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# Development of hierarchical simulation framework for design and optimization of molecular based flash cell

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**Introduction:** The field of molecular electronics continues to spur interest in the quest for miniaturization and reduction of operational power of electron devices. Most of the systems described in the literature are based on organic molecules, such as benzene, ferrocene and fullerenes [1]. However, the use of inorganic molecules known as polyoxometalates (POMs) (see Fig.1 and Fig.2) could offer several important advantages over the conventional and organic based devices. The interest in POMs for flash cell applications stems from the fact that POMs are highly redox active molecules and that they can also be doped with electronically active heteroatoms [3]. They can undergo multiple reversible reductions/oxidations, which makes them attractive candidates for multi-bit storage in flash memory cells. Our recent work showed that POMs are more compatible with existing CMOS processes than organic molecules and they can replace the polysilicon floating gate in contemporary flash cell devices [2]. In this work, we discuss a further improvement and development of our simulation framework and models, e.g. Poisson distribution of the molecules in the oxide, introducing a various device geometry such as FDSOI and nanowires and improved simulation flow.

**Simulation Methodology and Results:** For the purpose of realistic simulations of molecular flash cells, we developed a simulation flow that links the density functional theory (DFT) to a 3D device simulator [4]. The main advantage of that framework is that once the charge for the POM is obtained from the DFT program, it is transferred to the 3D numerical TCAD simulator where a drift-diffusion transport formalism is applied. In this way the computation flow has capabilities to evaluate not only the material capabilities and characteristics but also the full flash cell performance.

In this study, an n-channel FDSOI flash memory cell with an 18 nm square gate has been designed (Fig.1). The POM clusters substitute the poly-Si floating gate (FG). Fig.2 shows a key result of the DFT calculations for three POM clusters. The energy levels of the highest occupied and lowest unoccupied molecular orbitals (HOMO and LUMO, respectively) for all molecules are favourably aligned below the conduction band of Si and they could be effectively insulated by a comparatively high potential barrier of SiO<sub>2</sub>. From this point of view, all three molecules are similar, however only the W<sub>18</sub>SeO<sub>3</sub> - [W<sub>18</sub>O<sub>54</sub>(SeO<sub>3</sub>)<sub>2</sub>]<sup>4+</sup> cluster shows numerous oxidation and reduction steps. As a result, in this work we concentrate our discussions on this specific molecule.

As a further step in our flash cell design, we consider correlation between different thicknesses of the tunneling gate oxides (T<sub>tnn</sub>) and difference of the threshold voltage (ΔV<sub>T</sub>) (Fig.3). Fig.3 reveals that flash cells with SiO<sub>2</sub> as a gate material have wider programming windows (ΔV<sub>T</sub>) in comparison to devices with Al<sub>2</sub>O<sub>3</sub> as a FG. Also, for SiO<sub>2</sub> gate materials the programming window has the highest value at T<sub>tnn</sub>=1.5 nm. However, a flash cell with 1.5nm SiO<sub>2</sub> might have poor retention characteristics. For this reason, here we study a cell with T<sub>tnn</sub>=4.5 nm and SiO<sub>2</sub> as a gate material.

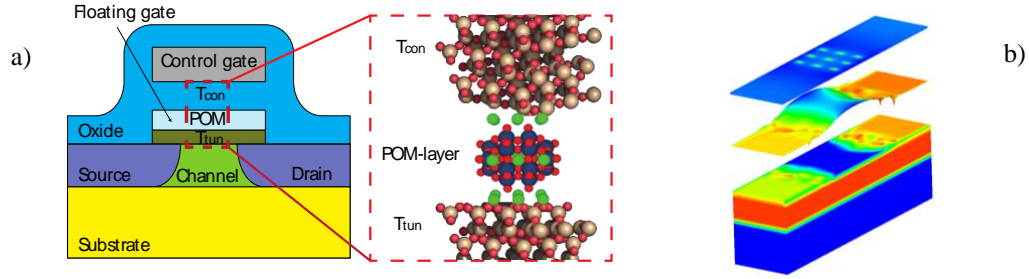
Fig. 4 threshold voltage variability (ΔV<sub>T</sub>) in three sets of 1,000 devices with POM molecules as a storage media. Each set has two sources of statistical variability, such as Random Dopant Fluctuations (RDF) and POMs fluctuations (POMF). It should be emphasised that for all three sets of 1,000 devices composing the ensembles, the number of POMs is constant and it equals nine. In the case of the RDF only calculations, the charge storage clusters are arranged in a regular grid of 3x3 POMs centered within the gate (Fig.1). In the POMF only calculations, the molecules are randomly displaced laterally. Finally, in the third case, both of these variations, i.e., RDF and POMF, are included. The following conclusions can be obtained from Fig. 4. Firstly, the curves presenting the PDF for all devices with RDF are broader in comparison to the POMFs only case. Secondly, the different bits do not overlap for this sample of 1,000 devices.

Fig.5 presents data for devices where the Poisson distribution in the POMs in the FG is considered. The actual Poisson distribution is presented in Fig.6 and it is identical for all devices. As shown in Fig.6, it is possible to have cells with as few as 1 molecule and as many as 19 POMs. Comparing the data from Fig. 4 and Fig. 5, is clear that the standard deviation is up to 5 times higher in comparison to the standard deviation for only 9 POMs in the FG. Also, the bits shown in Fig. 5 are much closer in comparison to those presented in Fig.4 and they overlap significantly.

