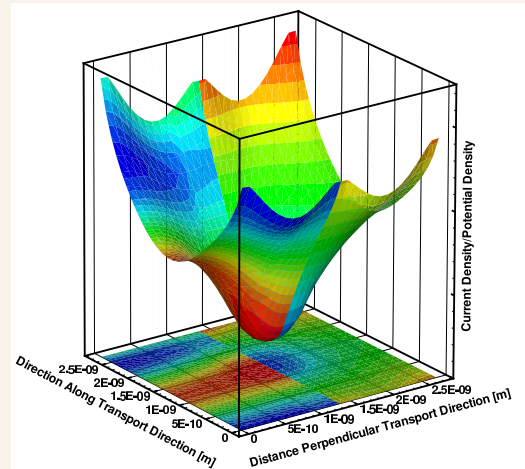


Quantum Simulation of Nanocrystalline Composite Thermoelectric Properties:

InterPACK Conference 2009



T.D. Musho¹ D.G. Walker²

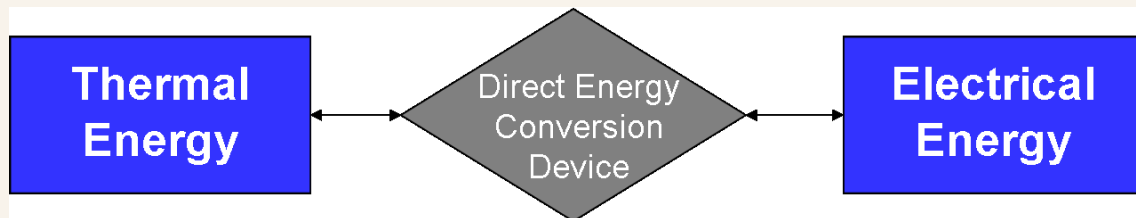
¹ Department of Material Science, Vanderbilt University, Nashville, Tennessee

² Department of Mechanical Engineering, Vanderbilt University, Nashville, Tennessee

Sponsor: NSF

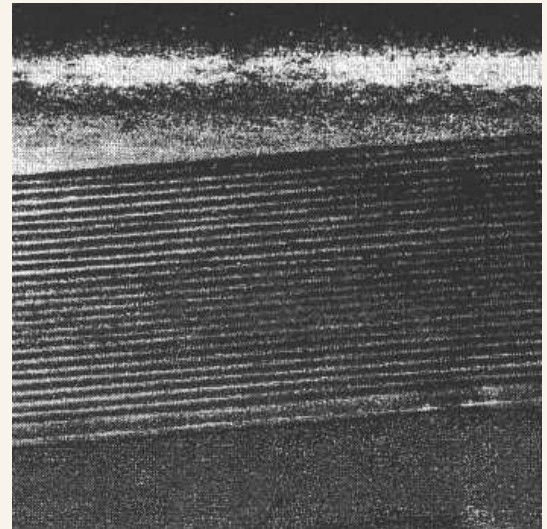
July 23, 2009

- 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

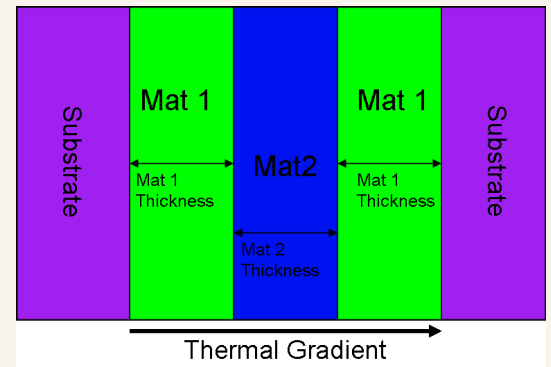
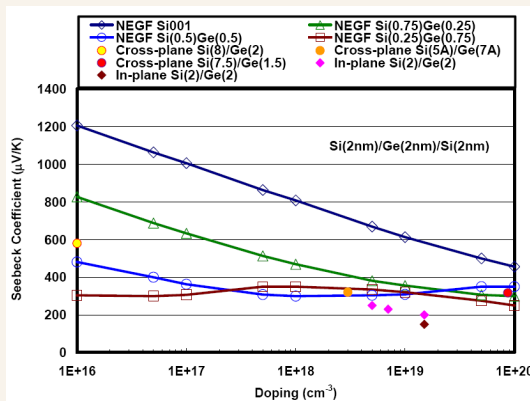




