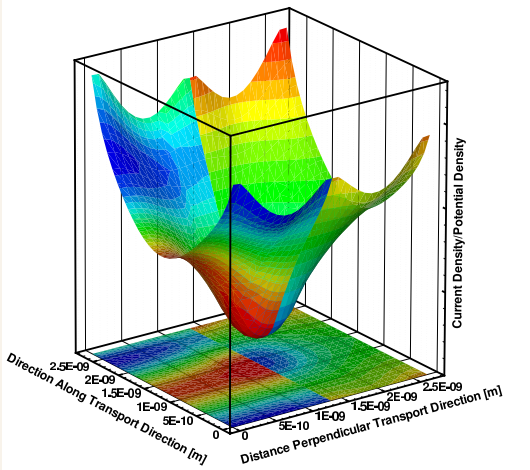
Quantum Simulation of Nanocrystalline Composite Thermoelectric Properties:

InterPACK Conference 2009



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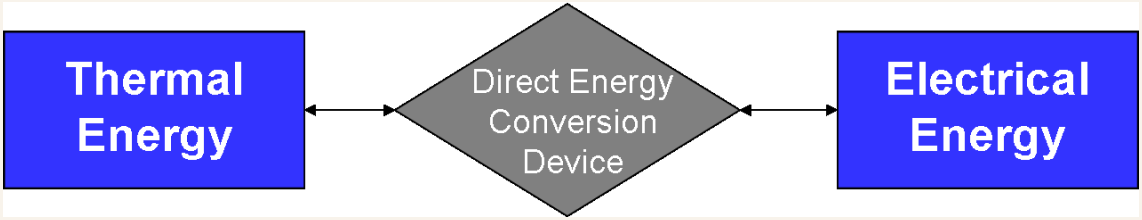
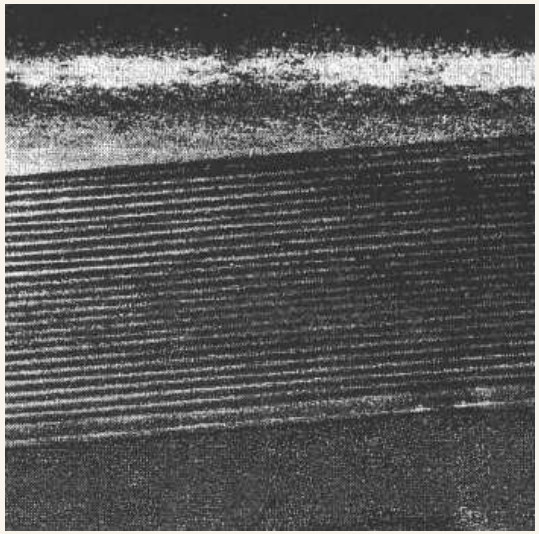
Motivation

- Direct Energy Conversion Devices
  - Thermoelectrics ($>$1 ZT)
  - Electric Cooler
- Nanostructured Material
  - Atom-by-Atom Basis
  - Quantum Confinement
- Wave Based Model
  - Quantum Mechanical Effects
  - Schrodinger-Poisson Solver
- Items of Interest
  - Electrical Transport
  - Device Trends
  - Optimal Device Spatial Parameters
    - Crystal Diameter
    - Crystal Spacing
  - Matrix and Crystal Material

