PCSI
Room Ballroom South - Session PCSI-WeM1
Ferroelectric & Neuromorphic Computing Materials

Moderator: Alec Talin, Sandia National Laboratories

8:30am **PCSI-WeM1-1 Emergent Phenomena at Ferroelectric/van der Waals Heterointerfaces*, Xia Hong,*** University of Nebraska - Lincoln **INVITED**

The heterointerfaces between ferroelectrics and two-dimensional (2D) van der Waals materials present a versatile platform for achieving novel interfacial coupling, nonvolatile field effect control, and nanoscale programmable functionalities.In this talk, I will discuss a range of emergent phenomena in ferroelectric/vdW heterostructures mediated by interfacial coupling of charge, lattice, and polar symmetry. By combining polarization doping with nanoscale domain patterning in a ferroelectric polymer P(VDF-TrFE) top-gate, we create directional conducting paths in an insulating 2D channel, which reveals highly anisotropic conductivity in monolayer (1L) to 4-layer 1T'-ReS$_2$ between the directions along and perpendicular to the Re-chain [1]. The interface-epitaxy between P(VDF-TrFE) and ReS$_2$ leads to large scale P(VDF-TrFE) thin films composed of highly ordered, close-packed, 10 and 35 nm wide crystalline nanowires [2]. We observe enhanced polar alignment, piezoelectricity, and Curie temperature in thin CuInP$_2$S$_6$ (CIPS) flakes prepared on ferroelectric oxide PbZr$_{0.2}$Ti$_{0.8}$O$_3$ (PZT), which can be attributed to the interfacial strain imposed by PZT [3]. An unconventional filtering effect of second harmonic generation signal is enabled by the polar coupling of 1L MoS$_2$ with either the polar domain or the chiral dipole rotation at the domain wall surface in PZT thin films or free-standing membranes [4,5]. Our study showcases the rich research opportunities offered by integrating ferroelectrics with 2D materials.

[1] D. Li *et al.*, Phys. Rev. Lett.**127**,136803 (2021).

[2] D. Li *et al.*, Adv. Mater.**33**, 2100214 (2021).

[3] K. Wang *et al.*, ACS Nano (2023). DOI: 10.1021/acsnano.3c03567

[4] D. Li *et al.*, Nat. Commun.**11**, 1422 (2020).

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9:10am **PCSI-WeM1-9 Impact of High-Power Impulse Magnetron Sputtering Pulse Width on the Nucleation, Crystallization, Microstructure, and Ferroelectric Properties of Hafnium Oxide Thin Films*, Samantha Jaszewski,*** Sandia National Laboratories

The impact of the high-power impulse magnetron sputtering (HiPIMS) pulse width on the crystallization, microstructure, and ferroelectric properties of undoped HfO$_2$ films is reported. HfO$_2$ films were sputtered from a Hf target in an Ar/O$_2$ atmosphere, varying the instantaneous power density by changing the HiPIMS pulse width with fixed time averaged power and pulse frequency. The pulse width is shown to affect the ion-to-neutral ratio in the depositing species with the shortest pulse durations leading to the highest ion fraction, as shown in Figure 1. *In-situ* X-ray diffraction measurements during crystallization demonstrate that the HiPIMS pulse width impacts nucleation and phase formation, with an intermediate pulse width of 110 µs stabilizing the ferroelectric phase over the widest temperature range. Although the pulse width impacts the grain size with the lowest pulse width resulting in the largest grain size (Figure 2), grain size does not strongly correlate with phase content or ferroelectric behavior in these films. These results suggest that precise control over the energetics of the depositing species may be beneficial for stabilizing the ferroelectric phase in this material.

9:15am **PCSI-WeM1-10 Fabrication and Gamma Radiation Effects on Endurance of Ferroelectric Hafnium Zirconium Oxide Capacitors*, M. David Henry*,** Sandia National Laboratories*; M. Lenox,* University of Virginia*; A. Hillsman,* North Carolina State University*; S. Jaszewski, G. Esteves,* Sandia National Laboratories, USA*; J. Jones,* North Carolina State University*; J. Ihlefeld,* University of Virginia

Ferroelectric hafnium zirconium oxide (HZO) is attracting significant interest in the semiconductor microelectronics industry with attributes including coercive voltages compatible with CMOS, retention of memory states after power down and reasonable polarizations achieved with films 8 to 15 nm thick.An immediate application of the HZO capacitors include non-volatile memory (NVM) with insertions in the back end of line (BEOL) fabrication.Although devices such as ferroelectric capacitors are most applicable for FeRAM integrations, subtle details in their fabrication including the electrodes used and thickness can have impact in the device performance metrics.

