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ABSTRACT:

Field-Driven Oxygen Drift and Its Impact on Ferroelectric HfO_2-Based Thin Films

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Ferroelectricity in HfO2-based thin films has drawn significant academic and industrial interest since its first report in 2011.[1-3] The ferroelectric response is primarily linked to the metastable orthorhombic phase (space group Pca21), whose formation and stability are highly sensitive to processing conditions, microstructure, and defect chemistry. In particular, the concentration of oxygen vacancies and their electric-field-driven drift have been widely reported as crucial factors governing polymorphism in HfO_2-based ferroelectric films, thereby strongly affecting ferroelectric properties and device reliability.

In this presentation, we provide an integrated review of how oxygen-vacancy concentrations and field-induced vacancy drift affect the relative phase fractions within HfO_2-based ferroelectric layers and how these shifts translate into changes in ferroelectric properties. We also discuss vacancy-mediated structural evolution under electrical stressing and its implications for functional performance. We further highlight recent results from our group using in situ grazing-incidence wide-angle X-ray scattering (GI-WAXS) to track, in real time, crystallographic phase evolution and strain development during electrical biasing and cycling. By combining these structural insights with electrical characterization, we elucidate the interplay among oxygen-vacancy drift, phase competition, and ferroelectric response. Finally, we discuss practical strategies to improve the performance and reliability of semiconductor devices employing HfO_2-based ferroelectric thin films.

[1] T. S. Boescke et al. Appl. Phys. Lett., 99, 102903 (2011).
[2] M. H. Park et al. Adv. Mater., 27, 1811 (2015).
[3] U. Schroeder and M. H. Park et al. Nat. Rev. Mater., 7, 653 (2022).