Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Thermoelectric Properties of Low-Dimensional Si and Ge Based Nanostructures NEOPHYTOS NEOPHYTOU, HANS KOSINA, Technical University of Vienna — Low-dimensional thermoelectric nanostructures based on Si and Ge are promising candidates for high performance energy conversion and generation applications. 1D nanowires (NWs) and 2D superlattices of Si, Ge and Si/SiGe have experimentally demonstrated excellent performance. In these confined systems the electrical conductivity, the thermal conductivity, and the Seebeck coefficient can be designed to some degree independently so as to achieve enhanced ZT values as compared to the related bulk material values. In this work, we calculate the thermoelectric coefficients of scaled Si and Ge NWs and thin-layers. We use the sp3d5s* tight-binding model for the electronic structure and linearized Boltzmann transport theory. Our calculations include structures of feature sizes up to 12nm containing over 5500 atoms. This study indicates that the confinement length scale can be exploited as a degree of freedom in designing the material properties. We examine n-type and p-type materials of different cross section sizes and confinement/transport orientations and provide optimization directions for power factor improvement. Finally, using measured values for the lattice thermal conductivity, the ZT is estimated.

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Date submitted: 05 Nov 2011 Electronic form version 1.4