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Reactions of water molecules at the Si/SiO2 interface I.G. BATYREV, L. TSETSERIS, Department of Physics and Astronomy, D.M. FLEETWOOD, R.D. SCHRIMPF, Electrical Engineering and Computer Science, S.T. PANTELIDES, Department of Physics and Astronomy, Vanderbilt University, Nashville, TN 37235 — Water molecules can be present to a varying degree at Si/SiO2 interfaces, either introduced by the oxidation process or through absorption from the atmosphere. Such water molecules may affect critically the electrical properties of metal-oxide-semiconductor (MOS) structures and devices. Here we present results of first-principles density-functional calculations of several pathways of water reactions near the Si/SiO2 interface. We found that (i) the presence of water molecules is energetically favored in the a-silica rings near the interface with an energy gain of ~ 0.3 eV relative molecule in vacuum; (ii) a water molecule causes depassivation of Si-H bonds with formation of a Si dangling bond, H_2 molecule and loose OH complex; (iii) a water molecule may passivate a Si dangling bond and form a loose OH complex; (iv) a water molecule may oxidize the Si-Si bonds and form a H_2 molecule. The interplay of reactions results in changes in interface-trap density. We compare the results with radiation-response measurements of nMOSFETS right after production and after 18 years of aging and explain the observed growth of interface trap density ($0.7\text{x}10^{11}\text{cm}^{-2}$) just after X-ray irradiation. This work was supported in part by the AFOSR and the US Navy.

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