Multiscale Modelling of Dielectric Breakdown in Amorphous HfO_2

Jack Strand[1,2] and Alexander Shluger[1]
[1]Department of Physics and Astronomy, University College London, Gower Street, London WC1E 6BT, UK
[2]Nanolayers Research Computing Ltd, 1 Granville Court, Granville Road, London, England, N12 0HL

Abstract Submission

We use a multi-scale modelling approach to study the time-dependent dielectric breakdown (TDDB) of an amorphous (a-) HfO_2 insulator in a metal-oxide-metal (MOM) capacitor. We focus on the role played by electron injection in the creation of oxygen vacancies, which eventually form the percolation path responsible for dielectric breakdown. Energy parameters characterizing the creation of oxygen vacancies and the tunneling process are calculated using Density Functional Theory (DFT), employing a hybrid density functional. The results demonstrate that the formation of oxygen vacancies facilitated by electron injection into the oxide represents a crucial step in the degradation process dominating the kinetics at common breakdown fields.

Introduction

Micro- and nano-electronic devices based on metal-oxide-metal (MOM) and complementary metal-oxide-semiconductor (CMOS) systems are the basis of modern technology. Over many decades, scaling down of transistor- and memory-device dimensions have led to exponential advances in computing power. This scaling has also led to the replacement of SiO_2 with higher dielectric constant materials, such as HfO_2. However, in spite of decades of perfection, oxides used in CMOS devices, including SiO_2 and HfO_2, are prone to many field-induced reliability issues[1]. Here, we present the results of multi-scale modelling which link the physical processes responsible for the field induced degradation of a-HfO_2 with the characteristics of time-dependent dielectric breakdown (TDDB), such as temporal evolution of current through the oxide and Weibull plots of TDDB.

Model

The model is based on previous work, which shows that electrons trap into deep, intrinsic states in HfO_2[2] (Fig. 1). The trapping of electrons facilitates the production of vacancies by lowering the activation energy for a vacancy-interstitial pair[3]. Trapping of electrons at vacancies also facilitates the production of additional vacancies (Fig. 2). We calculate a range of parameters associated with these defects and reactions and use this parameterize a device level simulation in the Ginestra®[4] code. Effects such as TAT, Fowler-Nordheim tunneling, heat generation and vacancy generation et cetera are all included. This allows us to simulate the time evolution current through a TiN/HfO_2/TiN subjected to electrical stress.

Results and Conclusion

The results show that the trap based model agrees well with experiment. We also gain an insight into the formation of the percolation pathway from the spatial distribution of generated vacancies (Fig. 3). This also confirms the Joule feedback mechanism, in which hard breakdown is caused by local heating around the percolation path, leading to a catastrophic increase and current and generation of vacancies.

References

[1] Wu, Ernest Y. "Facts and myths of dielectric breakdown processes—Part I: Statistics, experimental, and physical acceleration models." IEEE Transactions on Electron Devices 66.11 (2019): 4523-4534.

[2] Strand, Jack, et al. "Intrinsic electron trapping in amorphous oxide." *Nanotechnology* 29.12 (2018): 125703.

[3] Strand, Jack, Moloud Kaviani, and Alexander L. Shluger. "Defect creation in amorphous HfO2 facilitated by hole and electron injection." *Microelectronic Engineering* 178 (2017): 279-283.

[4]"Applied Materials Ginestra®" [Online] Available: https://www.appliedmaterials.com/us/en/semiconductor/ginestra-software.html"

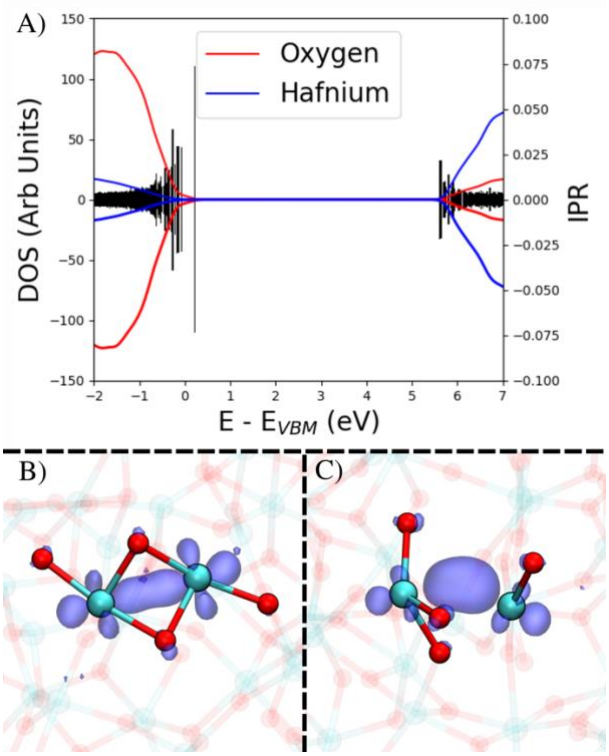

Fig. **1**. A) Projected density of states (lineplot) of a bulk, defect free amorphous HfO_2 model. Barplot shows the inverse participation ratio (IPR) of the KS states. High IPR indicates that the electron state is localized. The spectrum shows that there is part-localisation near the valence and conduction band edges. B) A single electron trap and C) A double electron trap in a-HfO_2.

