

Multiscale simulation of lateral charge loss in Si₃N₄ 3D NAND flash based on density functional theory

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Received 20 April 2019, revised 24 June 2019

Accepted for publication 2 July 2019

Published 24 July 2019



Abstract

Multiscale simulation combining density functional theory of defect physics and charge transport calculation is carried out to understand the intrinsic mechanism of the lateral charge loss in silicon nitride (Si₃N₄)-based 3D NAND flash memory. In this work, the defects' structures, trapping centers, and trap levels are investigated by *ab initio* calculations. Wherein, the focus is put on the nitrogen vacancy (V_N), puckered nitrogen vacancy (V_NP) and H-/O-incorporation. It shows that the V_NP and O atom will introduce extremely shallow electron traps which can be eliminated by the H passivation. The stability of several kinds of defects is also studied. To shed new light on the impact of trap levels on the charge de-trapping and the lateral charge loss, numerical simulations are performed with the drift-diffusion model and Poole–Frenkel model.

Keywords: silicon nitride, 3D NAND flash memory, trap levels, lateral charge loss

(Some figures may appear in colour only in the online journal)

1. Introduction

Charge-trap (CT) memory with Si₃N₄ as the storage layer has attracted great attention as a promising solution for future planar and three-dimensional (3D) vertical NAND flash technology [1]. However, the lateral charge spreading strongly degrades the reliability of CT memories [2, 3]. Due to the special structure and fabrication process of 3D NAND flash memory, the gate stack is formed on the whole sidewall of vertical memory holes and the storage layer cannot be separated between cells. In other words, shared CT layer between word-lines (WLs) would cause severer lateral charge loss [4–7]. Even worse, after long time data retention, the diffused charge may reach the neighboring cells and alter their storage states.

The charge loss in 3D NAND flash memory has been observed in previous experimental studies [4], in which

the shallow traps are suspected to be the dominant factor. However, the exact nature of the defect related to the charge loss remains unclear. In addition, quantitative modeling considering the trap levels, electrostatics, and various carrier transport mechanisms is necessary to understand the lateral charge loss phenomena as schematically depicted in figure 1. The previous modeling studies mainly focused on the vertical charge loss, however, the lateral charge loss modeling is rarely investigated [8, 9].

In this work, we present a comprehensive investigation of charge loss in 3D NAND flash memory with a focus on the puckered nitrogen vacancy and its incorporation with hydrogen and oxygen elements [10]. By combining the charge trapping/de-trapping model and carrier transport model with density functional theory (DFT)-based atomistic calculations, a multi-scale simulation is carried out for a quantitative prediction on the origin of lateral charge loss.

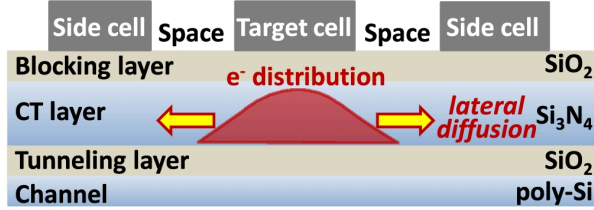


Figure 1. Schematic view of the lateral charge loss in 3D NAND flash memory cell.

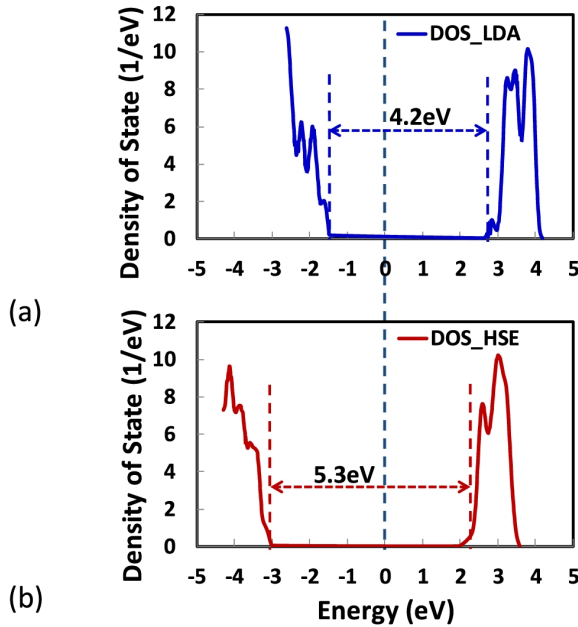


Figure 2. (a) Density of state calculated by LDA (b) and HSE. Compared with LDA, HSE get a better accuracy band gap.

