



Quantum Simulation of Nanocrystalline Composite Thermoelectric Properties

Properties

T.D. Musho¹, D.G. Walker²

¹ Vanderbilt University, Department of Material Science, ² Vanderbilt University, Department of Mechanical Engineering.
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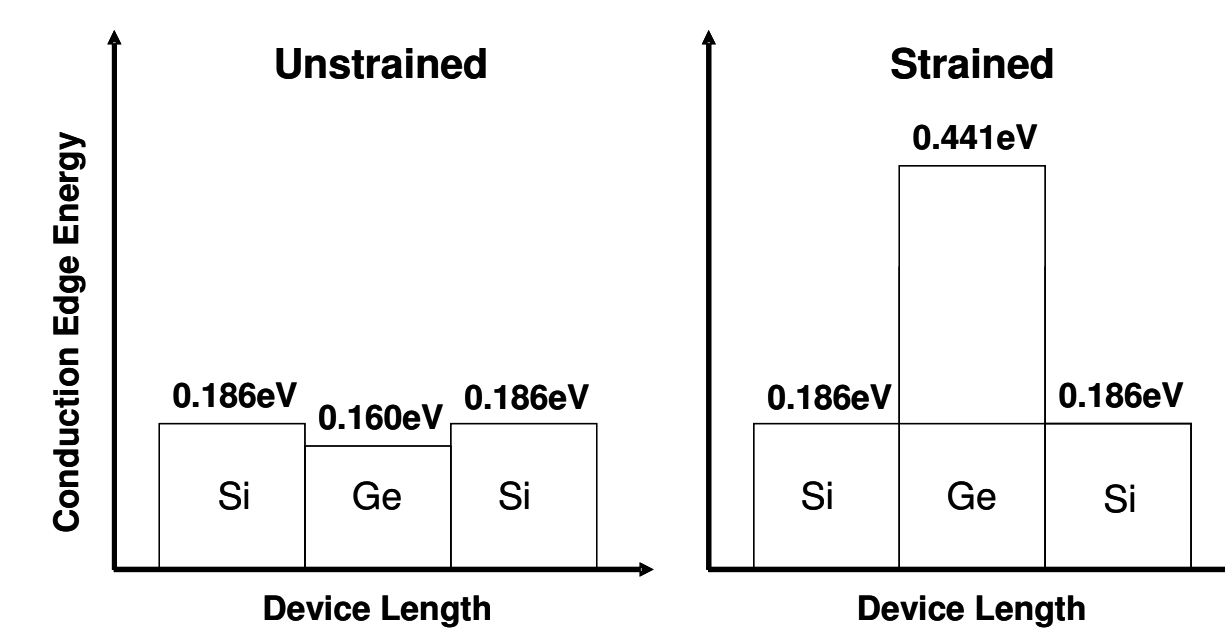
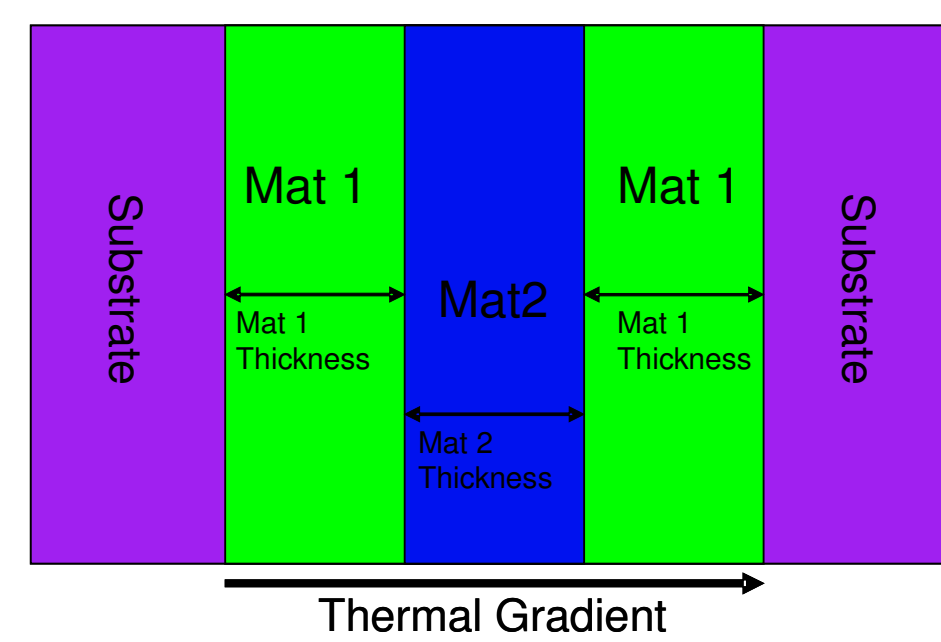
Introduction