This work investigates electrode configurations, including W and TiN, ferroelectric thickness and anneals utilized in BEOL processes for effects on endurance and polarization.Insertion of thin linear dielectrics, 1 nm of alumina on the bottom electrode, is also investigated to determine properties impactful to FeRAM circuit design. To determine the stability of the film, device polarization and endurance was measured after 5 MRad of Co^{60} gamma cell irradiation over differing voltage rails and cycling frequencies.This work extends the knowledge base of ferroelectric HZO with radiation effects for non volatile memory applications in CMOS.

9:20am **PCSI-WeM1-11 Design of Memristive Devices Towards Neuromorphic Computing*, Aiping Chen,*** Los Alamos National Laboratory **INVITED**

Current digital computing based on Von Neumann architecture suffers from several key bottleneck including von Neumann bottleneck, Moore's law, and the breakdown of Dennard scaling. Developing new computing platforms provide solutions towards Beyond Moore's computing. Recently, emergent devices such as memristive switching devices have been used to emulate some brain functions including synaptic behavior and neuronal behavior and therefore they have been proposed for developing low-power neuromorphic computing. Oxide-based memristive devices with excellent scalability have the potential to revolutionize not only the field of information storage but also neuromorphic computing.

In this talk, I will first discuss some basics of the brain, brain-inspired neuromorphic computing and artificial intelligence. In the second part of my talk, I will then discuss the roles of defects and interfaces on switching behavior in different types of memristive devices and their impacts on neuromorphic computing. Material systems have profound effects on switching behavior. For example, ferroelectric and non-ferroelectric systems show completely different switching behavior [1-2]. Defects also dominate the switching behavior. Figure 1 compared switching behavior in a variety of materials with different type of defects. Among different types of switching, filament-type switching and interface-type switching are two most distinct switching modes. I will focus on a specific interface-type switching we observed in Au/Nb:SrTiO$_3$ system [3]. It shows the switching is controlled by protons in the environment. We also explored the applications of such systems for neuromorphic computing applications [4].

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10:05am **PCSI-WeM1-20 Neuromorphic Memristors with TiO$_2$ and a-IGZO Bilayer Structure*, Jae-Yun Lee,*** College of Electrical and Computer Engineering, Chungbuk National University, South Korea*; H. Zhao, X. Wang, S. Shi,* College of Electrical and Computer Engineering, Chungbuk National University, South Korea, China*; B. Lee, S. Kim,* College of Electrical and Computer Engineering, Chungbuk National University, South Korea

In recent years, ReRAM devices have gained significant attention in neuromorphic applications and hardware-based artificial intelligence [1–2]. Specifically, the resistive memory devices exhibit ultrafast read and write speeds, high retention time [3], low voltage operation and low power consumption, emerging an attractive research target from the perspective of the modern low-cost portable devices [4].

Our proposed device performance and physical properties of the fabricated ReRAM devices were assessed at various annealing temperatures. The analysis from XPS results confirms that the device operation was mostly driven by the density of oxygen vacancies in the TiO$_2$ and a-IGZO bilayer structure. The optimal density of oxygen vacancies in the a-IGZO causes the drift of O^{2-} ions to and from the TiO$_2$ layer that induced a significant variation in the resistivity of the device, providing switching behavior.

10:10am **PCSI-WeM1-21 Origin of Large Electro-Optic Response in Ferroelectrics*, Alex Demkov*,** *I. Kim, T. Paoletta, S. Apte,* The University of Texas at Austin

Integrated silicon photonics experiences a revolution [1]. The key element of this technology is an optical modulator (OM) playing a role similar to that of a usual transistor. OMs based on a phase shifter using a linear electro-optic (EO) effect are an attractive option for building ultra-compact, fast and low power OMs [2]. Linear EO effect can be only observed in non-centrosymmetric materials, such as ferroelectrics, which started a search for ferroelectrics that can be integrated with Si and maintain a strong EO effect in thin films [3]. Ab initio calculations became an indispensable tool in this search [4].

We will discuss our recent progress in understanding the microscopic mechanism behind the EO response in three ferroelectrics successfully integrated on Si:$BaTiO_3$ (BTO), $LiNbO_3$ (LN) and $Sr_xBa_{1-x}Nb_2O_6$ (SBN). There are three parts to the EO effect in a ferroelectric, they are ionic, piezo and electronic contributions [5,6]. In different materials, different components of the EO tensor are dominated by different contributions. This has implications for the device design, depending on the temperature and frequency range. For example, optical quantum computing occurs at cryotemperatures (when optical phonons are frozen out), and thus has rely on the electronic and piezo contributions. On the other hand, at high RF frequencies, only the ionic and electronic contributions survive. On the fundamental level, our results support the notion that P4mm BTO is a dynamic average of lower symmetry Cm structures (Fig. 1). We also discover that in SBN, surprisingly the major contribution to the EO effect comes from high frequency optical phonons (Fig. 2). And in LN, ferroelectricity and the EO response are essentially decoupled.

The work is supported by the AFOSR under Award No FA9550-18-1-0053.

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