2. Atomic defect modeling

Atomic defects in the Si_3N_4 CT layer are calculated by DFT with plane wave pseudopotentials as implemented in the GPU accelerated PWmat package [11]. DFT provides information on the electronic properties and chemical bonding of a material. It follows from the Hohenberg–Kohn theorems [12]: The electron density of a system uniquely determines its ground state information hence the basic properties of the system under consideration. A 280-atom rectangular (a , b , and $c = 12.9879$ Å, 14.9971 Å, and 14.3566 Å) supercell is built to simulate the bulk $\beta\text{-Si}_3\text{N}_4$ (space group $P6_3/m$). On one hand, the $\beta\text{-Si}_3\text{N}_4$ crystalline phase is thermodynamically more stable at all temperatures than other phases [13]. On the other hand, the amorphous SiN_x , which is usually used for 3D NAND flash memory application, has similar local structures as crystalline $\beta\text{-Si}_3\text{N}_4$ [6]. Generalized gradient approximation–Perdew–Burke–Ernzerhof (GGA–PBE) exchange–correlation functional is used in the geometry optimization with a residual force of 0.01 eV Å^{-1} as the convergence criteria. For the self-consistent calculation, various approximations used in the

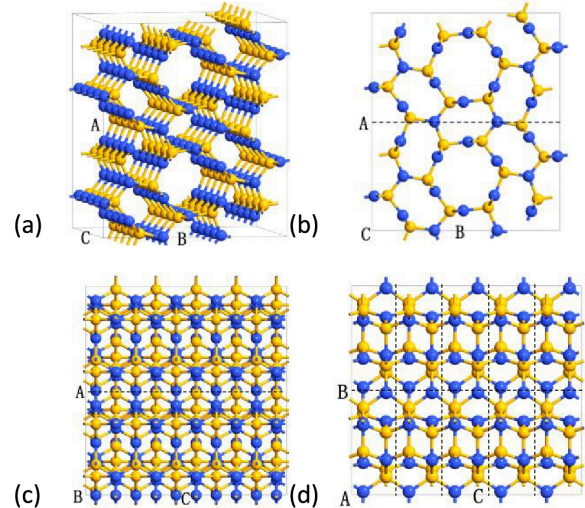


Figure 3. (a), (b) The supercell structure and (c), (d) their side views, including 280 atoms (expand the unit cell with $2 \times 1 \times 5$ at the A , B , and C direction respectively, $A = 12.9879$ Å, $B = 14.9971$ Å, and $C = 14.3566$ Å).

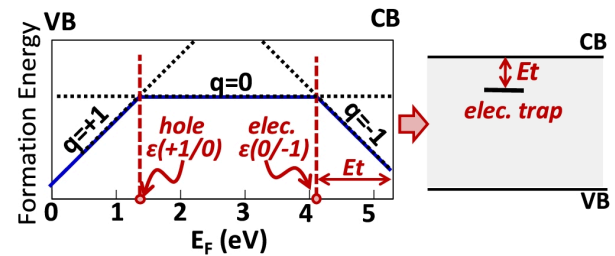


Figure 4. Schematic diagram of the transition level and electron trap level.

literature need proper justification for the accurate calculation of material properties. Exchange–correlation functional was initially based on local measurements of the homogeneous electron gas and gradient-corrected modifications. However, these functionals suffer from one key shortcoming that is particularly relevant to the study of defects in solid-state systems. They tend to give underestimated band gaps, both local-density approximation (LDA) and GGA. In addition, these underestimated band gaps lead to large uncertainties in the localized defect level positions. In this work, therefore, the hybrid functional, Heyd–Scuseria–Ernzerhof (HSE), is used for self-consistent calculations and the correct band gap of 5.3 eV can be achieved which shows significant improvement compared to the LDA, as shown in figure 2. Wherein, the kinetic energy cutoff for wave-functions is set as 50 Ry . Reciprocal space is sampled at the Γ -point which is sufficient because of the large supercell.

To build the supercell structure, we convert the hexagonal primitive cell to the rectangular cell as our unit cell. Then we repeat the unit cell for 2, 1, and 5 times at the A , B , and C directions, respectively. The final supercell structures are shown in figures 3(a)–(d).

