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**First-principles calculations of mobilities in novel MOSFETs**

MATTHEW EVANS, Vanderbilt University, SOKRATES PANTELIDES, Vanderbilt University — Nanoscale metal-oxide-semiconductor field-effect transistors (MOSFETs) incorporating novel materials demonstrate unusual electron transport behavior. Straining the silicon lattice results in significant increases in electron and hole mobility. However, mobility calculations using standard approximations have difficulty explaining this increase. MOSFETs using novel gate dielectrics (e.g. hafnium oxide) have mobilities that are much lower than MOSFETs using silicon dioxide as the dielectric. “Interface quality” has been invoked as a likely cause of this difference, but few attempts have been made to tie the mobility decrease to scattering mechanisms associated with the novel dielectric structure. In this talk, we report results of mobility calculations in MOSFETs with a strained-Si channel and with alternate gate dielectrics. The calculations employed a recently developed first-principles method based on atomic-scale interface models.[1] Changes in the local environment of atomic-scale interface roughness defects are shown to potentially account for the increase in mobility under strain. Interstitial Hf defects near the silicon-oxide interface can act as traps and are shown to impact the mobility in MOSFETs with hafnium oxide gate dielectrics. [1] M. H. Evans, X.-G. Zhang, J. D. Joannopoulos, and S. T. Pantelides, *Phys. Rev. Lett.*, v. 95, p. 106802 (2005).

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