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Thermoelectric Power Factor Engineering of Low-Dimensional and Nanocomposite Si Nanostructures NEOPHYTOS NEOPHYTOU, HANS KOSINA, Tecnical University of Vienna, Institute for Microelectronics — By employing nanostructured materials the thermoelectric figure of merit ZT has been raised to unprecedented large values, with a present record of ZT=2.4. Even in traditionally poor thermoelectric materials such as Si, high ZT values were achieved. The improvement was a result of the drastic reduction in the thermal conductivity, which could be suppressed close or even below the amorphous limit. Since thermal conductivity reduction is reaching its limits, additional benefits resulting from electronic structure engineering have to be investigated. In this work we theoretically provide design directions for the thermoelectric power factor (comprising Seebeck coefficient and electrical conductivity) and thermal conductivity in nanostructured Si channels. We consider 1D nanowires, 2D ultra-thin layers, and nanocomposite Si-based materials. We employ semiclassical Boltzmann transport and use both atomistic and continuum calculations for the electronic and phononic structure of the materials. This study examines how length scale can be exploited as a degree of freedom in designing the nanoscale thermoelectric material properties.

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