Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

First Principles Study of Strain Effects on the Electronic Properties in Silicon Nanowires XIHONG PENG, Phys. Dept. Rensselaer Polytechnic Institute, SANAT KUMAR, Dept. Chemical Engineering, Columbia Univ., SAROJ NAYAK, Phys. Dept. Rensselaer Polytechnic Institute — Silicon nanowires have drawn much attention in the past decades due to their potential applications in many fields, such as optoelectronics, micro- and nano- electronics. The study of size dependence on the band gap of silicon wires have been addressed both using theoretical methods and experimental techniques. In parallel, industry routinely applies strain to engineer the electronic properties in bulk Si. In present work, using first principles density functional theory we have studied the uniaxial strain effects on the electronic properties in Si nanowires with lateral dimension up to 5 nm. We discovered that the strain effects on the band gap display qualitatively new trends for the nanowires smaller than $\sim$5 nm. In Si bulk, indirect band gap decreases linearly with hydrostatic compression, while the band gap is increasing with uniaxial compressive strain for wires smaller than 2 nm. In the intermediate size range 2$\sim$5 nm, the band gap decreases both with compressive and tensile strains, exhibiting an approximately parabolic behavior. Finally we will present our results of strain effect on the effective masses of electrons and holes in nanowires that may have immense impact on future nanoelectronics devices.

Xihong Peng
Phys. Dept. Rensselaer Polytechnic Institute

Date submitted: 20 Nov 2006 Electronic form version 1.4