Comparison Between Bulk and FDSOI POM Flash Cell: A Multiscale Simulation Study

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Abstract—In this brief, we present a multiscale simulation study of a fully depleted silicon-on-insulator (FDSOI) nonvolatile memory cell based on polyoxometalates (POMs) inorganic molecular clusters used as a storage media embedded in the gate dielectric of flash cells. In particular, we focus our discussion on the threshold voltage variability introduced by random discrete dopants (random dopant fluctuation) and by fluctuations in the distribution of the POM molecules in the storage media (POM fluctuation). To highlight the advantages of the FDSOI POM flash cell, we provide a comparison with an equivalent cell based on conventional (BULK) transistors. The presented simulation framework and methodology is transferrable to flash cells based on alternative molecules used as a storage media.

Index Terms—Device variability, molecular electronics, multiscale modeling, nonvolatile memory (NVM), polyoxometalates (POM).

I. INTRODUCTION

OVER the last couple of decades, flash cells have undergone aggressive scaling reaching the 15-nm half-pitch (F) mark. This has been accompanied by scaling of a tunnel oxide thickness to improve the programming/erasing performance. At the same time, an interpoly dielectric thickness has been reduced to keep the capacitance coupling ratio at an almost constant value to achieve acceptable ratios between the control and floating gate (FG) voltages [1]. However, further scaling of the current NAND flash memory cells faces significant challenges including: 1) strong coupling between FGs in neighboring cells [2]; 2) charge loss from the FG [3]; and 3) random dopant fluctuations (RDF) that induce variability in flash cells [4].

Nanocrystals and charge-trapping memories have been proposed aiming to improve the flash cell performance [5], [6].

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II. FDSOI VERSUS BULK FLASH CELL PERFORMANCE

However, the random number and position of the traps create a significant additional variability in the threshold voltage of the programmed flash cells [7], [8]. One possible option for an improvement is to replace the nanocrystals/random defects with molecules [9], [10]. Among the possible candidates are polyoxometalate (POM) molecules, metal oxide clusters, where the metal atoms are usually group 5 or group 6 transition metals (W, Mo, …) in their highest oxidation state [11], [12]. POMs have attractive properties for potential nonvolatile memory (NVM) application due to their ability to undergo stable, multiple, and reversible oxidation/reduction processes. Moreover, the embedding of numerous types of POMs with SiO2 has been experimentally demonstrated as advantageous for the NVM application [13], [14]. This, in combination with the self-assembly of the POMs, is expected to yield a low-voltage threshold (Vt) variability.

To explore the full potential and POM-based flash cell technology, we compare multiscale computational simulations of fully depleted silicon-on-insulator (FDSOI) and conventional (BULK) POM flash memory cells. In addition, we provide a comparison with new and some of the previously reported results of the simulation of the BULK POM flash memory cell [15], [16]. Extensive information about the cell design and the simulations methodology is available in [16].

Fig. 1. Schematic of a single-transistor FDSOI memory cell, indicating the aimed substitution of the poly-Si FG with an array of POM molecules (POM layer). Legend: W—blue, O—red, Si—brown, and point charges representing the surrounding counter cations—green.
nine POMs placed in a perfect grid in the FG. The distance between the POMs molecules is 3 nm to exclude physical overlap between the two structures, which is in agreement with the experiments [13], [14]. The total oxide (SiO2) thickness is 20 nm, including the POMs layer (Fig. 1). The tunneling oxide (Tun) is 4.5 nm (3-nm high-quality SiO2 and 1.5-nm POMs layer), the bottom oxide is 15-nm thick, and the entire gate-stack is identical to our previously published work [16].

To investigate the device performance, we consider the [W18O54(SO3)]2− POM cluster as a charge storage center, having three easily accessible redox states. These are the parent (n = 4), 1x reduced (n = 5), and 2x reduced (n = 6) states. The parent flash cell has zero total charge in the FG because, even though the nine [W18O54(SO3)]2− POMs are negatively charged, their charge is neutralized by the positively charged cations, which are represented by point charges in our simulations (Fig. 1). In the case of the 1x reduced NVM cell, the total amount of charges in the FG is −9 q (q—unit charge of electron). Correspondingly, the 2x reduced transistors have −18 q in comparison with the parent structure.

