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Theoretical Investigation of the Hafnia-Hafnium Interface in RRAM Devices ANDREW O'HARA, The University of Texas at Austin, GENNADI BERSUKER, SEMATECH, ALEXANDER DEMKOV, The University of Texas at Austin — Oxide based resistive-switching memory devices (RRAM) utilizing hafnia (HfO_2) as the dielectric serve as an attractive option for embedded non-volatile memory systems. Successful operation requires a degree of oxygen deficiency caused by application of a forming voltage. A recent approach to help facilitate this has been the use of an oxygen gettering layer overlaying hafnia. Using density functional theory (DFT) in the local density approximation (LDA), we construct and study a hafnia-hafnium interface to understand the reducing and gettering properties. With this interface, we compare two routes to the creation of substoichiometric hafnia: formation of oxygen vacancies that leave hafnium unoxidized and migration of oxygen to hafnium to form an extended Frenkel pair (FP). Our work shows that the presence of the interface lowers the vacancy formation energy by 1.1 eV from the bulk value of 7.5 eV. Using the nudged-elastic band method, we show that not only is the formation energy lower for an extended FP, but that the barrier to formation of the shortest such FP is only 1.3 eV implying the favorability of such defects. Finally, we study the diffusion of oxygen in bulk hafnium to learn how the defect would behave after disassociation of the FP.

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