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Ferroelectricity in nanoscaled ZrO2 thin films and their promising application in energy storage capacitors

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Zirconia and hafnia based thin films have attracted considerable attention in the last decade due to the existence of a ferroelectric behavior at the nanoscale, which can enable the downscaling of the next-generation of non-volatile memory and energy storage devices [1,2].
In this presentation an overview regarding the recent advances on these materials will be given [2]. Then, our most recent results on this topic will be discussed. The effect of the insertion of a thin dielectric HfO2:Al2O3 (HAO) layer, with a thickness ranging from 2 to 8 nm, on the tunability of the ferroelectric and energy storage characteristics of ZrO2 films is presented [3]. An optimal combination of high energy density of 54.3 J/cm3 and good storage efficiency of 51.3% is obtained for the ZrO2 film capacitors with a 2 nm-thick HAO insert layer. These values correspond to an increase of ˜ 55% and ˜ 92%, from the respective values of pure ZrO2 film capacitors. Moreover, special attention will be given to the existence of a novel rhombohedral R3m phase in ZrO2 thin films [4]. This presentation relates experimental structural studies to density-functional theory (DFT) calculations to disclose this novel rhombohedral R3m phase in epitaxially-strained (111)-oriented ZrO2 thin films, grown by ion-beam sputtering deposition technique on (111)-Nb:SrTiO3 substrates. Comprehensive local and macroscopic ferroelectric characterization reveals that these ZrO2 films display a switchable ferroelectric polarization reaching 20.2 μC/cm2 with a coercive field of 1.5 MV/cm. Interestingly, these films show a wake-up free ferroelectric behaviour.

References

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