- 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.
- 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.

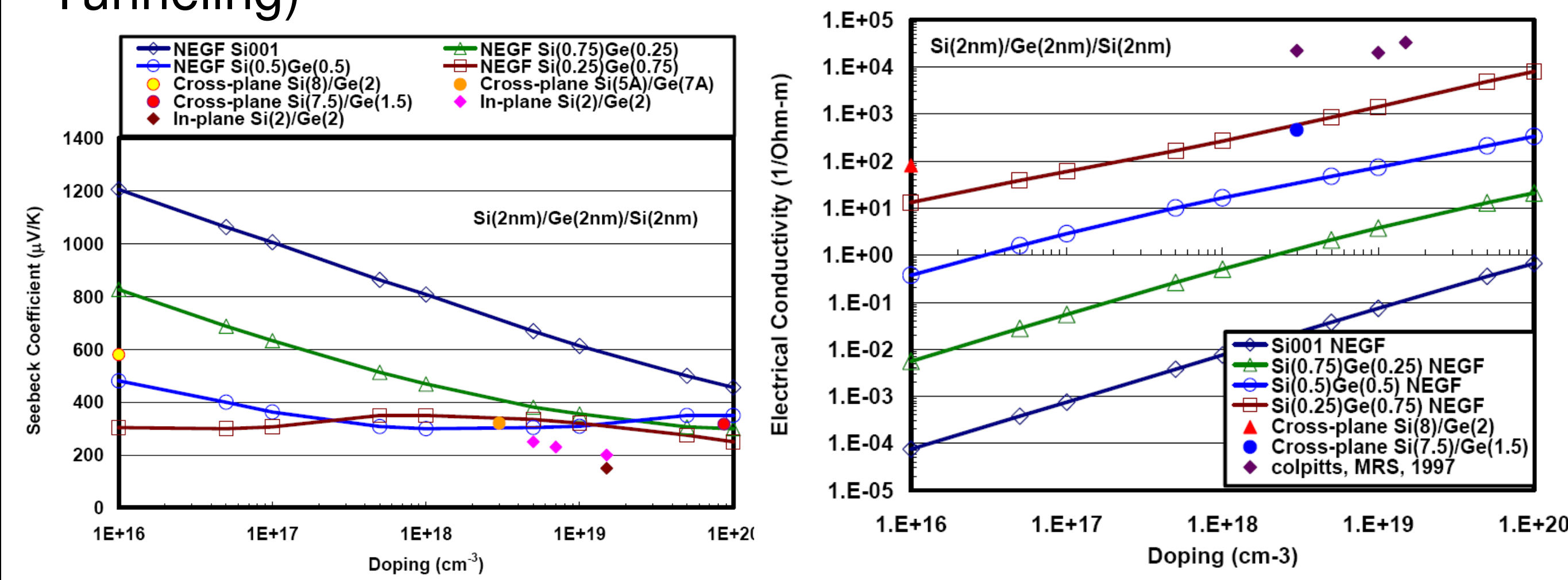
• Thermoelectric Figure of Merit $ZT = \frac{S^2 \sigma T}{\kappa}$

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)



• A. Bulusu and D. G. Walker, "Quantum Modeling of Thermoelectric Properties of Si/Ge/Si Superlattices," accepted for publication, IEEE Transactions on Electron Devices, Vol. 55, No. 1, pp. 423-429, January, 2008.

