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First-principles calculations of mobilities in MOSFETs GEORGE HADJISAVVAS, LEONIDAS TSETSERIS, MATTHEW EVANS, SOKRATES PANTELIDES, Vanderbilt University — Nano-scale MOSFETs demonstrate interesting electron transport behavior. Straining the silicon lattice results in significant increases in carrier mobility up to 100%. Transport properties are known to depend also on the presence of interface traps. Due to their significance, a large number of studies have obtained mobilities, but in an empirical and semi-classical fashion, whereas, in nano-devices quantum mechanical effects and atomic-scale structural details are the key factors of mobility calculations. Here we use a recently developed method[1] for first-principles calculations of mobilites within DFT to probe the effect of strain and interface point defects (e.g., dangling bonds) on mobilities in double gate ultra-thin SOI (UTSOI) MOSFETs. The transport properties are described in a fully self-consistent quantum mechanical fashion and mobilities are calculated within the Born approximation. The results show that biaxial tensile strain is shown to significantly increase carrier mobility in UTSOI devices by suppressing the effective scattering from atomic-scale interface inhomogeneities; the effect of dangling bonds on mobility in a UTSOI channel is weaker than in conventional MOSFETs because the carrier density peaks at the center of the channel. This work was supported in part by NSF Grant ECS-0524655 and by AFOSR Grant 4224224232. [1] M.H. Evans et al., Phys. Rev. Lett. **95,** 106802 (2005).

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