Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

First-principles calculation of phonon-limited mobility in silicon[1]
YUNING WU, XIAOGUANG ZHANG, Department of Physics and Quantum Theory Project, University of Florida, SOKRATES PANTELIDES, Department of Physics and Astronomy, Vanderbilt University — We introduce a new first-principles method to calculate phonon-scattering-limited electron mobilities. The lifetime of a Bloch state due to scattering is represented by an imaginary electron self-energy which is extracted from the complex band structure of a supercell that contains the phonon vibrations within the frozen-phonon approximation. The phonon vibrations are modeled by a set of configurations generated from a Monte Carlo simulation. Mobility contributions are dominated by electrons on the transverse ellipsoids with low effective mass and long lifetime. The results indicate that high-mobility channels form a conduction network above the percolation threshold. As a result the Matthiessen's rule does not hold for phonon scattering. The overall mobility is evaluated through the configurational average of the percolation-dominant resistor network. The calculated electron mobility agrees with available experimental data.

[1]This work is supported by the LDRD program at ORNL. Portion of this research was conducted at the Center for Nanophase Materials Sciences, which is a DOE Office of Science User Facility.

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Date submitted: 13 Nov 2014 Electronic form version 1.4