Session 40: Modeling and Simulation - Simulation and Modeling of Advanced Process and Emerging Memory
Wednesday, December 5, 1:30 PM
Continental Ballroom 7-9
Co-Chairs: S-D Kim, SK Hynix
J. Kang, Peking University

1:35 PM - 2:00 PM
40.1 Physics of hole trapping process in high-k gate stacks: A direct simulation formalism for the whole interface system combining density-functional theory and Marcus theory, *Y.-Y. Liu, X. Jiang, Chinese Academy of Sciences*

Charge trapping defects in high-κ dielectrics and at their interfaces are known to be a challenging obstacle for the silicon based modern transistors. To facilitate the solution of such problems, a deeply physical understanding of the charge trapping process at atomistic scale is mandatory. As such, we propose, for the first time, a direct method to calculate the exact hole trapping rates explicitly in the high-***k*** gate stack consisting of silicon channel, SiO2 interfacial layer and HfO2. The physics of multiple path (trap locations) hole trapping processes is revealed by combining density-functional theory and Marcus theory. The roles of physical quantities including defect reorganization, coupling constant and Gibbs free energy are discussed. It is suggested that oxygen vacancies at high-***k*** interface with interfacial layer SiO2 are dominant hole traps under NBTI stress. The developments and findings provide not only a deep physical insight into the hole trapping related reliability degradation mechanism, but also a new simulation framework.

2:00 PM - 2:25 PM
40.2 Parasitic Surface Reactions in High-Aspect Ratio Via Filling using ALD: A Stochastic Kinetic Model, *T. Muneshwar, G. Shoute, D. Barlage*, and K. Cadien*, Synthergy Inc., *University of Alberta*

A scalable kinetic Monte-Carlo model (sKMC) of molecular transport for atomic layer deposition (ALD) for high aspect-ratio (AR) features is developed. Surface coverage is a critical parameter studied here in detail. The capabilities of the stochastic model provide insight into challenges in growing ALD films in high-AR via structures faced by the industry, including the effects of parasitic surface reactions resulting in poor coverage. Furthermore, we provide experimental results verifying the model's prediction by growing ALD SiNx on high-AR via structures. By compensating for the processing errors corroborated by the model, we experimentally improved sidewall coverage from 70% to 92%.

2:25 PM - 2:50 PM
40.3 Physics-based modeling of volatile resistive switching memory (RRAM) for crosspoint selector and neuromorphic computing, *W. Wang, A. Bricalli, M. Laudato, E. Ambrosi, E. Covi, and D. Ielmini, Politecnico di Milano*

Volatile resistive switching memory (RRAM) is raising strong interest as potential selector device in crosspoint memory and short-term synapse in neuromorphic computing. To enable the design and simulation of memory and computing circuits with volatile RRAM, compact models are essential. To fill this gap, we present here a novel physics-based analytical model for volatile RRAM based on a detailed study of the switching process by molecular dynamics (MD) and finite-difference method (FDM). The analytical model captures all essential phenomena of volatile RRAM, e.g., threshold/holding voltages, on-off ratio, and size-dependent retention. The model is validated by extensive comparison with data from Ag/SiOx RRAM. To support the circuit-level capability of the model, we show simulations of crosspoint arrays and neuromorphic time-correlated learning.

2:50 PM - 3:15 PM

40.4 Analytic Model for Statistical State Instability and Retention Behaviors of Filamentary Analog RRAM Array and Its Applications in Design of Neural Network, *P. Huang, Y. C. Xiang, Y. D. Zhao, C. Liu, B. Gao*, H. Q. Wu*, H. Qian*, X. Y. Liu, J. F. Kang, Peking University, *Tsinghua University*

For the first time, an analytic model is presented for the statistical state instability and retention behaviors of filamentary analog resistive random access memory (RRAM) array. In the model, the diffusion of oxygen vacancy (VO), the Brownian-like hopping of VO during the diffusion process and the recombination of VO are considered. The statistical state instability and retention behaviors of different states under various temperatures are accurately described by the model, which is verified by the measured data of 1Kb filamentary analog RRAM (FA-RRAM) array. Furthermore, the analytic model is successfully implemented to evaluate and optimize the reliability of FA-RRAM based multi-layer neural network. Guided by the model, optimized synapse structures and refresh operation are proposed to significantly enhance the reliability of FA-RRAM based neural network.

3:15 PM - 3:40 PM

40.5 Evidence of Magnetostrictive Effects on STT-MRAM Performance by Atomistic and Spin Modeling, *K. Sankaran, J. Swerts, R. Carpenter, S. Couet, K. Garello, R. F. L. Evans*, S. Rao, W. Kim, S. Kundu, D. Crotti, G. S. Kar, and G. Pourtois, imec, *University of York*

We demonstrate, using an atomistic description of a 30nm diameter spin-transfer-torque magnetic random access memories (STT-MRAM), that the difference in mechanical properties of its sub-nanometer layers induces a high compressive strain in the magnetic tunnel junction (MTJ) and leads to a detrimental magnetostrictive effect. Our model explains the issues met in engineering the electrical and magnetic performances in scaled STT-MRAM devices. The resulting high compressive strain built in the stack, particularly in the MgO tunnel barrier, and its associated non-uniform atomic displacements, impacts on the quality of the MTJ interface and leads to strain relieve mechanisms such as surface roughness and adhesion issues. We illustrate that the strain gradient induced by the different materials and their thicknesses in the stacks has a negative impact on the tunnel magneto-resistance, on the magnetic nucleation process and on the STT-MRAM performance.