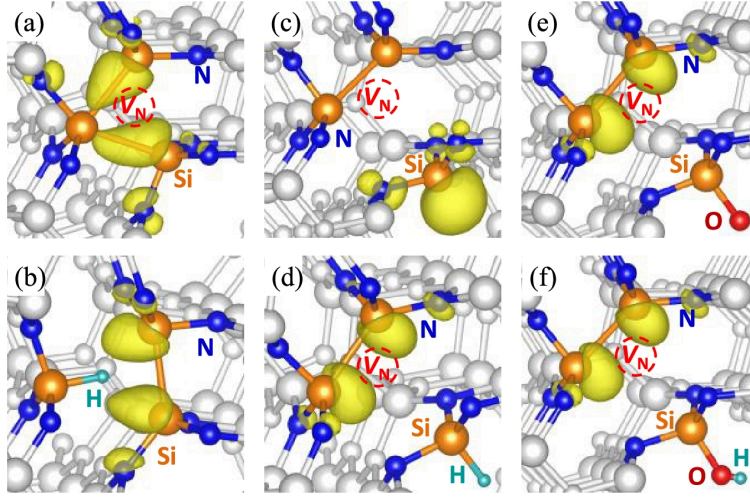


Figure 5. Atomic structures of calculated defects and the lowest unoccupied state using an iso-value of $0.05 \text{ \AA}^{-3/2} \text{ eV}^{-1/2}$ for (a) V_N and (b) its H passivation, (c) puckered V_N (V_NP) and (d) its H passivation (V_NP-H_i), (e) interstitial O atom near the V_N (V_N-O_i) and (f) its H passivation.

2.1. Formation energy

The formation energy for a defect α in the charge state q can be described by equation (1) [14]:

$$\Delta H_f(\alpha, q) = E(\alpha, q) + \sum n_i \mu_i + qE_F + qV, \quad (1)$$

where $\Delta E(\alpha, q) = E(\alpha, q) - E(\text{host}) + \sum n_i E(i) + q\varepsilon_{VBM}(\text{host})$, with n_i the number of atoms of type i removed from the supercell, μ_i the chemical potential of constituent i referenced to elemental solid/gas with energy $E(i)$, q the number of electrons transferred from the supercell to the reservoirs in the formation of the defect, E_F the Fermi level with reference to the valence band maximum (VBM) of the host. The electrostatic potential correction, ΔV , is included to align the potential of the defect supercell with the host [15].

Although the electronic structure far from the neutral defect would be very similar to that of the perfect bulk, the charge density and the average electrostatic potential in this region might differ from each other by a constant. This is because of the convention of setting the average Hartree potential over the supercell to zero in DFT calculations and possibly to variations in the average value of the local pseudopotential which depends on the number and kind of atoms in the supercell [16]. Therefore, a localized change in the potential in the near region needs to be compensated by a constant shift of the potential across the cell in simulation. The alignment term ΔV is obtained by comparing the electrostatic potential difference in the supercell with and without defect. To avoid the large variation of a single point's electrostatic potential, we adopt the average electrostatic potential of a unit cell. The average electrostatic potential V is obtained from the unit cell which is far from the point defect in the supercell, and the reference electrostatic potential V_{ref} is obtained from the same unit cell in the supercell without point defect. The ΔV equals to $V - V_{ref}$.

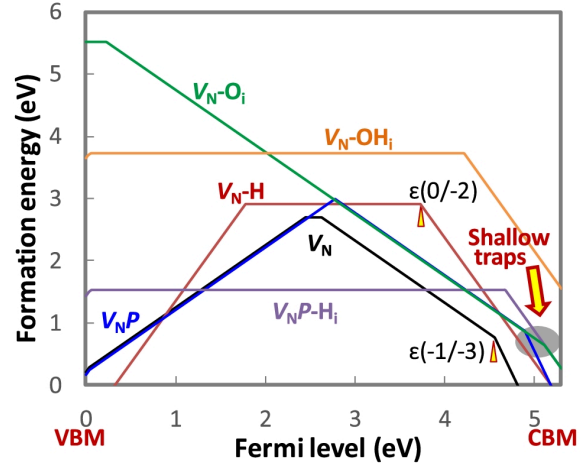


Figure 6. The formation energy of defects (Si rich). The V_NP and V_N-O_i induce shallow traps and the H passivation will deepen the trap levels of V_N , V_NP , and V_N-O_i .

