Abstract for an Invited Paper
for the MAR07 Meeting of
The American Physical Society

Computational Thermoelectrics.

PAUL VON ALLMEN, NASA-Jet Propulsion Laboratory, California Institute of Technology

For several decades the thermoelectric properties of materials have attracted moderate interest in the solid state physics community. It was believed that bulk materials such as Bi2Te3 have come close to the maximum attainable figure of merit ZT. The resulting efficiency for energy conversion and other applications was seen as insufficient to spur more detailed theoretical studies. In the 80's and 90's the expansion of material fabrication technologies allowing for the fabrication of nano-patterned systems and the theoretical prediction that ZT can reach values in nanostructures far larger than in bulk materials have spurred a renewed theoretical interest in thermoelectric properties. This presentation will offer a review of the computational efforts undertaken to achieve a quantitative description of the thermoelectric properties of nano-patterned materials. Evaluating ZT requires the computation of the electronic contribution to the electrical and thermal conductivities and the Seebeck coefficient, and the lattice contribution to the thermal conductivity. A brief overview of the methods mostly used in evaluating these transport properties will be given. Semiclassical approaches relying on a solution of the Boltzmann transport equation for both electrons and phonons will be described as well as Green-Kubo and non-equilibrium transport techniques. Examples will be given for bulk semiconductors such as silicon, germanium and bismuth telluride. Atomic level calculations of the thermoelectric properties for semiconductor nanostructures will also be presented. The lattice contribution to the thermal conductivity is of particular importance to maximize ZT for semiconductors. Beside the Boltzmann transport equation approach, other methods use the fluctuation-dissipation theorem or non-equilibrium molecular dynamics. Numerical results will be shown for bulk materials and nanostructures. Concluding remarks will offer an estimate of the currently achievable accuracy on the prediction of thermoelectric properties and will outline the path for improvements.