Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Ab initio modeling of interfacial oxygen defects in ultrathin high-k gate dielectric stacks BLANKA MAGYARI-KOPE, Stanford University, ERIC COCKAYNE, NIST, YOSHIO NISHI, Stanford University — As the thickness of the metal-oxide-semiconductor field-effect transistor (MOSFET) is further reduced, and the gate dielectric is under constant voltage, traps due to defects are generated and may form a conductive path. At a critical density of defects this may lead to gate dielectric breakdown. First principles methods based on density functional theory and non-equilibrium Green's function calculations are employed to calculate the tunneling current through ultrathin oxide layers of HfO_2 and SiO_2 in a gate stack structure with Pt metal electrode. The microscopic effects of the oxygen defects formation on the electronic transport through the gate oxides are analyzed and discussed. A number of interface models are constructed that include oxygen vacancies at various interfaces and isolated oxygen vacancy defects in the bulk oxide. The band offsets and the tunneling currents are calculated as a function of defects positions in the gate dielectric.

Blanka Magyari-Kope
Stanford University

Date submitted: 20 Nov 2008 Electronic form version 1.4