The chemical potential of the atom i , μ_i , depends on the experimental conditions. Under the Si-rich condition, to avoid precipitation of the Si elements, the chemical potential is limited by: $\mu_{Si}^{max} = \mu(\text{Si bulk}) = 0$. In addition, μ_{Si} and μ_N are limited to the value of maintaining Si_3N_4 . Therefore, $3\mu_{Si} + 4\mu_N = \Delta H_f(\text{Si}_3\text{N}_4) = E(\text{Si}_3\text{N}_4) - 3E(\text{Si}) - 4E(\text{N})$. For impurity atoms like H atom and O atom, their chemical potentials are limited by the formation of SiH_4 and SiO_2 .

2.2. Transition level

The value of E_F where the charge state q_1 and q_2 exhibit the same formation energy, $\Delta H_f(\alpha, q_1) = \Delta H_f(\alpha, q_2)$, is

Table 1. Summary of our calculation results compared with some of the other works' calculations [18, 20–22].

Defect type	Electron trap levels					
	[20]	[21]	[22]	[18]	[17]	This work
V_N	(0/−1) 2.67	(0/−1) 2.6	(−1/−3) 1.3	(0/−1) 2.3	(0/−1) 2.3	(−1/−3) 0.74
$V_N\text{-H}$	—	(0/−1) 1.8	(0/−2) 1.8	(0/−1) 1.2	(0/−1) 0.9	(0/−2) 1.56
$V_N\text{P}$	—	—	—	—	(0/−1) 2.0	(−1/−3) 0.37
$V_N\text{P-H}_i$	—	—	—	—	(0/−1) 0.6	(0/−2) 0.58
$V_N\text{-O}_i$	—	—	—	—	—	(−1/−2) 0.18
$V_N\text{-OH}_i$	—	—	—	—	—	(0/−2) 1.08

defined as the transition level $\varepsilon(q_1/q_2)$. From the formation energy defined in equation (1), $\varepsilon(q_1/q_2)$ can be derived as:

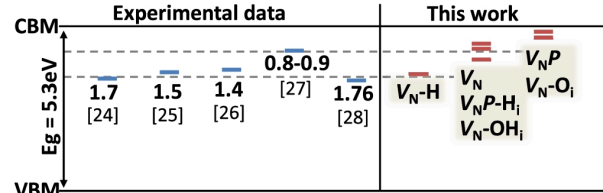
$$\varepsilon(q_1/q_2) = \frac{E(\alpha, q_1) - E(\alpha, q_2) + q_1\Delta V_1 - q_2\Delta V_2}{(q_2 - q_1)} - \varepsilon_{VBM}(host).$$

For the example shown in figure 4, the three lines represent three charge states: +1, 0, and −1. At the cross point of the line $q = 0$ and the line $q = -1$, the formation of the −1 state equals to the value at the neutral state. By increasing E_F , the stable charge state shifts from the neutral state to the negatively charged state. The corresponding E_F at the cross point is the transition level. Define the energy from the transition level to the conduction band minimum (CBM) as the electron trap level (E_t).

Some typical defects' atomic structures are illustrated in figure 5. All these defects are relaxed at a neutral state. The lowest unoccupied states are visualized using an iso-value of $0.05 \text{ \AA}^{-3/2} \text{ eV}^{-1/2}$. Previously, we have found that the V_N has the lowest formation energy, making it the most common defect in Si-rich Si_3N_4 . There are also some other research works [17] that claim the existence of the puckered configuration of V_N , just like the puckered O vacancy in SiO_2 , in which a silicon atom with a dangling bond is pushed into the outward, as described in figure 5(c). The puckered configuration has been designed to investigate an isolated Si dangling bond. Here, both $V_N\text{P}$ and V_N defects are studied comparably, including their impacts of H/O-incorporations. From their atomic structure, we can see that the V_N can form two Si–Si bonds where the lowest unoccupied state is localized. Compared with V_N , $V_N\text{P}$ forms a Si–Si bond with a dangling bond of Si that contributes to the lowest unoccupied state.