The related ID−VG characteristics for the FDSOI and BULK cells are shown in Fig. 2. All characteristics are aligned in order for the parent structures of the FDSOI and BULK transistors to have identical Vt determined by a current criterion of the 10−7 A drain current (black curves in Fig. 2 intersect at drain current = 10−7 A). Several important observations can be made from the data presented.

First, because the short-channel effects are less pronounced in the FDSOI cell in comparison with the BULK flash cell, the FDSOI cell has lower leakage current, higher drive current, and steeper subthreshold slope in comparison with the BULK devices.

Second, our calculations show a reduction of threshold voltage shift (∆VT) between the parent, 1x reduced, and 2x reduced configurations for the FDSOI devices in comparison with the BULK cells. Narrowing of ∆VT between discussed states in FDSOI, if compared with the BULK cell, is clearly visible in Fig. 3. Fig. 3 also compares the analytical results of ∆VT versus Qs, obtained from the sheet-charge approximation (SCA), with the results from the 3-D simulations. The values of ∆VT for transition from the parent to 1x reduced state are 1.17 and 0.95 V for the BULK and FDSOI structures correspondingly. In the case of transition from the 1x reduced to 2x reduced state for the BULK transistor, the value is 1.16 V and for the FDSOI structure it is 0.84 V.

The right-hand side of Figs. 3 and 4 reveals the charge distribution in the middle of the channel for the BULK and FDSOI structures. The plot in Fig. 3 shows that the maximum of the 1-D electron density distribution in the channel is farther away from the surface in the FDSOI devices in comparison with the BULK structures. This is also visible in Fig. 4, where the dashed lines represent the charge centroids for the FDSOI and BULK devices. Due to the fact that the charge for the FDSOI transistor is farther from the Si/SiO2 interface in comparison with the BULK device, the influence of a trapped charge in the FG on the VT shift is smaller. Hence, the current flow through the channel in the FDSOI case is less disturbed by the number and the position of the POMs in the FG in comparison with the BULK structure.

Having established that the FDSOI cell has better ID−VT characteristics with narrowing of ∆VT window if compared with the BULK cell, it is important to investigate how sources of statistical variability (SV) determine the VT distribution in the FDSOI and the BULK flash cells.

### III. Statistical Variability

Consistently with our previous work [16], we introduced two principal sources of SV. The first source of SV (RDF)
and it is known to have a dominant impact on their threshold voltage variability [4]. The dopants profile used in the source/drain (S/D) follows the Gaussian distribution. The second source of SV is the random distribution of the position of the POMs in the FG along both the channel length and width, termed POM fluctuations (POMF). Ultimately, both the spatial position and number of the POMs could vary. However, in this brief, we present the results based only on a constant number of nine POMs in the FG. The fixed number and relatively low number of POM molecules gives us the opportunity to easily establish the relationship between the molecule position in the FG and the behavior of the flash cell.

We consider statistical ensembles of 2000 flash cells each in the statistical numerical device simulations. In the first set of simulations, we analyze the RDF mainly not only in the S/D regions of the FDSOI cell, but also in the channel of the BULK cell. Simultaneously, the nine POMs are arranged in a $3 \times 3$ grid in the FG. In the second set of simulations, called POMF, the position of the nine molecules along channel length and width is randomly varied but the flash cells have continuous doping. Finally, in the third set of simulations, marked as RDF$+$POMF, the combination of the RDF and the random lateral distribution of the position of the nine POMs in the oxide is considered.

In Tables I and II, under the heading Nominal $V_T$, three distinct $V_T$ values for the smooth FDSOI and BULK devices are reported correspondingly. The tables also report the average ($\mu$) and the standard deviation ($\sigma$) of the three $V_T$s for the simulated ensembles with variability. The corresponding values of $V_T$ are shown in Figs. 5–7 in terms of probability density function (pdf) for each ensemble and each state, comparing the FDSOI and BULK distributions. Based on the presented data, several observations can be made.