- Non-Equilibrium Green's Function (NEGF) Method
- Superlattice Structure
 - 1d Heterostructure, Silicon-Germanium junction
- Electrical Transport
 - Quantum Confinement
 - Tunneling Effects
 - Increased Density of States (DOS)



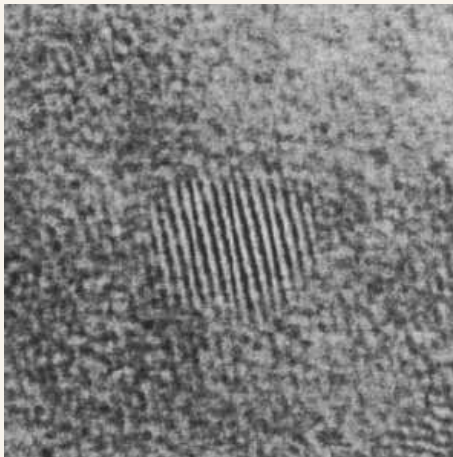
Nozik, Annu. Rev. Phys. Chem. 2001. 52:193231



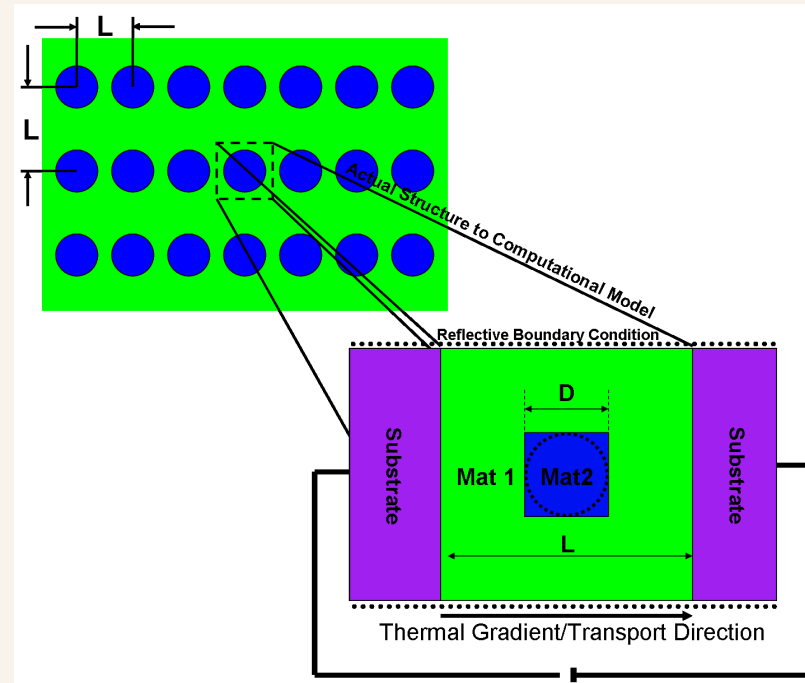
