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Thermoelectric Properties of Gated Silicon Nanowires

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-abstract-

Silicon nanostructures exhibit thermal conductivities close to the amorphous limit, which make them very promising thermoelectric materials. Room temperature figure of merit ZT=0.5 was recently demonstrated in Si nanowires (NWs) and nanomeshes. With the thermal conductivity, however, reaching its limits, additional benefits resulting from the electronic power factor need be investigated. In this work we theoretically investigate the thermoelectric performance of gated p-type Si NWs of diameters from D=5nm to D=20nm using atomistic calculations for electrons and phonons and linearized Boltzmann transport theory. We examine NWs in the [100], [110] and [111] transport orientations. The thermoelectric performance is found to be strongly anisotropic, with the [111] NWs having the highest and the [100] NWs the lower power factor. We demonstrate that field modulation of the carrier density can provide 4-5x higher power factors than what can be achieved in doped NWs. This is a result of the much higher electrical conductivity achieved by electric field modulation. The Seebeck coefficient is lower in field modulated channels, but the overall power factor is higher.

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