

Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

First-principles calculations of mobilities in ultra-thin double-gate MOSFETs OSCAR D. RESTREPO, KALMAN VARGA, Vanderbilt University, BLAIR TUTTLE, Vanderbilt University & Penn State Erie, SOKRATES T. PANTELIDES, Vanderbilt University & Oak Ridge National Laboratory — Carrier mobilities in MOSFETs are usually simulated by employing empirical scattering models. These methods do not take into account quantum mechanical effects with atomic-scale structural resolution, which are key elements to describe transport at the nano-scale. We use a novel first-principles approach to calculate mobilities in ultra-thin SOI MOSFETs [1]. For this report, we use newly constructed interface models of Si(100) and amorphous SiO₂. Straining the silicon lattice results in significant increases in carrier mobility. We distinguish between the strain enhancement due to the change in velocities and the enhancement coming from the change in scattering potential. We also compare our calculations with experimental values for mobility degradation caused by radiation induced Coulomb scattering centers. We are able to quantify the contribution to the total mobility from various types of scattering centers, namely, from atomic-scale interface roughness (oxide protrusions, suboxide bonds) and scattering from point defects (dangling bonds, hydrogen). This work was supported by NSF Grant ECS-0524655. [1] M. H. Evans et al., Phys. Rev. Lett. 95, 106802 (2005).

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Date submitted: 02 Dec 2007

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