Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Interface effects on calculated defect levels for oxide defects[1]

ARTHUR EDWARDS, Air Force Research Laboratory, HUGH BARNABY, Arizona State University, PETER SCHULTZ, Sandia National Laboratories, ANDREW PINEDA, Air Force Research Laboratory — Density functional theory (DFT) has had impressive recent success predicting defect levels in insulators and semiconductors [Schultz and von Lillienfeld, 2009]. Such success requires care in accounting for long-range electrostatic effects. Recently, Komsa and Pasquarello have started to address this problem in systems with interfaces. We report a multiscale technique for calculating electrostatic energies for charged defects in oxide of the metal-oxide-silicon (MOS) system, but where account is taken of substrate doping density, oxide thickness, and gate bias. We use device modeling to calculate electric fields for a point charge a fixed distance from the interface, and used the field to numerically calculate the long-range electrostatic interactions. We find, for example, that defect levels in the oxide do depend on both the magnitude and the polarity the substrate doping density. Furthermore, below 20 Å, oxide thickness also has significant effects. So, transferring results directly from bulk calculations leads to inaccuracies up to 0.5 eV– half of the silicon band gap. We will present trends in defect levels as a function of device parameters. We show that these results explain previous experimental results, and we comment on their potential impact on models for NBTI.

[1]Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the United States Department of Energy's National Nuclear Security Administration under co

Arthur Edwards
Air Force Research Laboratory

Date submitted: 15 Nov 2013 Electronic form version 1.4