Nanocrystalline Composite



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



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



Band Structure

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

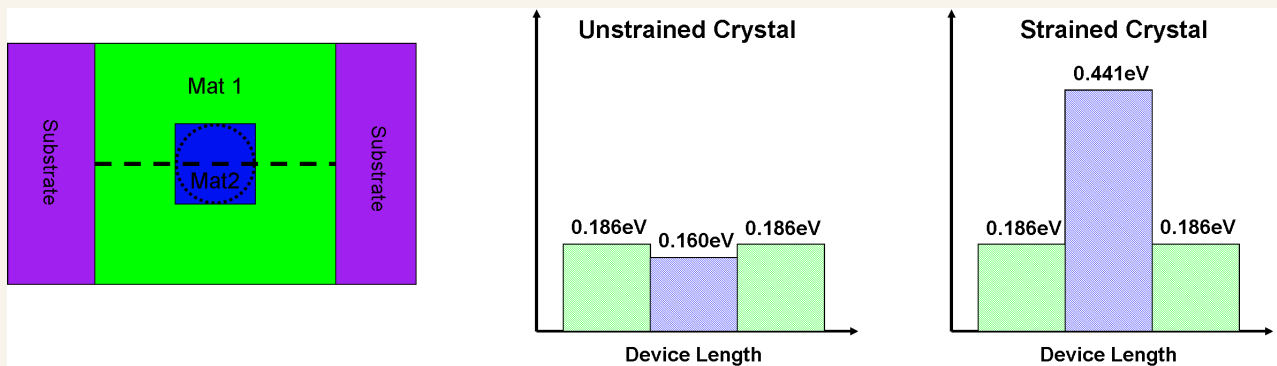
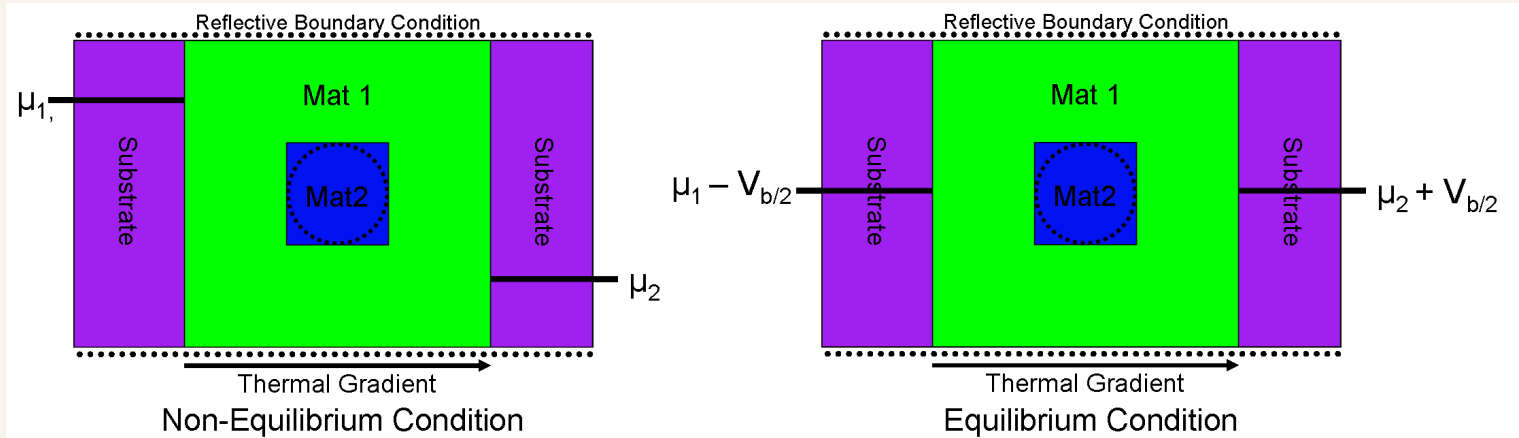
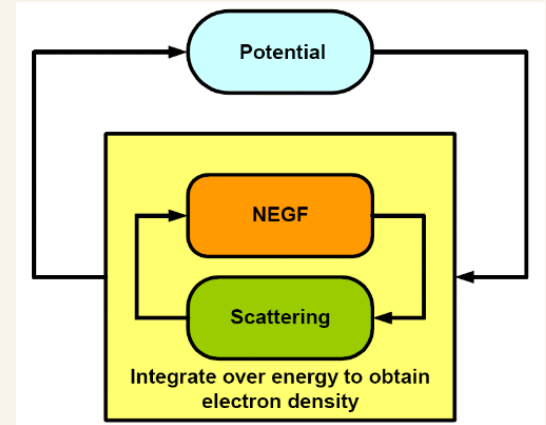


