Introduction

- Nanostructured devices have been proposed as potentially good thermoelectric energy conversion devices.
- Nanoscale performance is not well captured with particle based theory.
- A novel computational approach was implemented to capture quantum effects (wave based model).
- Quantum simulations of superlattice film devices have previously been analyzed.
- Quantum simulations of a two-dimensional nanocrystalline composites (NCC) are currently of interest.
- NCC’s electrical transport has not been studied extensively.
- Results have the potential to aid in the design of NCC structures for future thermoelectric devices.
- Thermoelectric Figure of Merit $ZT = \frac{S^2 \sigma T}{K}$

Previous Research (Superlattice)

- Non-equilibrium Green's function (NEGF) approach
- Si/Ge/Si-Superlattice Structures – Film
- Effects of Quantum Confinement
- Increased Density of States
- Increased Transport – Quantum Effects (Band Narrowing, Tunneling)

New Structure (NCC)

- Evolve 1D NEGF -> 2D NEGF
- Geometry Simplification
- Reflective Boundary Condition
- Material – Silicon, Germanium

Crystal Diameter Effects

- Competing effects between Seebeck and Conductivity

Thermoelectric Application

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

Conclusion

- Straining of the NCC crystal structure due to difference in lattice constant is a critical mechanism in electrical transport.
- NCCs’ have greater Seebeck than homogeneous Si device
- Optimization of NCC Thermoelectric Devices
  - Larger Conductivity for germanium crystal in silicon over silicon crystal in germanium.
  - Small crystal size preferred < 50% Device Size.
  - Crystal spacing in transport direction ~ 50% Crystal Size
  - Optimal Power Factor has yet to be determined based on device size >5nm (it is noted for large devices that scattering becomes dominant, thus affecting performance.)
  - Further investigation of thermal conductivity is required to determine figure of merit for corresponding NCC structures.

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