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Is the oxygen vacancy the dominating charge trap in hafnia based MOSFETs? JACOB GAVARTIN, DAVID MUNOZ-RAMO, ALEXANDER SHLUGER, MARSHALL STONEHAM, University College London, U.K., GENNADI BERSUKER, SEMATECH, TX, U.S.A. — One of the factors affecting performance of high-k based MOSFETS is the instability of the threshold voltage, V_T, attributed to a high concentration of the carrier traps in the dielectric stack. Bulk oxygen vacancies in HfO_2 had been suggested as dominating electric traps, although this has not been unambiguously proved. We present ab initio calculations of the vacancies and divacancies in the monoclinic HfO_2 with the charge states +2,+1,0,-1,-2. Recent electrical I-V measurements probing V_T relaxation under pulsed electrical stress [1] infer that: 1. The charge trapping under the applied stress is significantly faster than de-trapping following stress release suggesting significance of lattice relaxation upon trapping. 2. The kinetics of this V_T relaxation is multiexponential with dominating activation energies in the range and 0.25-0.45 eV. We juxtapose the experimental data with the energetic parameters obtained from the calculations and consider whether the charge trapping and de-trapping by the variously charged vacancy levels accounts for all available experimental trends. [1] R. Choi, S.C. Song, C.D. Young, G. Bersuker, B.H. Lee, Appl. Phys. Lett. 87, 122901 (2005).

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