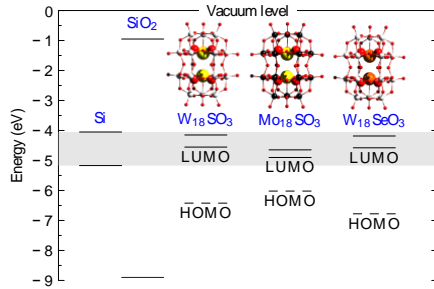
**Conclusions:** In this work, we compare the statistical threshold voltage variability of the molecular based 18-nm FDSOI flash cells. Two sources of statistical variability, RDF and POMF, are discussed. We establish that the RDF variability is the dominant factor, which influences the V<sub>T</sub> distribution. Most importantly, we show that controlling the number of POMs in the oxide is critical in order to achieve the optimal device performance.

## Reference:

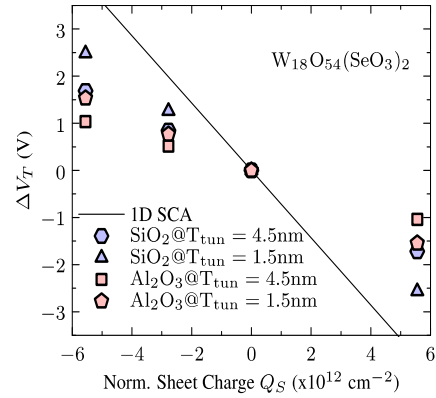
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[3] L. Vihla-Nadal, *et al.*, *Nat. Rev. Mat.*, vol. 2, p. 17054 (2017). [4] V. P. Georgiev *et al.*, *IEEE-TED*, vol. 62, p. 680, (2015).



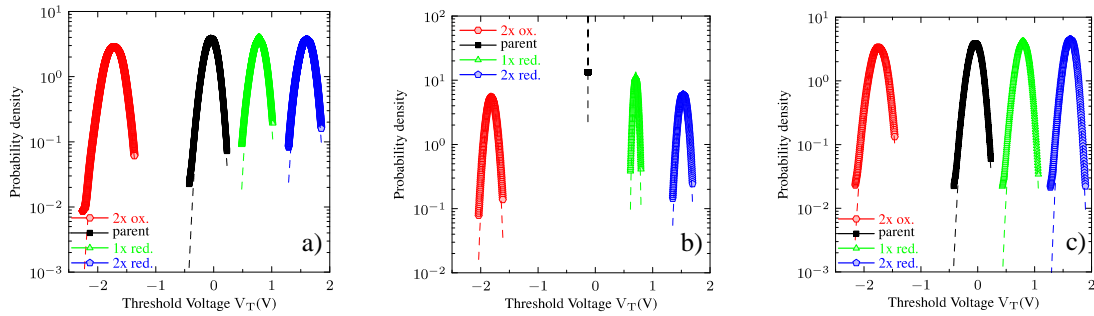
**Fig. 1.** a) Schematic representation of a single-transistor FDSOI non-volatile memory cell, indicating the aimed substitution of the poly-Si floating gate (FG) with an array of polyoxometalate clusters (POM layer). The green balls are point charges representing the cations, which surround each POM in the experiment. b)– 3D electrostatic potential in oxide and the substrate. Fingerprint of the 3x3 POMs in the gate and the random dopant in the source and the drain are clearly visible.



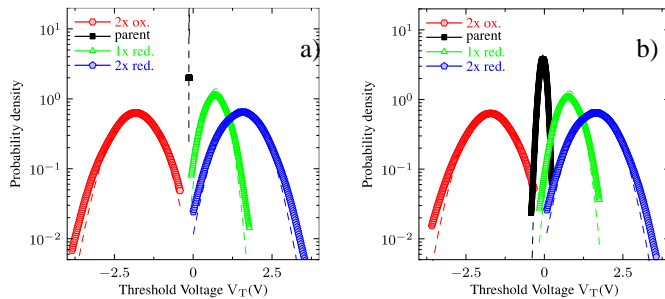
**Fig. 2.** Energy diagram comparing the conduction and valence band edges of Si and SiO<sub>2</sub> relative to the HOMO and LUMO levels of three POMs. Ball-and-stick view (insert) of three non-classic Wells-Dawson structure W<sub>18</sub>SO<sub>3</sub> - [W<sub>18</sub>O<sub>54</sub>(SO<sub>3</sub>)<sub>2</sub>]<sup>4-</sup>; M<sub>18</sub>SO<sub>3</sub> - [M<sub>18</sub>O<sub>54</sub>(SO<sub>3</sub>)<sub>2</sub>]<sup>4-</sup> and W<sub>18</sub>SeO<sub>3</sub> - [W<sub>18</sub>O<sub>54</sub>(SeO<sub>3</sub>)<sub>2</sub>]<sup>4-</sup>.



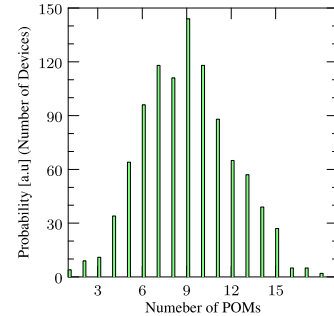
**Fig. 3.** Comparison between sheet charge approximation (SCA) and the numerical results of the simulated flash cell for two gate materials (SiO<sub>2</sub> & Al<sub>2</sub>O<sub>3</sub>) at two T<sub>tun</sub> oxide values (4.5 nm & 1.5 nm).



**Fig. 4.** Probability density function (PDF) of the V<sub>T</sub> for each bit of 1,000 devices: a) with *RDF only*, b) with *POMF only* and c) with combined variability (*RDF with POMF*). Dashed line is a Gaussian fit.



**Fig. 5.** Probability density function (PDF) of the V<sub>T</sub> for each bit of 1,000 devices: a) without *RDF and with Poisson POMF* and b) with *RDF and Poisson POMF*.



**Fig. 6.** Histogram of the number of POMs for ensembles of 1,000 devices with POMF used in the Poisson distribution case.