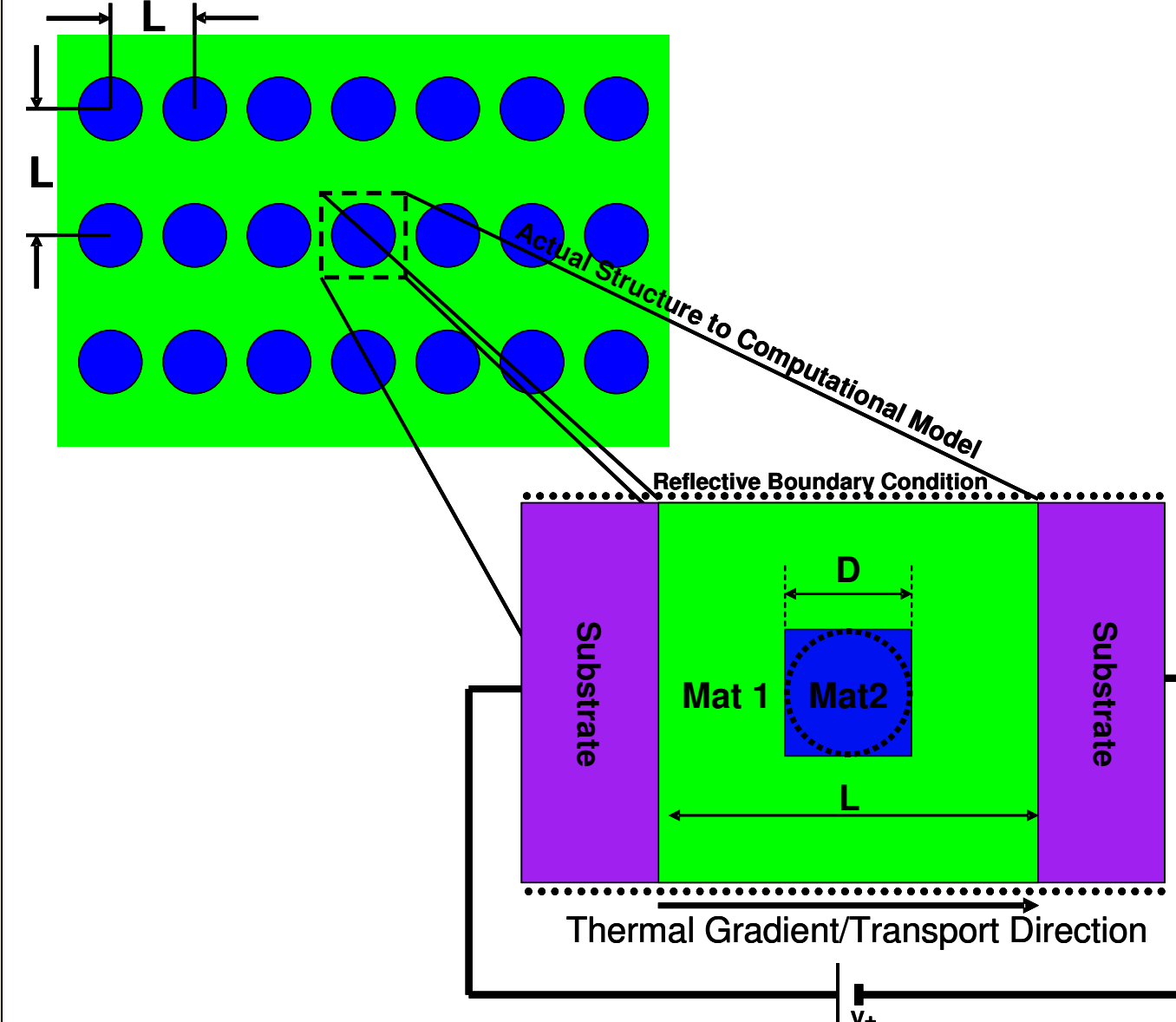
• Van de Walle, C. G., 1989 "Band lineups and deformation potentials in the model-solid theory". Physical Review B, 39(3), Jan., pp. 1871-1883

• Terence Musho; Greg Walker (2008), "Thermoelectric Power Factor Calculator for Superlattices," DOI: 10254/nanohub-r5602.2.

