Abstract Submitted
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Thermoelectric Properties of Silicon Nanowires: a Computational Study[1] E. B. RAMAYYA, I. KNEZEVIC, University of Wisconsin - Madison — We present a detailed simulation of electronic and thermal transport in thin, highly doped silicon nanowires, surrounded by a native oxide. Electronic states are found from a self- consistent Poisson-Schrödinger solver within the effective mass framework. Confined acoustic phonon dispersions are calculated from the elastic continuum equation with the free- standing boundary conditions, appropriate for Si surrounded by the acoustically softer SiO_2. Transport of charge and heat is described by solving the Boltzmann transport equations for both electrons and acoustic phonons using the ensemble Monte Carlo technique. We see little increase in the phonon-drag portion of the Seebeck coefficient over the bulk value, and obtain the total Seebeck coefficient in agreement with experiment. Boundary roughness scattering indeed proves to have a significant effect on both electronic and thermal transport, and we discuss a novel method to account for the phonon boundary scattering, which supplants the use of the phenomenological specularity parameter. We demonstrate that indeed the room-temperature figure of merit in thin wires reaches values close to 1, and discuss options for its further enhancement.

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