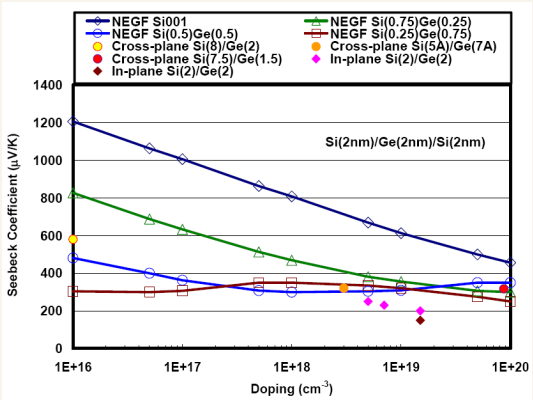


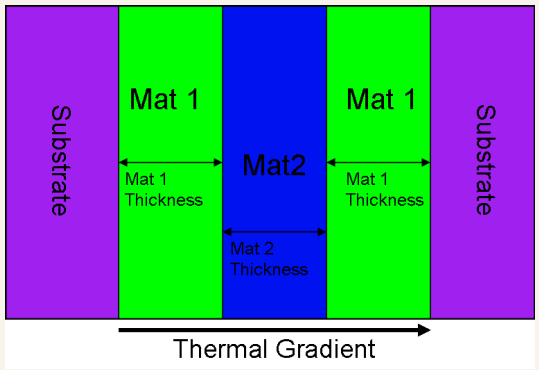
Previous Research

- Non-Equilibrium Green's Function (NEGF) Method
- Superlattice Sturcture
  - 1d Heterostructure, Silicon-Germanium junction
- Electrical Transport
  - Quantum Confinement
  - Tunneling Effects
  - Increased Density of States (DOS)



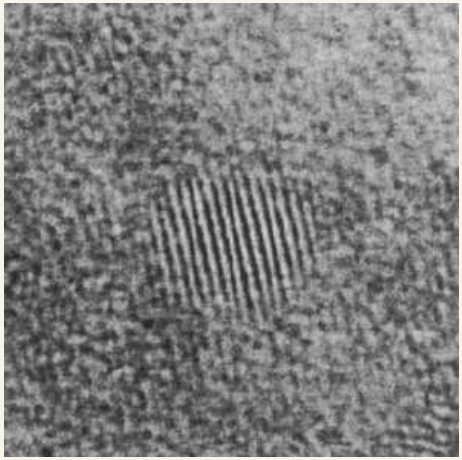
Nozik, Annu. Rev. Phys. Chem. 2001. 52:193231





Nanocrystalline Composite

- Nanostructure
  - 2d Heterostructure, Silicon-Germanium junction
- Electrical Transport
  - Quantum Confinement
  - Planar Transport
  - Increased Sufrace to Volume



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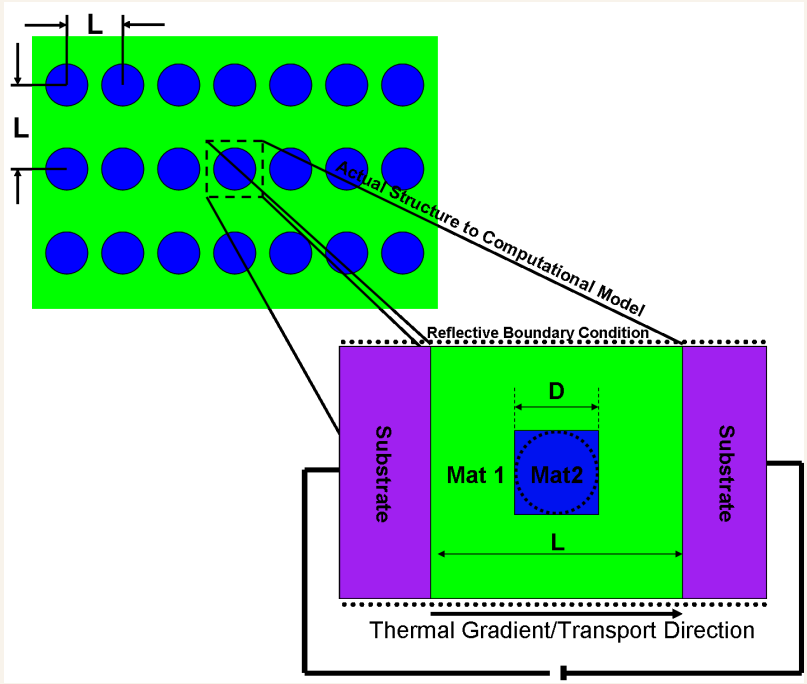


Band Structure

- Straining of Crystal
  - Difference in lattice constant
  - Deformation Potential
- Silicon-Germanium Structure
  - Crystal Material Strained

