Modeling Thermoelectric Properties of Nanofilms and Nanowires

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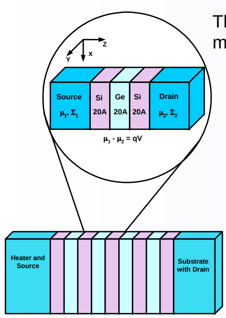
Abstract

- Improving efficiency of thermoelectric energy conversion devices is a major challenge in microelectronics industry. Superlattices were proposed to improve ZT due to reduced thermal conductivity.
- Quantum confinement effects significantly decrease electrical conductivity of nanofilms and nanowires compared to the bulk.
- Size quantization effects found to dominate performance of nanoscale energy conversion devices offsetting benefits gained through reduced thermal conductivity of superlattices.

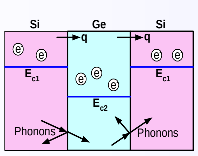
Nanoscale Effects

- Decrease in device dimensionality increases the Seebeck coefficient of the device.
- Decrease in nanofilm thickness leads to electron confinement resulting in reduced electrical conductivity.
- Decrease in electrical conductivity dominates over increase in Seebeck coefficient leading to poor device performance.

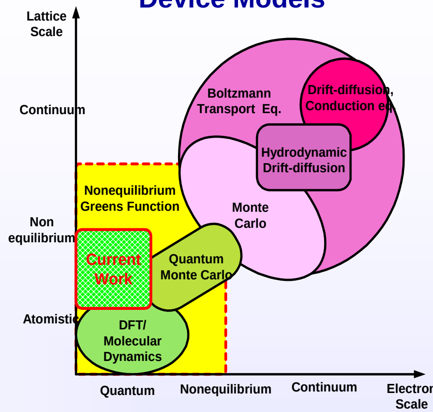


Thermoelectric figure of merit

$$ZT = \frac{S^2 \sigma T}{\kappa}$$



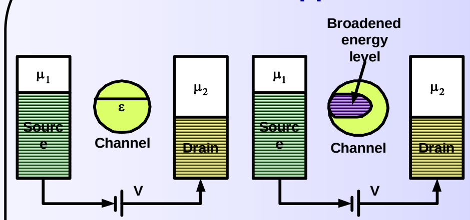
Device Models



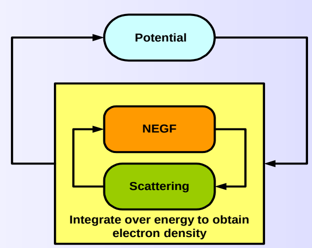
Nonequilibrium Green's Function (NEGF)

- NEGF method does not require a statistical distribution of carriers within the device.
- Can be used to solve extreme nonequilibrium problems.
- Allows inclusion of quantum effects such as tunneling and diffraction, not usually possible through classical models.

NEGF Solution Approach

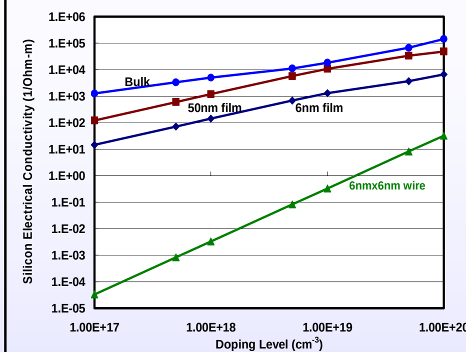


Channel energy level near the contacts are broadened due to difference in channel and contact density of states.



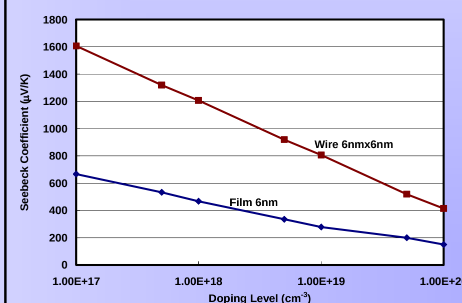
Channel current is calculated self-consistently by calculating change in channel electron density with change in channel potential.

Nanoscale Effects on Electrical Conductivity of Silicon Films and Wires



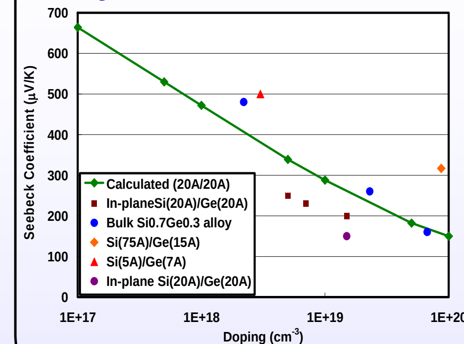
- Quantum confinement in thin films leads to increased spacing between the electron energy levels, decreasing the electrical conductivity.
- Reducing dimensionality from nanofilm to nanowire increases confinement effects further decreasing the electrical conductivity.

Nanoscale Effects on Seebeck Coefficient of Silicon Films and Wires



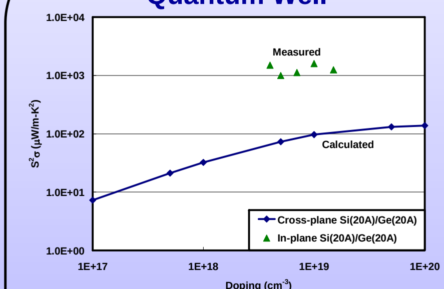
- The voltage for which the thermal current due to a heated drain is balanced by the field current is the Seebeck voltage.
- Reduced dimensionality results in increased density of states per unit volume near the conduction band edge resulting in higher Seebeck coefficients.
- Reduced dimensionality of the nanowire compared to the nanofilm results in higher Seebeck coefficient of the wire.

Seebeck Coefficient of Si/Ge/Si Quantum Well Structure



NEGF successfully predicts Seebeck coefficient of Si/Ge/Si quantum well structure.

Power Factor of Si/Ge/Si Quantum Well



- NEGF calculations performed on single layer of Si/Ge/Si superlattice layer.
- Experiments usually carried out on 1200 layers of superlattices on strained substrate.

Conclusions

- NEGF can be successfully used to model nanoscale device characteristics .
- Quantum effects such as confinement can be easily included while predicting thermoelectric properties of nanofilms and nanowires.
- Size quantization effects have to be taken into consideration when designing nanoscale thermoelectric structures.

References

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- A. Bulusu and D. G. Walker, Coupled Quantum-Scattering Modeling of Thermoelectric Properties of Si/Ge/Si Quantum Well Superlattice, IMECE 2006.
- T. Koga, S. B. Cronin, M. S. Dresselhaus, J. L. Liu and K. L. Wang, Experimental Proof-of-Principle Investigation of Enhanced $Z_{3D}T$ in (001) Oriented Si/Ge Superlattices, Apl. Physics Letters, 77, 10, 2000.