ATOMISTIC MECHANISMS FOR POLARIZATION SWITCHING AND WAKEUP IN HFO_X-BASED FERROELECTRICS

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Recently, with the development of the *o*-HfO_2, the ferroelectrics have regained the increased interest in the device community. In an attempt to understand the atomistic mechanisms driving the polarization switching, we observe a fine balance between dipole-field energy and anion drift force that defines the switching mechanism during polarization reversal. We show that constrained relaxation can lead to 90° polarization rotation (domain deactivation). Intrinsically, the Si/V_O-doping can switch faster than undoped HfO_2 or HfZrOx.[1] By simulating the switching barrier heights in strained HfO_2 systems, we predict what type of crystalline structures might phase-transform during the wakeup phase of the ferroelectric operation.[2]

Keywords
Orthorhombic HfO_2, ferroelectric switching.

References
[1] S. Clima et al., IEDM (2020).
[2] S. Clima et al., IEDM (2018).