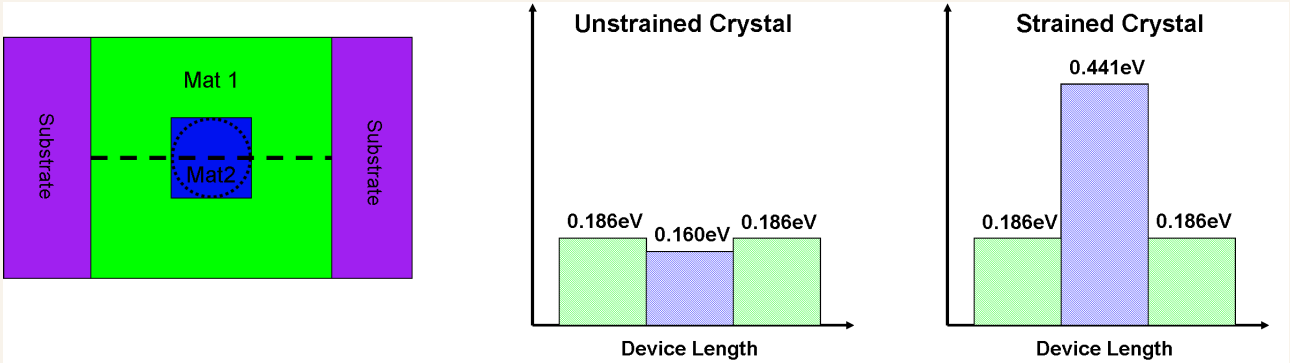


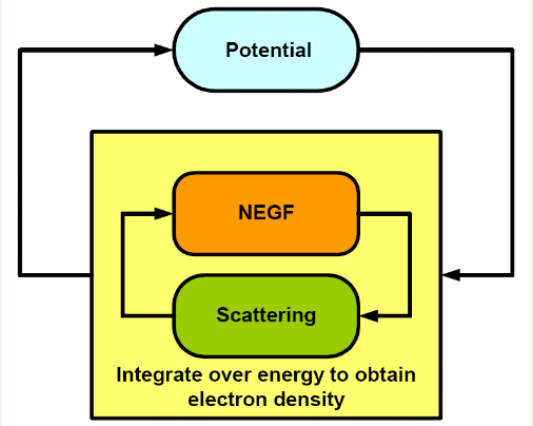
Table 1: Conduction Band Edge with Strain (E_f = 0.1)

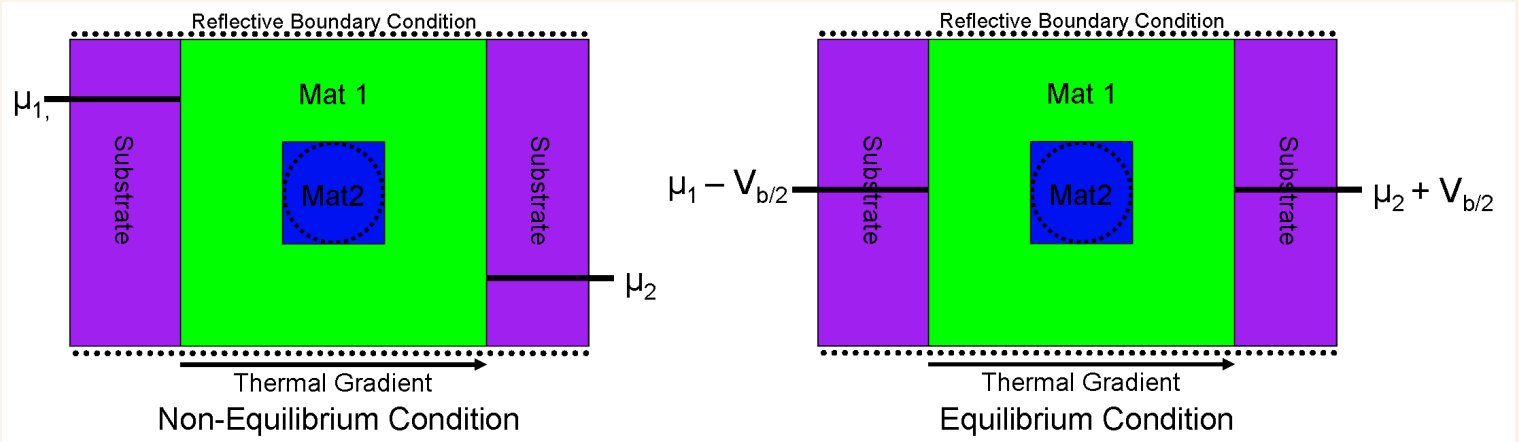
Device	Mat1 E_c [eV]	Mat2 E_c [eV]
Si-Ge	0.186	0.602
Ge-Si	0.160	-0.266
Si-Si	0.186	0.186
Ge-Ge	0.160	0.160

