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New SiOH complexes and proton release mechanism in silica as a source of Si/SiO_2 interface-trap build up I.G. BATYREV, S.T. PANTELIDES, Department of Physics and Astronomy, Vanderbilt University, M.P. RODGERS, D.M. FLEETWOOD, R.D. SCHRIMPF, Electrical Engineering and Computer Science Department, Vanderbilt University — Water molecules in SiO_2 have been studied extensively in the context of reliability of electronic devices. Here we report results of new density-functional first-principles calculations and experimental data that demonstrate a key role of H_2O molecules in the long-term degradation of MOSFETs by increases in interface-trap densities. A new low energy complex formed by H_2O has been identified. The complex consists of two SiOH groups located on neighboring rings. The energy of the complex is 0.3 eV lower than that for the free interstitial water molecule in the ring of ~ 0.7 nm. The two silanol groups have different local topology, which results in different ability of the SiOH elements to capture holes and release protons under X-irradiation. The release of H^+ has a barrier of the reaction ~ 0.45 eV and is accompanied by creation of a peroxy-type structure inside network ring. The released protons can diffuse or drift (driven by electric fields) to the interface, where they depassivate dangling bonds by forming H_2 molecules. We will present experimental data on the radiation response of devices that have been in storage for 20 years. The results are consistent with the theoretical picture, when water molecules are responsible for a substantial increase of interface-trap densities over time.

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