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H-shuttling within a Hf-defect complex in Si/SiO2/HfO2 structures A.G. MARINOPOULOS , I. BATYREV, X. ZHOU, R. SCHRIMPF, D. FLEETWOOD, S.T. PANTELIDES, Vanderbilt University, Department of Physics and Astronomy — It was recently shown that, following irradiation of Si-SiO2/HfO2 structures by X-rays or constant-voltage stress, both oxide- and interface-trap densities exhibit oscillations with switch-bias annealing that are much larger than those previously observed in Si/SiO_2 devices. Here we describe a particular defect complex that can account for the observations. The complex comprises a suboxide Hf-Si bond and an interfacial dangling bond (P_b center). With the aid of first-principles calculations we show that this defect possesses a symmetric double-well minimum and can provide trapping sites for H atoms near the interface. In the first site, the H atom passivates the dangling bond; in the second site the H atom resides near the center of the Hf-Si bond. A moderate intervening barrier (1.2 eV) suggests a relatively easy hopping of H atoms between these two energy minima, aided by the applied field and temperature. This shuttling mechanism can explain the observed oscillations in the interface trap densities during switched-bias conditions. This work was supported in part by the AFOSR and the DOE.

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