Van de Walle, C. G., Physical Review D, 39(3),Jan.,pp. 1871-1883

Computational Method

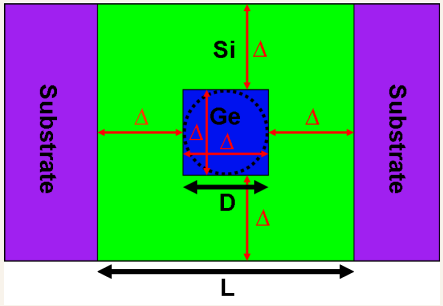
- Wave Based Model
  - Non-Equilibrium Green's Function (NEGF) Method
  - Self Consistent Schrodinger-Poisson Solver
- 2d Effective Mass Hamilitonian
- 2d Spacially Varying Dielectric Potential
- Ballistic Transport

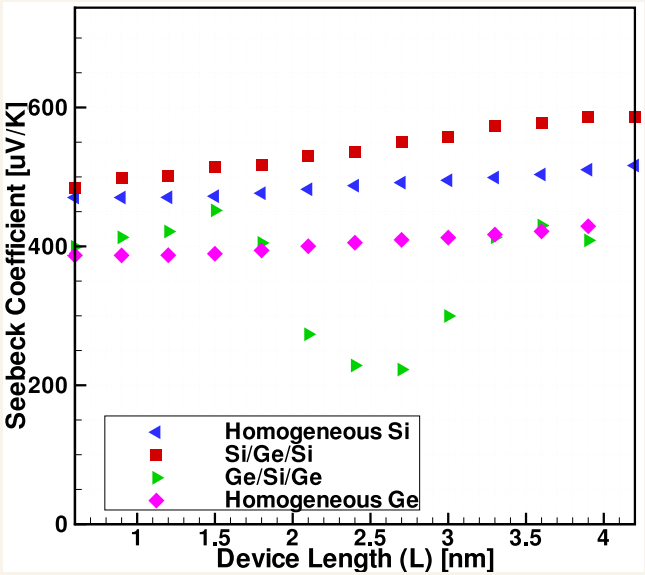


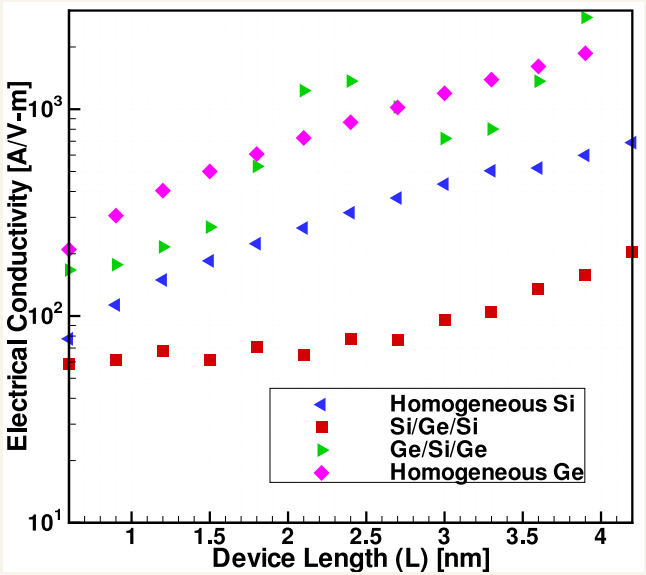