Figure 6 shows the extracted formation energies at Si rich condition. The horizontal axis is the Fermi level and the slope represents the charge state (q) of the supercell. From the formation energies, one can find that the V_N forms three transition levels, $\varepsilon(+1/0)$, $\varepsilon(0/−1)$ and $\varepsilon(−1/−3)$. With H passivation, $V_N\text{-H}$ defect forms two transition levels, $\varepsilon(+2/0)$ and $\varepsilon(0/−2)$. Compared with the single transition level $\varepsilon(0/−1)$ [18], those transition levels present more details of Si_3N_4 charge properties.

In comparison to V_N with the trap level E_t of 0.74 eV, $V_N\text{P}$ shows a shallower trap level ($E_t = 0.37$ eV). With interstitial O atom nearby V_N ($V_N\text{-O}_i$), it drags the nearby nitrogen atom and transforms the puckered form. It results in an extremely shallow electron trap ($E_t = 0.18$ eV). Electrons trapped by this extremely shallow trap can easily get de-trapped after

**Figure 7.** Comparison of the electron trap levels between experimental data and the calculated results in this work [23–27].

charging. In addition, when a single H exists beside the defects $V_N\text{-O}_i$, the trap level ($V_N\text{-OH}_i$) tend to be deeper ($E_t = 1.08$ eV). Based on the above analysis, it is reasonable to conclude that the H passivation could deepen various trap levels including V_N , $V_N\text{P}$, as well as $V_N\text{-O}_i$. In other words, H process optimization could be the key point to improve the stability of charged electrons both at the interface and in the bulk Si_3N_4 .

The trap levels reported in the literature and this work are compared in table 1. Compared with the single transition level $\varepsilon(0/−1)$ in previous research, our study provided more accurate trap levels because that more charge states are taken into consideration. Compared with the experiments (figure 7), we can find that the 1.4–1.7 eV traps might be contributed by $V_N\text{-H}$ defect. The 0.8–0.9 eV traps could be contributed by the V_N , $V_N\text{P-H}$ and $V_N\text{-OH}_i$ defects. As to shallow traps under 0.8 eV, they are still difficult to detect due to experiment accuracy, such as the approach named 'trap spectroscopy by charge injection and sensing (TSCIS)' [19].

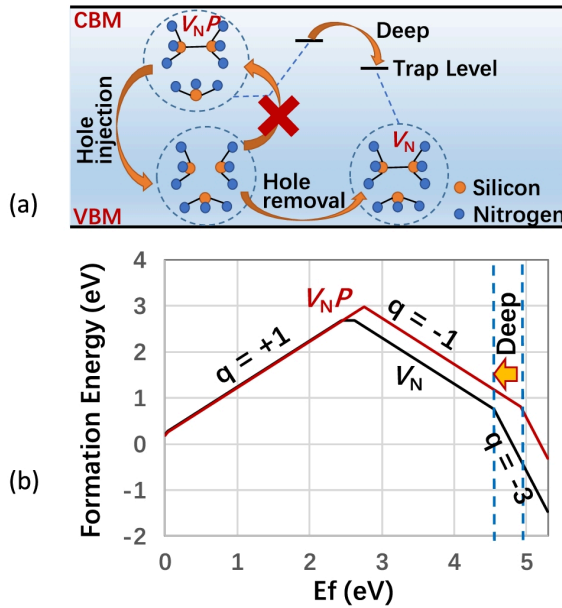
2.3. Defects stabilization with electron/hole injection

Taking the charge-injection-induced structural relaxation of each defect into consideration, we studied the stability of pre-existing defects in Si_3N_4 CT layer by calculating several typical defects in [9], as summarized in table 2. The defects include the substitutional site and the interstitial site, and the substitutional atoms include H, O and Si atom while the interstitial atoms include H and O atom. It is found that most of the defects are stable with electron/hole injection except $V_N\text{P}$, $\text{H}_N\text{-H}_i$, and $\text{Si}_N\text{-H}$.

