Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Optimization of thermoelectric properties in cross-plane superlattices - A 1D NEGF Study MISCHA THESBERG, MAHDI POURFATH, Vienna Univ of Technology, NEOPHYTOS NEOPHYTOU, University of Warwick, HANS KOSINA, Vienna Univ of Technology — Thermoelectric materials utilize carrier energy filtering through potential barriers to achieve improvements in the Seebeck coefficient. Barriers, however, tend to drastically reduce the electrical conductivity, and power factor improvements are difficult to be realized. In this work we present a fully quantum mechanical simulation study of thermoelectric transport in the presence of barriers for energy filtering. For this, we use the non-equilibrium Green's function (NEGF) method, including both acoustic and optical phonons. We show that power factor improvements can be achieved by properly adjusting a series of interrelated parameters: i) the position of the Fermi level, ii) the width, size and shape of the barriers as well as the separation between them, iii) the optical phonon energies. Our results provide insight on how to optimize superlattices and nanocomposite materials for enhanced thermoelectric properties.

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Date submitted: 13 Nov 2014 Electronic form version 1.4