Matrix and Crystal Material

- Increased Diameter of Crystal and Spacing Proportionally. D = L/3



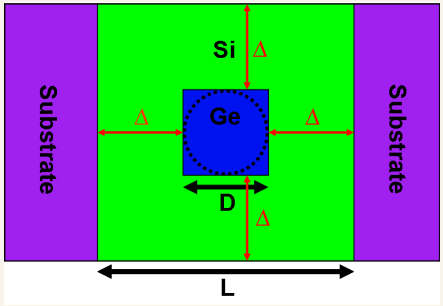


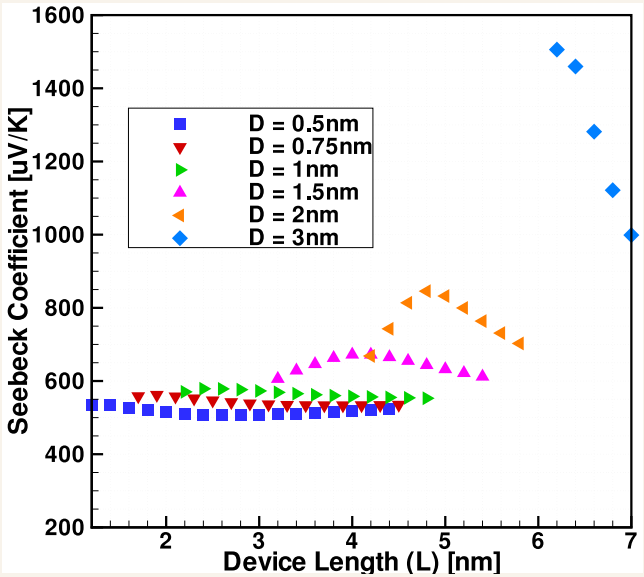


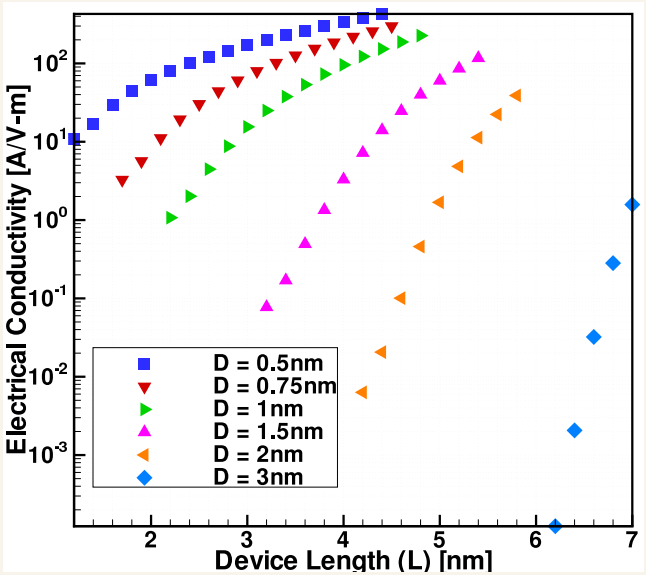
- Silicon Matrix, Germanium crystal has greatest Seebeck.
- Straining of the Silicon crystal results in degeneracy.

Crystal Spacing Effects

- Maintain crystal diameter and increase spacing between nearest neighbor crystal.