First, in the FDSOI case, the nominal (smooth) devices for each bit have lower $V_T$ in comparison with the BULK structures. The average value of $V_T$ for 2000 cells at each bit, for both types of flash cells, is close to the values for the nominal transistors. More importantly, the conclusion established in Section II for the nominal cells, in which the difference between each state in the FDSOI cell is smaller if compared with the BULK transistors, is still valid for $\mu V_T$.

Second, the RDF has a dominant impact on the dispersion of $V_T$ in both types of POM-based flash cells, as reflected in the values of $\sigma V_T$. In addition, $\sigma V_T$ for the RDF ensembles and the RDF$+$POMF ensembles is almost four times larger in the BULK cells in comparison with the FDSOI case. Moreover, Figs. 5 and 7 reveal that the states in the BULK case overlap significantly even at the value before $1 \sigma$, while in the FDSOI

**Table I**

<table>
<thead>
<tr>
<th>Bit</th>
<th>Nominal $V_T$</th>
<th>RDF 2000 devices</th>
<th>POMF 2000 devices</th>
<th>RDF$+$POMF 2000 devices</th>
</tr>
</thead>
<tbody>
<tr>
<td>Redox state</td>
<td>$V_T$ $(V)$</td>
<td>$\mu V_T$ $(V)$</td>
<td>$\sigma V_T$ $(mV)$</td>
<td>$\mu V_T$ $(V)$</td>
</tr>
<tr>
<td>(1) parent</td>
<td>1.778</td>
<td>1.821</td>
<td>44.8</td>
<td>1.778</td>
</tr>
<tr>
<td>(2) 1x red</td>
<td>2.948</td>
<td>2.976</td>
<td>443</td>
<td>2.945</td>
</tr>
<tr>
<td>(3) 2x red</td>
<td>4.107</td>
<td>4.122</td>
<td>437</td>
<td>4.089</td>
</tr>
</tbody>
</table>

**Table II**

<table>
<thead>
<tr>
<th>Bit</th>
<th>Nominal $V_T$</th>
<th>RDF 2000 devices</th>
<th>POMF 2000 devices</th>
<th>RDF$+$POMF 2000 devices</th>
</tr>
</thead>
<tbody>
<tr>
<td>Redox state</td>
<td>$V_T$ $(V)$</td>
<td>$\mu V_T$ $(V)$</td>
<td>$\sigma V_T$ $(mV)$</td>
<td>$\mu V_T$ $(V)$</td>
</tr>
<tr>
<td>(1) parent</td>
<td>-0.056</td>
<td>-0.052</td>
<td>98</td>
<td>-0.129</td>
</tr>
<tr>
<td>(2) 1x red</td>
<td>0.902</td>
<td>0.784</td>
<td>84</td>
<td>0.716</td>
</tr>
<tr>
<td>(3) 2x red</td>
<td>1.743</td>
<td>1.615</td>
<td>77</td>
<td>1.546</td>
</tr>
</tbody>
</table>
case, the overlap is almost at $3\sigma$. Hence, the dispersion of the $V_T$ in the FDSOI case is significantly reduced in comparison with the BULK structure. Another notable feature in the trends of $\sigma V_T$ for the ensembles with RDF is its decrease with the increase of the net negative charge stored in the oxide. This is ascribed to the increasing control of the stored charge over the channel conductance. This effect is more pronounced for the FDSOI cells.

IV. Conclusion

In this brief, we study the nominal and statistical behaviors of the FDSOI and BULK molecular-based flash cells using hierarchical numerical simulations. Two main sources of SV are considered such as RDF and POMF. The results of our analysis highlight that the difference between the threshold voltage shift in the FDSOI structures is smaller in comparison with the BULK case. Second, the FDSOI flash cell has significantly smaller variation of $V_T$ in comparison with the BULK case. Hence, the dispersion of the $\alpha$-window of a flash cell with molecular metal–oxide–storage, $\alpha - \{\text{W}_{18} \text{O}_{54}(\text{SO}_3)_2\}^{4-}$ and $\alpha - \{\text{W}_{18} \text{O}_{54}(\text{SO}_3)_2\}^{5-}$, is ascribed to the increasing control of the stored charge over the channel conductance. This effect is more pronounced for the FDSOI cells.

REFERENCES


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