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Review of State of the Art Technologies used to Improve Performance of Thermoelectric Devices

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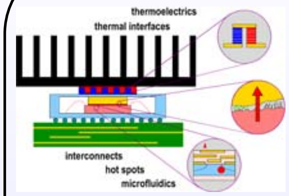
Abstract

- Improving efficiency of thermoelectric energy conversion devices is a major challenge in microelectronics industry.
- Reduction in device size expected to produce limitless improvement in performance. Nanoscale superlattices proposed to improve ZT due to reduced thermal conductivity and increased Seebeck coefficient.
- Size quantization effects found to dominate performance of nanoscale energy conversion devices offsetting benefits gained through reduced thermal conductivity of superlattices.
- Semi-classical transport models used to predict ZT can effectively predict thermoelectric performance of bulk materials. Quantum corrections commonly required to include confinement effects.
- Nonequilibrium Green's function method proposed to couple quantum and scattering effects to predict thermoelectric performance.
- NEGF found to be a valuable tool to predict and design nanostructures for energy conversion devices.

Thermoelectric Figure of Merit



$$ZT = \frac{S^2 \sigma T}{\kappa} \qquad COP = \frac{\frac{ZT_C^2}{2} - \Delta T}{ZT_H T_C}$$

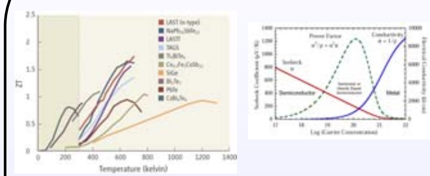
Localized heating and Cooling. Low noise, reliable, rugged and environment friendly.

Growing need to reduce dependence on non-renewable energy resources.

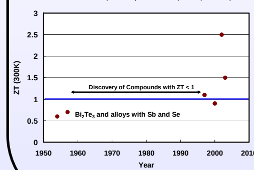
Increase vehicle fuel economy ⇒ need to harness waste heat.

ZT ≥ 3 can produce COP values better than bottoming cycles and vapor compression Cycles.

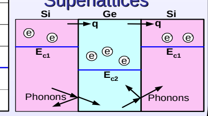
Thermoelectric Material Performance



Robert. F. Service, et.al., Science, 311, 1860, 2006.

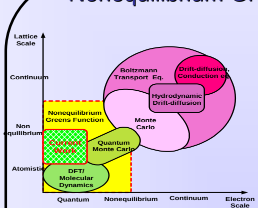


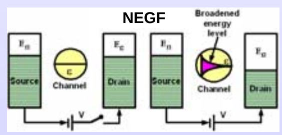
Nanostructured Superlattices

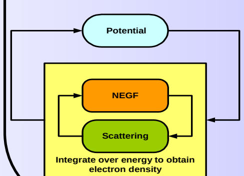


Reproduced from A, Majumdar, Science, 303, 2004

Nonequilibrium Green's Function Method

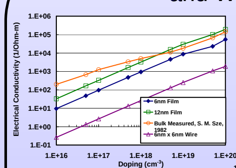


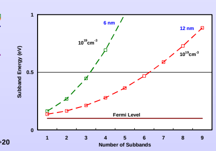




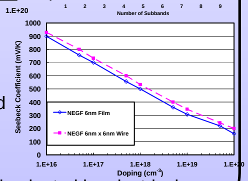
Broadening of energy density of states near source and drain contacts leads to current flow. NEGF does NOT require a statistical distribution of carriers within the device ⇒ can be used to solve extreme nonequilibrium problems. Can include quantum effects such as tunneling and diffraction, not usually possible through classical models.

Nanoscale Effects on Silicon Films and Wires



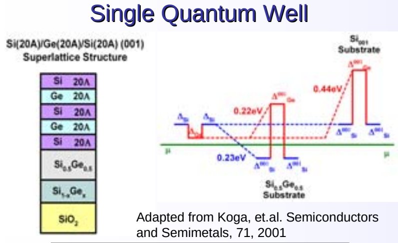


Reduced dimensionality ⇒ increased density of states per unit volume near the conduction band edge ⇒ higher Seebeck coefficient of the wire.

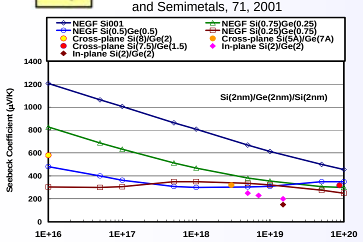


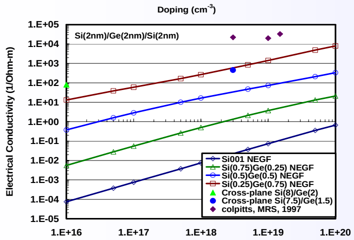
Power factor is dominated by electrical conductivity. 72% decrease in power factor of 6nm films compared to 12nm films.

Thermoelectric Properties of Strained Single Quantum Well

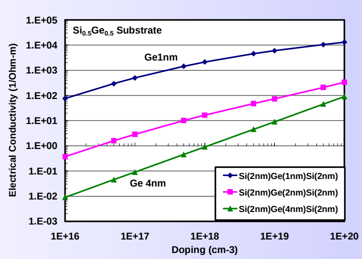


Adapted from Koga, et.al. Semiconductors and Semimetals, 71, 2001

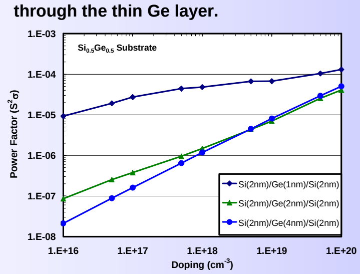




Effect of Germanium Barrier Thickness

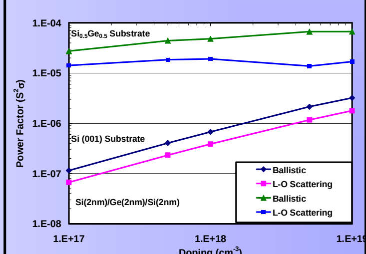


Ge 1nm barrier thickness provides highest electrical conductivity due to tunneling through the thin Ge layer.



For high doping, superlattice with Ge 4nm layers has similar power factor as Ge 2nm. Problems with interlayer diffusion can be avoided by using thicker Ge layers.

Electron-Phonon Scattering in Strained Si(2nm)/Ge(1nm)/Si(2nm) Superlattices



Superlattice with $Si_{0.5}Ge_{0.5}$ substrate showed 64% decrease with scattering compared to 43% decrease with Si(001) substrate.

Seebeck oscillations result in better performance of 10^{18}cm^{-3} doping compared to 5×10^{18}cm^{-3} for $Si_{0.5}Ge_{0.5}$ substrate.

For Bi_2Te_3/Sb_2Te_3 6nm period superlattices with cross-plane ZT ~2.5, power factor values of 40-60(10^{-4} W/K^2-m) were reported.

Harman et.al. Science, 297, 2002.

Conclusions

Contrary to popular belief, small may not always be better.

Materials selection is still very important for thermoelectric performance.

By modulating substrate strain, thicker barrier layers with lower doping give optimum thermoelectric performance in superlattices.

NEGF is a valuable design tool that couples quantum and scattering effects to study thermoelectric performance of nanostructured energy conversion devices.

References

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