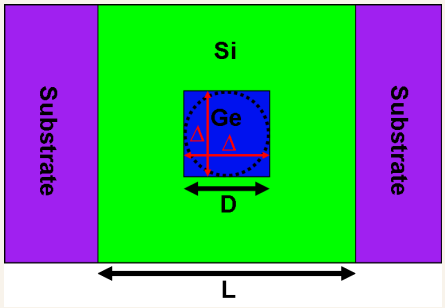


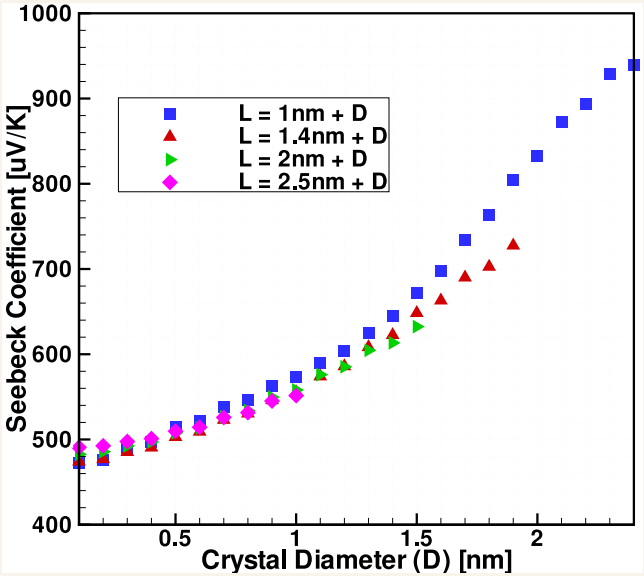


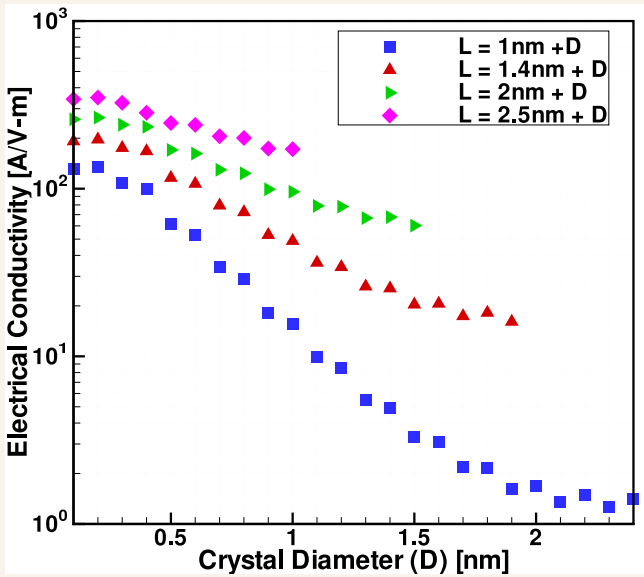
- Maxinum in Seebeck is evident for larger crystals.
- Locus of optimal crystal spacing.

Crystal Diameter Effects

- Maintain crystal spacing and increase crystal diameter.





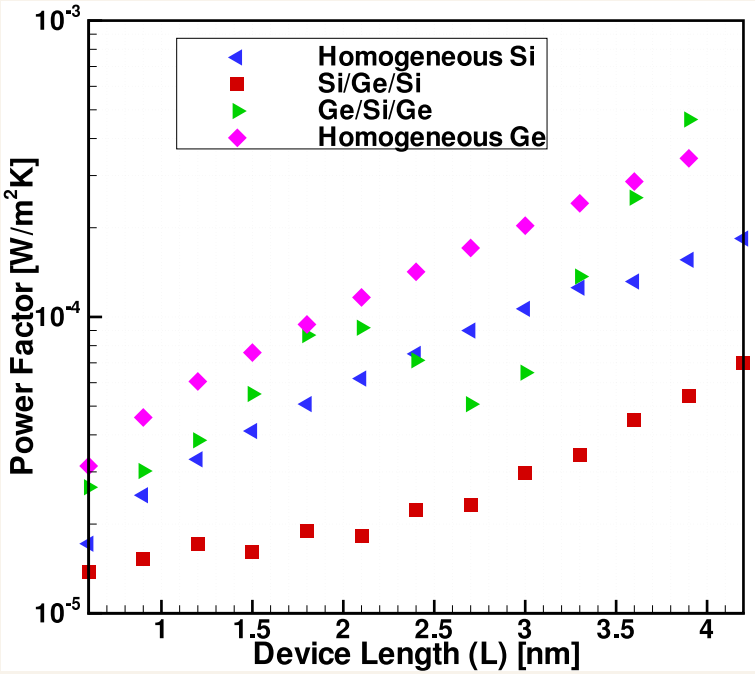


- Competing effects between Seebeck and Conductivity.

Thermoelectric Application

- Figure of Merit

$$ZT = \frac{S^2 \sigma T}{k} \quad (1)$$



- Homogeneous Ge proves to have greatest Power Factor.
- Ge/Si/Ge has greater power factor than Si/Ge/Si.
- Power Factor has strong dependence on electrical conductivity which can be controlled by parameters such as doping.

Conclusion

- Straining is a critical mechanism in electrical transport
- NCCs' have greater Seebeck than homogenous homogeneous Si
- Optimization of NCC Thermoelectric Devices
  - Greater Seebeck for silicon crystal in germanium matrix
  - Small crystal size preferred $<$ 50% device size
  - Crystal spacing in transport direction 50%
  - Optimal Power Factor has yet to be determined based on device size. $>$ 5nm
- Further investigation of thermal conductivity is required to determine complete figure of merit.