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First-principles calculation of mobilities in nano-MOSFETs

MATTHEW EVANS, Massachusetts Institute of Technology, XIAOGUANG ZHANG, Oak Ridge National Laboratories, JOHN JOANNOPOULOS, Massachusetts Institute of Technology, SOKRATES PANTELIDES, Vanderbilt University — As metal-oxide-semiconductor field-effect transistors enter the nanoscale regime, the usual approximations made in mobility calculations fail to account for observations because wave penetration in the gate oxide becomes significant and the effective-mass approximation breaks down. We introduce a novel method for first-principles calculations of carrier mobilities in ultrathin silicon-on-insulator channels. The method is based on density functional theory and Green's functions. The silicon-oxide interface is treated at the atomic-scale, so that all wave functions extend on both sides of the interface. Interface roughness is included in terms of deviations from an abrupt interface (e.g. suboxide bonds, oxide protrusions) acting as scattering centers. Scattering from impurities (e.g. dopants, nitrogen, hydrogen) is also included. A dynamical approach to optical phonon scattering has been developed, including phonon-plasmon interactions. Initial results reveal the importance of the atomic scale in controlling the effects of interface roughness.

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