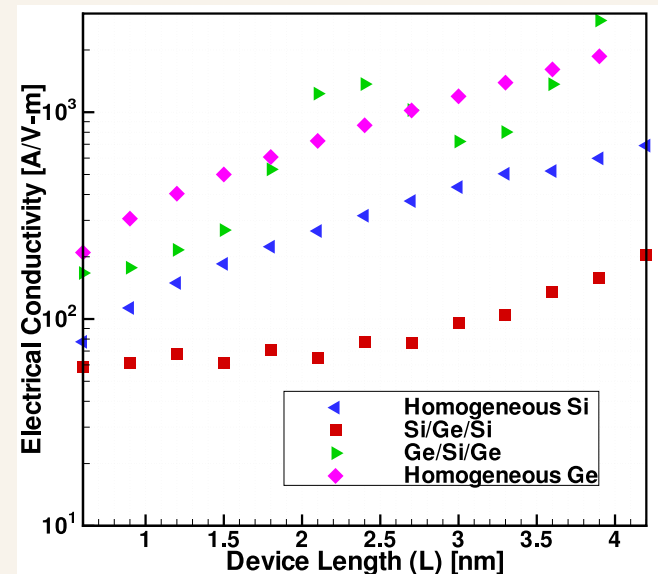
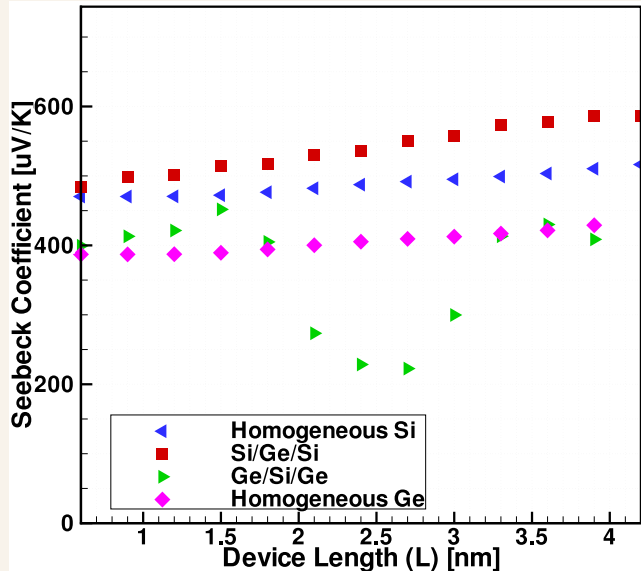
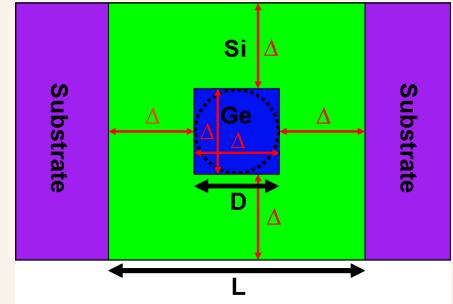
Table 1: Conduction Band Edge with Strain ($E_f = 0.1$)