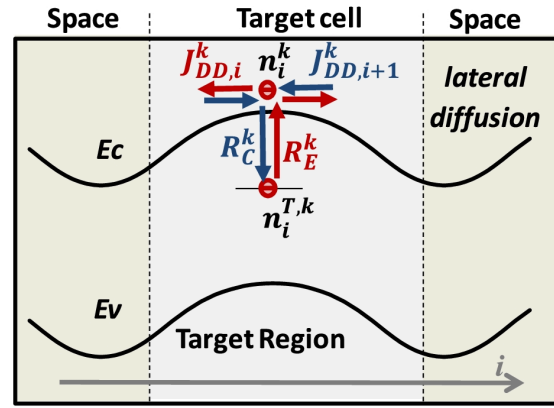
Based on our calculation, we find that the only three defects $V_N\text{P}$, $\text{H}_N\text{-H}_i$, and $\text{Si}_N\text{-H}$ have irreversible structural transformation along with charge injections. $\text{Si}_N\text{-H}$ defect has deep levels at the initial state and the final state, so impacts of its instabilities on memory reliabilities might be ignorable.

Table 2. Summarized stabilities of defects in Si₃N₄ CT layer. The defects include the substitutional site and the interstitial site. The substitutional atoms include H, O and Si atom while the interstitial atoms include H and O atom.

Defect type	e^- injection	h^+ injection	Initial state	Final state
V_N	Reversible	Reversible	$0.74 (-1/-3) e$	—
V_{N-H}	Reversible	Reversible	$1.56 (0/-2) e$ $1.80 (+2/0) h$	—
$V_N P$	Reversible	Irreversible	$0.37 (-1/-3) e$	$0.74 (-1/-3) e$
$V_N P-H_i$	Reversible	Reversible	$0.58 (0/-2) e$	—
H_N	Reversible	Reversible	$1.77 (+2/0) h$ $1.56 (-2/0) e$	—
H_N-H_i	Reversible	Irreversible	$3.74 (+1/-1) e$ $0.81 (-1/-2) e$	$2.88 (+1/-1) e$
O_N	Reversible	Reversible	$5.15 (+2/0) h$	—
O_N-H_i	Reversible	Reversible	$2.47 (+2/0) h$ $0.24 (0/-2) e$	—
V_N-O_i	Reversible	Reversible	$5.10 (0/-1) e$ $0.18 (-1/-2) e$	—
V_N-OH_i	Reversible	Reversible	$1.08 (0/-2) e$	—
Si_N	Reversible	Reversible	$3.34 (+1/0) h$ $1.69 (-1/0) e$	—
Si_N-H	Irreversible	Reversible	$1.46 (0/-2) e$	$1.41 (0/-2) e$ $2.01 (+2/0) h$

**Figure 8.** (a) Unstable $V_N P$ defect is transferred into V_N defect w/ positive charge injection; (b) the electron trap level of V_N ($\epsilon(-1/-3) = 0.74$ eV) is deeper than $V_N P$ ($\epsilon(-1/-3) = 0.37$ eV).

H_N-H_i has one shallow electron trap level (0.81 eV) and one deep trap level (3.74 eV) at the initial state while there is only one deep trap level at the final state. In the case of $V_N P$ defect, it could be transformed to V_N defect when there exists a positive charge (h^+) injection (figure 8(a)), and the V_N defect could not get back to $V_N P$ defect structure at both the neutral state and the charged state. In other words, it is an irreversible transformation from $V_N P$ defect to V_N defect. More importantly, based

**Figure 9.** Discretization of the fluxes for each site. The fluxes are coupled by two continuity equation: one for the free electrons in the conduction band (CB): n_i^k and the one for the trapped electrons $n_i^{T,k}$.

on calculated formation energies shown in figure 8(b), it is found that the electron trap level of V_N ($\epsilon(-1/-3) = 0.74$ eV) is deeper than that of $V_N P$ ($\epsilon(-1/-3) = 0.37$ eV). Thus, it is reasonable to believe that the extremely shallow trap ($V_N P$) is not stable and can be transformed to stable shallow trap (V_N) during P/E cycling.

3. Lateral charge loss simulation

To understand the relationship between the above-calculated trap levels and the retention performance of 3D NAND flash memory, a 1D model for the lateral charge loss has been carried out based on drift-diffusion carrier transport model and Poole-Frenkel charge trapping/de-trapping model. The

conduction mechanisms of the lateral charge loss include the electron emission/capture via charge trapping defects calculated in the previous section and drift-diffusion above the conduction band of the CT layer.

