Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Hydrogen-induced defect generation in amorphous SiO_2 MASAYASU MIYATA, Seiko-Epson Corp., ADRI C.T. VAN DUIN, JAMIL TAHIR-KHELI, WILLIAM A. GODDARD III, MSC, Caltech — Dielectric breakdown of thin silicon oxides (SiO_2) of metal-oxide semiconductor field-effect transistors is a long-standing problem. The breakdown is generally recognized to be due to the accumulation of defects in the oxide. An amorphous SiO_2 (a-SiO_2) has been known to have very few defects, thanks to its strong and flexible network of Si-O bonds. Then, why are defects created in this good insulator? The hydrogen related chemistry model has the potential to explain dielectric breakdown, but it is still unclear how hydrogen could generate the energy required to break Si-O bonds. Using the quartz structure, molecular dynamics simulations have been executed with Reax Force Field (ReaxFF) method that is fitted to give first principle energy profiles. In these simulations we found that at elevated temperatures a meta-stable structure of hydrogen attached to Si- O bond is formed, which we will refer to as the Attached Radical (Att_ Rad). Att_Rad has a degenerated half-filled electronic level, so will be good candidate for breakdown precursor. We will discuss its structure and energetics, comparing to the state with hydrogen at interstitial site. Using ReaxFF, we also managed to obtain a defectless a-SiO_2 structure and found that the Att_Rad state is significantly more stable in a-SiO_2 compared to quartz, indicating that this state might initiate dielectric breakdown in Si/a-SiO_2 interfaces.

Masayasu Miyata
Seiko-Epson Corporation

Date submitted: 04 Jan 2005

Electronic form version 1.4