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

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



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

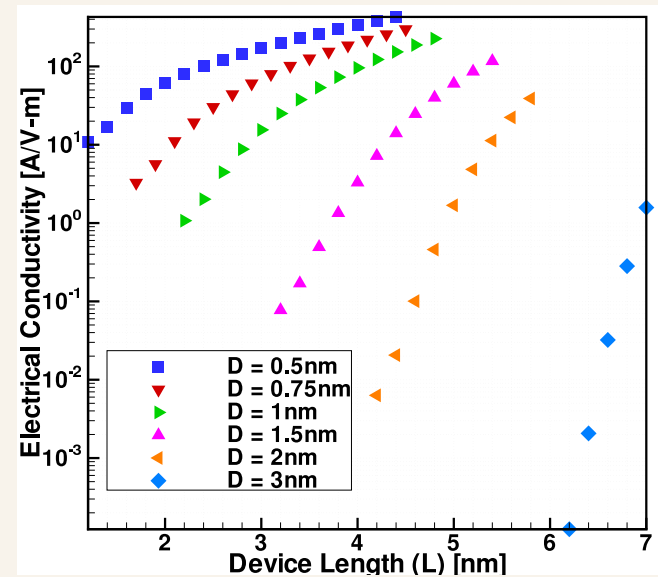
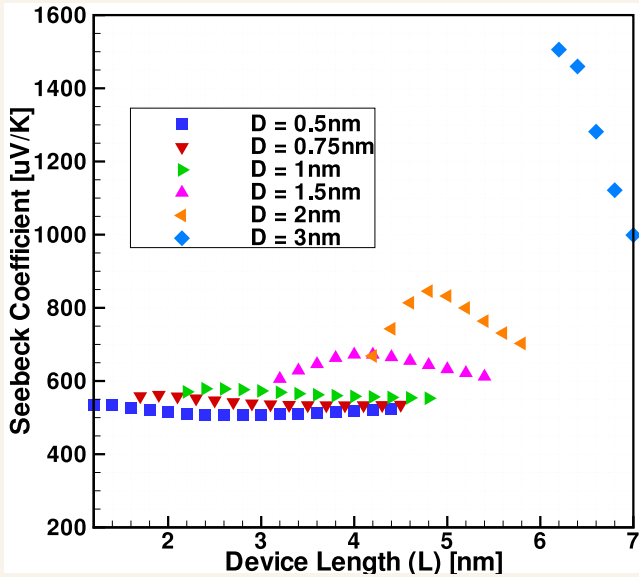
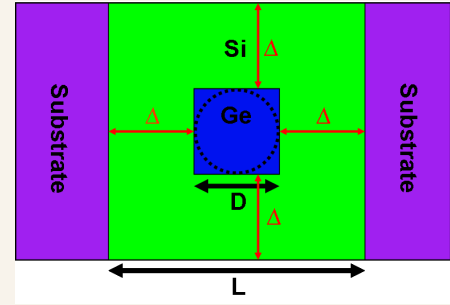


- Silicon Matrix, Germanium crystal has greatest Seebeck.
- Straining of the Silicon crystal results in degeneracy.