Figure 9 shows the balance of the fluxes for each site. The fluxes are described by two coupled continuity equations: one for the free electrons in the CB ($n(x)$) and the other one for the trapped electrons ($n^T(x)$). Self-consistent calculation of the continuity equations and the Poisson equation leads to the spatial distribution of electron charge density and potential profile over time. For numerical calculation, a discretization in space and time (i and k , respectively) is adopted:

$$\frac{n_i^k - n_i^{k-1}}{\Delta t} = -\frac{J_{DD,i+1}^k - J_{DD,i}^k}{q\Delta x} - R_{C_i}^k n_i^k + R_{E_i}^k n_i^{T,k} \quad (2)$$

$$\frac{n_i^{T,k} - n_i^{T,k-1}}{\Delta t} = R_{C_i}^k n_i^k - R_{E_i}^k n_i^{T,k} \quad (3)$$

$$\frac{V_{i+1}^k + V_{i-1}^k - 2V_i^k}{\Delta x^2} = q \frac{n_i^k + n_i^{T,k}}{\epsilon_0 \epsilon_N}. \quad (4)$$

At each time, the nonlinear equations are solved with the full Newton scheme. The electron emission (R_E) influences the free electrons (n_i^k) and the trapped electrons ($n_i^{T,k}$) as described in equations (2) and (3). The electron emission R_E is mainly depended on the trap level (E_t), described by the Poole-Frenkel equation:

$$R_E(x) = \nu_{PF} \cdot \exp\left(\frac{\beta \sqrt{F(x)} - E_t}{KT}\right), \beta = \sqrt{\frac{e^3}{\pi \epsilon_0 \epsilon_r}}. \quad (5)$$

$F(x)$ is the electric field at position x inside the Si_3N_4 layer, and for the retention condition with no extra electric field, it equals to the gradient of the electric potential. ν_{PF} is the attempt to escape frequency for emission, here equals 5×10^7 [8]. The free electron capture rate is:

$$R_C(x) = C_C(N_T - n^T(x)) \quad (6)$$

where C_C is the capture coefficient, $n^T(x)$ is the electron density trapped in defects, and N_T is the total defects' density in Si_3N_4 . Here, we adopt $C_C = 5 \cdot 10^{-14} \text{ m}^3 \cdot \text{s}^{-1}$, $N_T = 4 \cdot 10^{25} \text{ m}^{-3}$ [8].

The electron transport in the CB of Si_3N_4 is described by the drift-diffusion equation:

$$J_{DD}(x) = q\mu \left(-n(x) \frac{\partial}{\partial x} V(x) + \frac{KT}{q} \frac{\partial}{\partial x} n(x) \right) \quad (7)$$

where μ is the electron mobility and adopted $1 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ [8], $n(x)$ the electron density in the conduction band, and $V(x)$ the electrostatic potential. To avoid stability issues related to Poisson/drift-diffusion coupling, J_{DD} (from $i = 0$ to $i = N - 1$) is written in the form proposed by [28]:

$$J_{DD,i+1}^k = \frac{\mu kT}{\Delta x} \left\{ \begin{aligned} &-n_{i+1}^k B\left[\frac{q}{kT}(V_{i+1}^k - V_i^k)\right] \\ &+n_i^k B\left[\frac{q}{kT}(V_i^k - V_{i+1}^k)\right] \end{aligned} \right\} \quad (8)$$

