

Session 16: Modeling and Simulation - Advanced Modeling of Ferroelectric Materials and Devices

Tuesday, December 4, 9:00 AM

Plaza A

Co-Chairs: R. Clerc, Institute d'Optique

Y. Chauhan, IIT Kanpur

9:05 AM - 9:30 AM

16.1 In-Memory Computing Primitive for Sensor Data Fusion in 28 nm HKMG FeFET Technology, *K. Ni, B. Grisafe, W. Chakraborty, A. K. Saha***, *S. Dutta, M. Jerry, J. A. Smith, S. Gupta***, and *S. Datta, University of Notre Dame*, **Purdue University*

In this work, we exploit the spatio-temporal switching dynamics of ferroelectric polarization to realize an energy-efficient, and massively-parallel in-memory computational primitive for at-node sensor data fusion and analytics based on an industrial 28nm HKMG FeFET technology [1]. We demonstrate:(i) the spatio-temporal dynamics of polarization switching in HfO₂-based ferroelectrics under the stimuli of sub-coercive voltage pulses using experiments and phase-field modeling; (ii) an inherent rectifying conductance accumulation characteristic in FeFET with a large dynamic range of $G_{max}/G_{min} > 100$ in the case of 3.0V, 50ns gate pulses; (iii) transition to more abrupt accumulation characteristics due to single/few domain polarization switching in scaled FeFET (34nm LG); and (iv) successful detection of physiological anomalies from real- world multi-modal sensor data streams.

9:30 AM - 9:55 AM

16.2 Experimentally Validated, Predictive Monte Carlo Modeling of Ferroelectric Dynamics and Variability, *C. Alessandri, P. Pandey, and A. C. Seabaugh, University of Notre Dame*

A physics based, predictive, circuit compatible Monte Carlo simulation framework for ferroelectric dynamics is developed. Polarization reversal data is used to extract the statistical distribution of the ferroelectric grains. With these parameters, the ferroelectric response to any arbitrary waveform, its scaling behavior, and variability are predicted without further calibration.

9:55 AM - 10:20 AM

16.3 Scalability Study on Ferroelectric-HfO₂ Tunnel Junction Memory Based on Non-equilibrium Green Function Method with Self-consistent Potential, *F. Mo, Y. Tagawa, T. Saraya, T. Hiramoto, M. Kobayashi, The University of Tokyo*

We have investigated scalability and design guideline of HfO₂-based Ferroelectric Tunnel Junction (FTJ) memory by employing numerical simulation which is based on Non-Equilibrium Green Function (NEGF) method and self-consistent potential, and calibrated by our experimental FTJ data, for the first time. Metal-Ferroelectric-Insulator-semiconductor (MFIS) FTJ shows a higher TER than Metal-Ferroelectric-Insulator-Metal (MFIM) FTJ with almost the same read current because of the large asymmetry of dielectric screening property in top and bottom electrodes. High read current can be obtained by thinner layers while high TER and low depolarizing field area maintained by adjusting bottom semiconductor electrode property. Based on these results, a guideline for designing MFIS structure FTJ to achieve high read current and high TER has been proposed. We have shown a potential for scaling the FTJ down to sub-20 nm diameter.

10:20 AM *Coffee Break*

10:45 AM - 11:10 AM

16.4 Role of Oxygen Vacancies in Electric Field Cycling Behaviors of Ferroelectric Hafnium Oxide, *C. Liu, F. Liu, Q. Luo***, *P. Huang**, *X. X. Xu***, *H. B. Lv***, *Y. D. Zhao, X.Y. Liu and J. F. Kang, Peking University*, ***Chinese Academy of Sciences*, ****University of Hong Kong*

Based on first principle calculations, a new mechanism of the oxygen vacancies(V_o) in the HfO₂-based ferroelectric devices is presented. In this mechanism, the V_o in m-phase HfO₂ not only serve as the electron traps but also emerge ferroelectricity besides the known o-phase HfO₂. And the increased remanent polarization during the “wake-up” process is mainly attributed to this part of V_o -m-phase HfO₂ ferroelectric cells. Based on the new mechanism, a Kinetic Monte Carlo (KMC) simulator is developed to quantify the typical electric cycling behaviors observed in the HfO₂-based ferroelectric devices, including the wake-up, fatigue, split-up, and breakdown effects. This new understanding establishes relationship between the V_o and the cycling behaviors, and further shows the connection between the dopant and the wake-up characteristics of HfO₂-based ferroelectric device.

11:10 AM - 11:35 AM

16.5 First-Principles Perspective on Poling Mechanisms and Ferroelectric/ Antiferroelectric Behavior of Hf_{1-x}Zr_xO₂ for FEFET Applications, *S. Clima, S.R.C. McMitchell, K. Florent*, L. Nyns, M. Popovici, N. Ronchi, L. Di Piazza, J. Van Houdt, G. Pourtois, imec, *University of Leuven, PLASMANT, University of Antwerp*

We investigate at the atomic level the most probable phase transformations under strain, that are responsible for the ferroelectric/ antiferroelectric behavior in Hf_{1-x}Zr_xO₂ materials. Four different crystalline phase transformations exhibit a polar/ non-polar transition: monoclinic-to-orthorhombic requires a gliding strain tensor, orthorhombic-to-orthorhombic transformation does not need strain to polarize the material, whereas tetragonal-to-cubic cell compression and tetragonal-to-orthorhombic cell elongation destabilizes the non-polar tetragonal phase, facilitating the transition towards a polar atomic configuration, therefore changing the polarization-electric field loop from antiferroelectric to ferroelectric. Oxygen vacancies can reduce drastically the polarization reversal barriers.