Crystal Spacing Effects



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

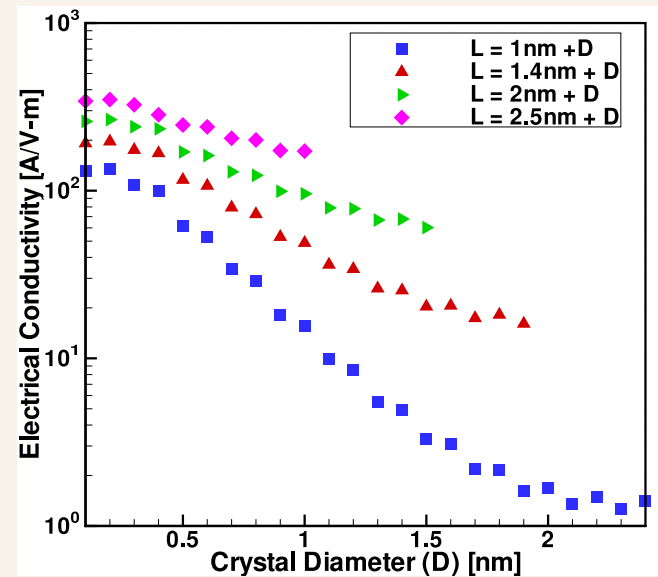
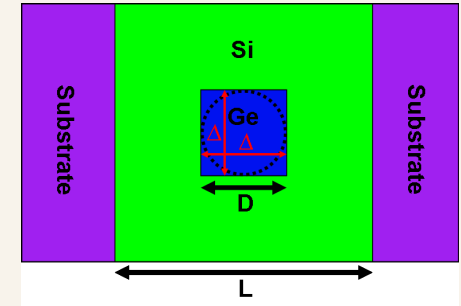
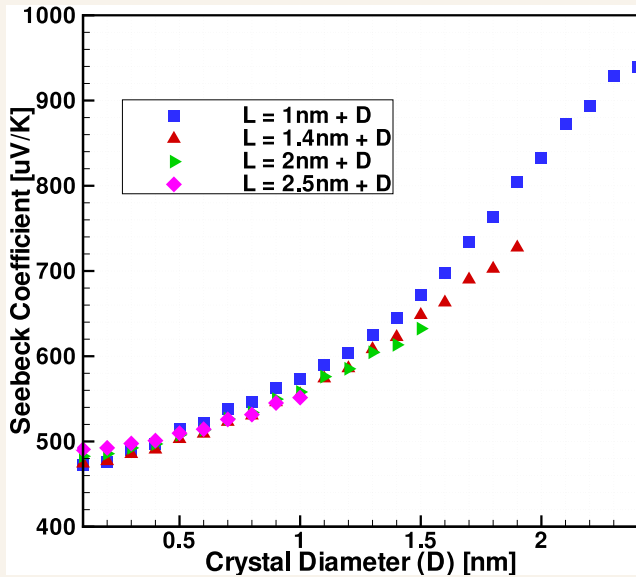


- Maximum in Seebeck is evident for larger crystals.
- Locus of optimal crystal spacing.

Crystal Diameter Effects



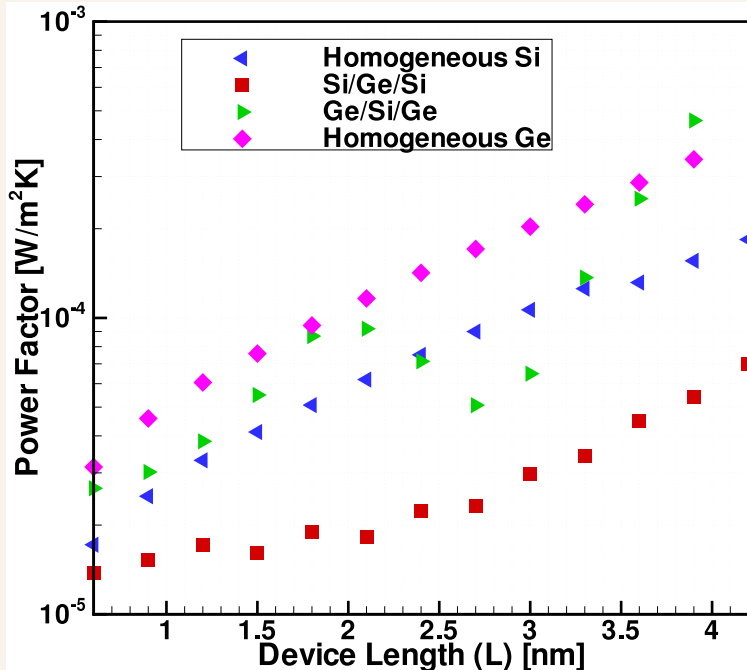
- Maintain crystal spacing and increase crystal diameter.



- Competing effects between Seebeck and Conductivity.

- 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.



- 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. $> 5\text{nm}$
- Further investigation of thermal conductivity is required to determine complete figure of merit.