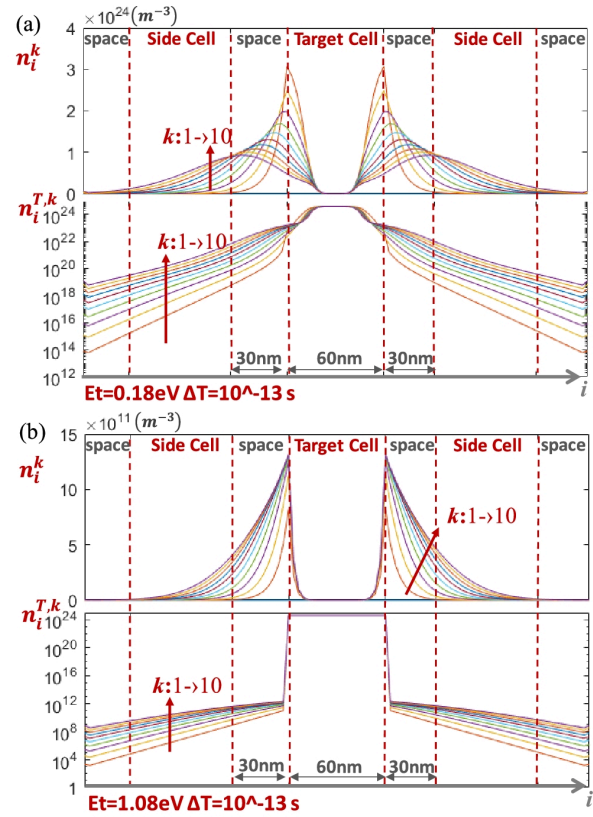


Figure 10. Distribution of electrons in the conduction band (up) and the traps (down) with (a) V_{N-O_i} with 0.18 eV trap level and (b) V_{N-OH_i} with 1.08 eV trap level.

where $B(x)$ is the Bernoulli function: $B(x) = \frac{x}{e^x - 1}$.

The boundary conditions are set by: $J_{DD,0}^k = J_{DD,N+1}^k = 0$.

As demonstrated in previous experimental work in [4, 5], a large difference in threshold voltage (V_{th}) shifts can be observed if adjacent cells have different states (neutral, erase, and program). Wherein, large V_{th} shifts can be observed when the adjacent cells of a programmed cell are at erasing states since much more charge will diffuse laterally to the space region. A model on the CT layer of 3D NAND flash memory with three adjacent cells and four space regions in between is built for the lateral charge loss simulation. The target cell is in the program state with electron existence. The adjacent cells and space regions are in the neutral state. There is no bias for both cells and space region at the retention condition, but the electron can diffuse to the space region and adjacent cells. In our simulation, only the lateral charge loss is considered to describe the processes of electron emission/trap and drift-diffusion. The widths of the cell and space region are set to 60nm and 30nm respectively. It is assumed that the target cell is in a charged state ($n^T(x) = 4 \cdot 10^{24} \text{ m}^{-3}$, $n(x) = 0$) while the two adjacent cells and spaces have no electron existence ($n^T(x) = 0$, $n(x) = 0$) in the initial of the simulation. By solving equations (2)–(4), redistributions of conduction band charge density at each time step are obtained. The impact of

the trap depth E_t on the charge density redistribution is then extracted.

As suggested by figure 10, it is concluded that the extremely shallow traps such as the case of V_N-O_i with $E_t = 0.18$ eV lead to extremely large lateral diffusion while the deep one (V_N-OH_i with $E_t = 1.08$ eV) does not affect much the charge distribution over time. The lateral diffusion will degrade the data retention performance since charge diffusion can change memory cell's V_{th} and cause more error bits: V_{th} of the programmed cell will be lower while that of neutral cells or erased cells will be higher on the contrary. The numerical simulation quantitatively indicates that the H passivation is a very effective solution of the lateral charge loss induced 3D NAND retention degradation. Our results in figure 10 agrees well with reported simulation results in [29], indicating that the process optimization to minimize shallow traps, such as the V_N-O_i defects close to the SiO_2/Si_3N_4 interface, could be the key point to suppress the temporal charge diffusion. Although some experimental work [4, 5] is designed to study the contribution of lateral charge loss qualitatively, it is still difficult to extract the lateral charge loss directly due to the complex 3D NAND structure (figure 1) and multiple impact factors like bi-directional vertical charge loss or redistribution, read disturb, testing time and so on. Special experiments are still necessary for comprehensive understandings on the shallow traps and traps' instabilities.

4. Conclusion

In this work, the nitrogen vacancy, puckered nitrogen vacancy, and their H-/O- incorporation in Si_3N_4 CT layer are investigated through comparative study to understand the physics of the charge diffusion in 3D NAND flash memory. It is found that the extremely shallow traps introduced by the O atom and the puckered V_N could be the main reason for the lateral charge loss. Hydrogen helps to eliminate all the aforementioned shallow traps. The stability of several kinds of defects is also studied. In addition, a numerical calculation is performed to intuitively illustrate the relation between the trap energy level and the lateral charge diffusion, showing that the shallow trap introduces large charge de-trapping, leading to terrible lateral charge diffusion between neighbor cells.

Acknowledgments

The authors acknowledge support from the China Key Research and Development Program (2016YFA0201802), the National Natural Science Foundation of China (61874068, 11574304, 11774338).

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