Defect generation in high-\( \kappa \) gate dielectric stacks: characterization and modelling
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INTRODUCTION

The generation of defects in p-Si/SiON/ZrO\(_2\)/TiN structures during electron injection from the TiN gate is studied. The data is consistent with a model considering the release of H\(^+\) (protons) at the anode, followed by the transport and trapping of H\(^+\) in oxide networks.

RESULTS AND DISCUSSION

The C-V characteristics (10kHz) of the structures are shown in Fig.1, before and after constant gate voltage stress at \(-3.6\) V. The generation of positive charges in the gate stack as well as defects at the Si/SiON interface is observed in Fig.1. Solid lines are fits to the data, assuming that the interface defects have an energetic distribution within the Si band-gap characteristic of P\(_{\text{in}}\) centers (1,2). The agreement between the model and data suggests the depassivation of Si=SiH caused by electron impact at the (100)/Si/SiON interface, and the subsequent release of hydrogen in the gate stack (3).

The density of positive charges N\(_p\) generated during the electrical stress is shown in Fig. 2 as a function of time for different values of \(V\) (stress voltage). One observes that N\(_p\) increases rapidly with time and saturates for t=600s, the saturation value increasing with \(V\).

The relative variation in the current density \(\Delta J_s/J_s(0)\) is presented in Fig.3 as a function of time for different values of \(V\). An increase in \(\Delta J_s(t)\) is observed, suggesting the generation of neutral defects in the gate stack, leading to the stress-induced leakage current (4).

The kinetics for positive charge and neutral defects generation in the gate stack can be explained by a dispersive hydrogen transport model. Once liberated at the Si/SiON interface, hydrogen can randomly hop in the gate stack, most probably in proton form (5). The proton can then be trapped in the SiON or ZrO\(_2\) network, leading to the generation of hydrogen-induced defects. The transport and trapping of H\(^+\) is modelled by a dispersive transport mechanism (6). The numerical simulations are shown in Figs. 2 and 3 as solid lines. The agreement between the data and the model is very good, and the comparison allows the determination of the defects centroid positions. It is found that the positive charge is located at about 7 Å from the Si/SiON interface, suggesting that this defect could be a Si=OH\(^+\) center (7). The neutral defect is found to be located in the ZrO\(_2\) layer, at about 11 Å from the TiN interface. This suggests that this defect could be a ZrOH and/or a ZrH center (8).

CONCLUSIONS

In conclusion, we suggest that the generation of defects in SiON/ZrO\(_2\) gate stacks during injection of electrons from the metal gate is related to the release of H\(^+\) at the Si/SiON interface, followed by the transport and trapping of H\(^+\) in oxide networks. This mechanism leads to the generation of hydrogen-induced positive charges and neutral defects in the SiON/ZrO\(_2\) stack.

REFERENCES


![Fig.1. C-V characteristics of a p-Si/SiON/ZrO\(_2\)/TiN structure (t=10kHz, 80μm×80μm area) measured before and after constant gate voltage stress at –3.6 V during 400 s. Solid lines are numerical simulations (3).](image1)

![Fig.2. Positive charge density N\(_p\) vs. time during constant gate voltage stress of the capacitors. Solid lines are numerical simulations.](image2)

![Fig.3. Normalized current density variation \(\Delta J_s/J_s(0)\) vs. time during constant gate voltage stress of the capacitors. Solid lines are numerical simulations.](image3)