Quantum Transport Properties in Nanocrystalline Composites for Thermoelectric Devices

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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 superlattice film devices have previously been analyzed.
• Quantum simulations of a two-dimensional nanocrystalline composites (NCC) are currently of interest.
• 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

• Nonequilibrium Green's function (NEGF) approach
• Si/Ge/Si-Superlattice Structures – Film

Method

1. Apply \( \Delta T \) to get \( V \)
2. Apply \( V \) to get \( I=0 \Rightarrow S=\Delta V/\Delta T \)

Device Size Effects

• Electrical Conductivity greatest in Si/Ge/Si structures
• Power Factor closely dependent on electrical conductivity

Doping Effects

• Seebeck less influenced by crystal size
• Conductivity has greater dependency on barrier width
• Optimal doping evident from maximum in power factor

Conclusion

• NCC structures have greater electrical conductivity over that of a superlattice structure.
• NCCs' have greater power factor than homogenous Si device
• Optimization of NCC Thermoelectric Devices
  • Devices favor germanium crystal in silicon over silicon crystal in germanium.
  • Small crystal size preferred < 50% Device 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.
• Kim (2006) experimental research of NCCs shows that thermal conductivity is greater for homogenous Si over NCC structures.
• Evolution of 2D NEGF method to 3D will allow for performance characterization of more complicated devices.