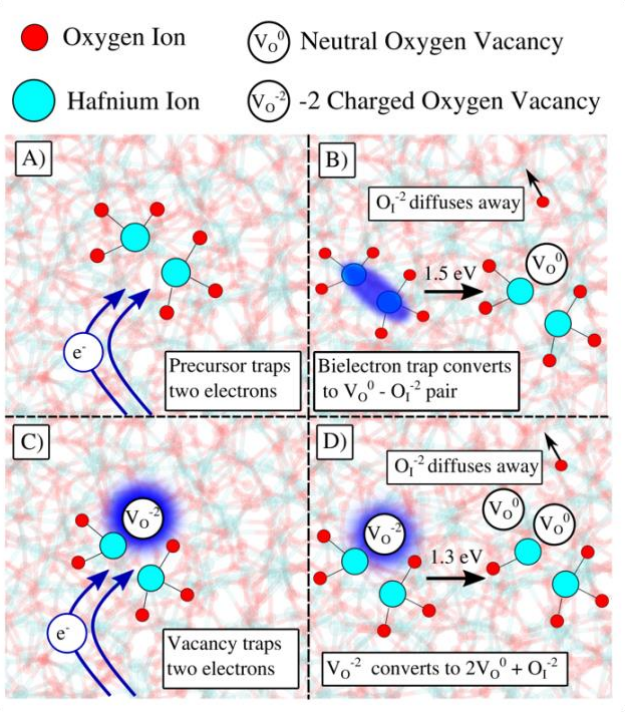

Fig. 2. Degradation model in amorphous HfO_2. A) The injection of electrons into the intrinsic trapping states shown in Fig 1. B) and Fig. 1C). B) The creation of a vacancy at the trap site. C) The injection of electrons into the vacancy, leading to negative charging. D) The generation of an additional vacancy.

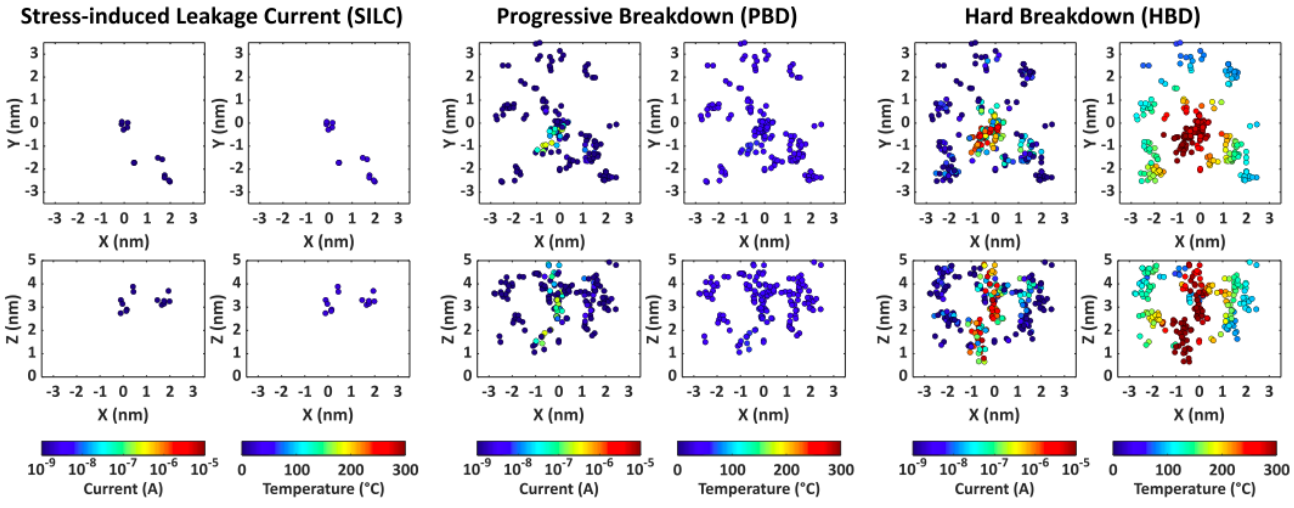

Fig. 3 Position, current and temperature of vacancies in a typical simulated device. Three different stages are shown: SILC, PBD and HBD. For each stage the top two panels show the X-Y projection of the simulation cell whereas the bottom two panels the X-Z projection. The bottom electrode is located at Z=0 and the top electrode is at Z=5 nm. Circles show O vacancies in the oxide. The colour of circles shows the values of current (left panels) and temperature (right panels) according to the colour coding schemes at the bottom of the figure. Initially, there is no clear percolation pathway or filament formation (in SILC and PBD). Eventually, at hard breakdown, a conducting filament indicated by a localised temperature and current increase has developed.