Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Tunneling properties of ultra-thin SiO_2 barriers: a first-principles study EUNJUNG KO, HYOUNG JOON CHOI, Department of Physics and IPAP, Yonsei University, Seoul, Korea — We performed first-principles simulations of the electron tunneling through ultra-thin SiO_2 barriers in Si(100)/SiO_2/Si(100) structures. The atomic structures of the Si/SiO_2 interfaces are generated by considering various silicon suboxide states observed in photoemission studies. For comparison, we also consider sharp Si/SiO_2 interfaces with dangling bonds. For each atomic structure, the tunneling conductance is calculated by a first-principles scattering-state method based on the *ab-initio* pseudopotentials and the density functional theory within the local density approximation. As a result we obtained the dependence of the tunneling probabilities on the oxide thickness and on the interfacial structures. Effects of the dangling bonds on the tunneling probabilities will also be discussed. Computational resource for this work is provided by KISTI under the 8th Strategic Supercomputing Support Program.

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Date submitted: 27 Nov 2007 Electronic form version 1.4