**Quantum Simulation of Si/Ge Nanostructured Thermoelectrics**

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**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 one-dimensional superlattice structures and two-dimensional nanocrystalline composites (NCC) were studied.
- Electrical transport has not been studied extensively in previous research.
- Results have the potential to aid in the design of nanostructures for future enhanced thermoelectric devices.
- Thermoelectric Figure of Merit $ZT = S^2 \sigma T / K$

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**Nanostructured Devices**

- **Si/Ge - Superlattice Structures (SL)**
- **Si/Ge – Nanocrystalline Composite (NCC)**

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**Computational Method**

- Schrödinger-Poisson Solver
- Self-consistent Calculation
- Ballistic Electron Transport
- Deformation Potential Lattice Strain
- SL – 1D Effective Mass Hamiltonian
- NCC – 2D Effective Mass Hamiltonian

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**SL Period Study**

- Seebeck become independent of layers when > 3
- As layers are added n-1 transmission peaks are evident

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**Local Density of States**

- Density of states shows periodic nature of electrons occupancy.
- As the Ge barrier gets smaller, tunneling effects increase.

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**NCC Size Effects**

- Seebeck greater for Si/Ge NCC Devices
- Seebeck maximized in 4 layer SL when Si/Ge layers are >3nm

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**Conclusion**

- SLs have limited Seebeck performance for more than 4 layers (Only need 4 layers to have equivalent performance of 100’s of layers)
- NCCs have greater Seebeck than homogeneous Si device
- Optimization of NCC thermoelectric devices is possible
  - Seebeck greater for germanium crystal in silicon over silicon crystal in germanium.
  - Small crystal size preferred < 50% device size or smallest.
  - 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 nanostructured devices.
- Kim (2006) experimental showed greater thermal conductivity for NCC structures over bulk material.
- Borca-Tasciuc experimental research of SLs showed greater than bulk alloy thermal conductivity could be achieved.

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**Thermoelectric Application**

- • Seebeck greater for Si/Ge NCC Devices
- • Seebeck maximized in 4 layer SL when Si/Ge layers are >3nm

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*References*