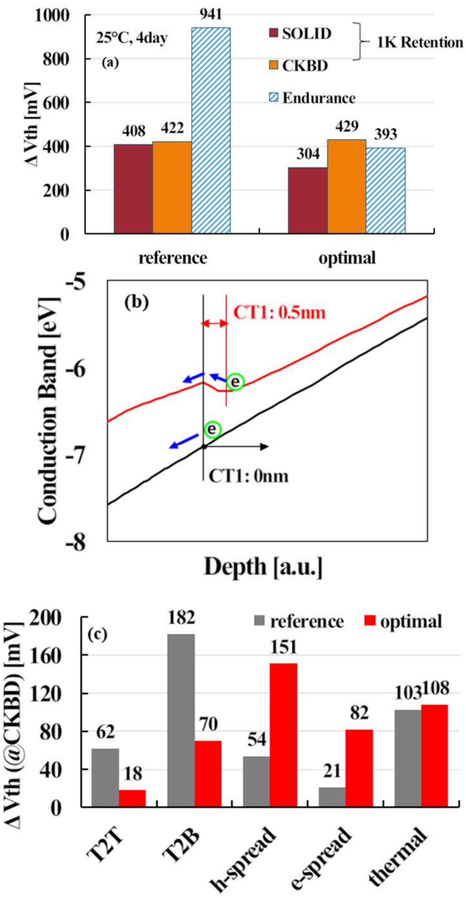


Fig. 9. (a) 1K retention (SOLID/CKBD, 25 °C, 4 day) & Endurance characteristics (b) Conduction band diagram during cycling (erase) voltage (c) component-wise 1K retention analysis

Nevertheless, under the optimized conditions proposed in this study, the retention slope improve from 22.75 mV/day to 15.25 mV/day over time, indicating enhanced long-term retention characteristics and the potential to meet the 10-year retention specification required for flash memory applications, as shown in Fig. 10.

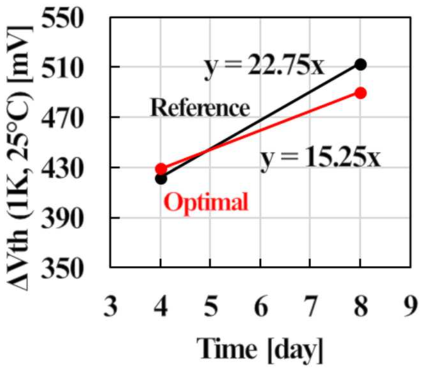


Fig. 10. Slope of 1K retention (25 °C) characteristics over time: (black) reference, (red) optimal nitrogen profile

IV. Conclusion

In this study, an atomistic-based TCAD simulator was developed to enable the optimization of material compositions and structural parameters for enhanced reliability in 3D VNAND flash memory. Through this simulation framework, we focused on improving reliability by engineering the composition of the ONO layers. The results demonstrated that mixed interfacial layers formed between individual dielectric layers play a critical role in trap generation within the TO layer during P/E cycling. Based on these findings, the compositions and thicknesses of the TO4, CT1, and CT regions were systematically optimized.

Specifically, by setting the nitrogen concentration of TO4 and CT to 43% and 50.1%, respectively, and the thickness of CT1 to 0.5 nm, a 58% improvement in 1K endurance and a retention enhancement of Δ104 mV were achieved compared to the baseline structure. Furthermore, the retention loss rate was reduced from 22.75 mV/day to 15.25 mV/day, demonstrating a significant improvement in long-term data retention performance.

Overall, the proposed simulation methodology and optimization strategy are expected to provide valuable guidelines for the development of highly reliable and durable 3D VNAND flash memory technologies.

References

[1] Woo Young Choi, Hyung Su Kown, Yong Jun Kim, Byungin Lee, Hyunseung Yoo, Sangmoo Choi, Gyu-Seog Cho, and Sung-Kye Park, “Influence of Intercell Trapped Charge on Vertical NAND Flash Memory”, *IEEE Electron Device Letters*, Vol. 38, No. 2, 2017

[2] G. Kresse and J. Furthmüller, “Efficient iterative schemes for ab initio total-energy calculations using a plane-wave basis set”, Phys. Rev. B, vol. 54, pp. 11169, 1996.

[3] G. Kresse and J. Furthmüller, “Efficiency of ab-initio total energy calculations for metals and semiconductors using a plane-wave basis set”, Comput. Mater. Sci. vol. 6, pp. 15, 1996.

[4] P. E. Blöchl, “Projector augmented-wave method”, Phys. Rev. B, vol. 50, pp. 17953, 1994.

[5] C.Sandhya “Study of P/E Cycling Endurance Induced Degradation in SANOS Memories Under NAND (FN/FN) Operation”, IEEE Trans. on Electron Devices, Vol 57, No 7, 2010.