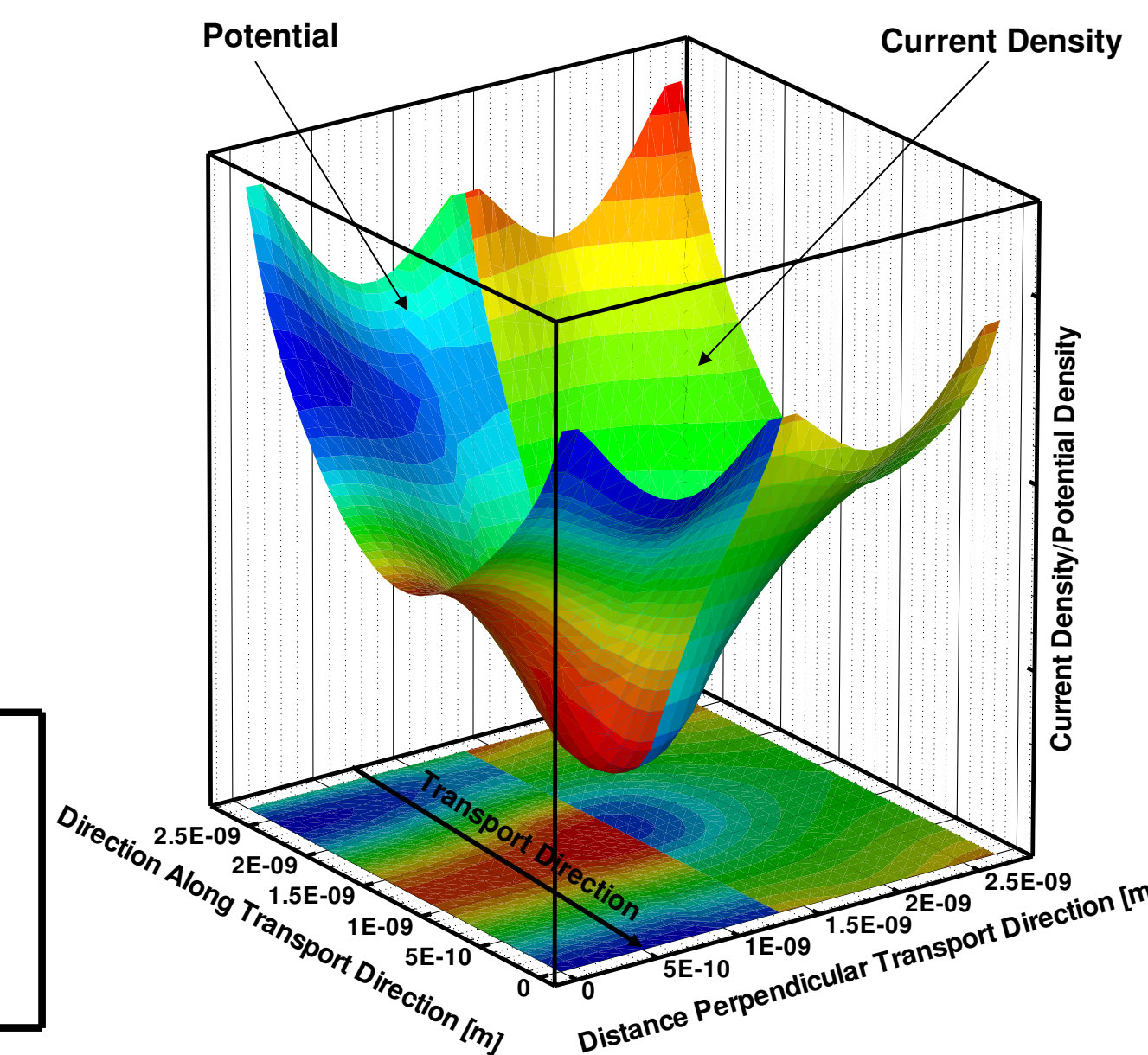
• Terence Musho; Greg Walker (2008), "Thermoelectric Power Factor Calculator for Nanocrystalline Composites," DOI: 10254/nanohub-r5603.4.

New Structure (NCC)

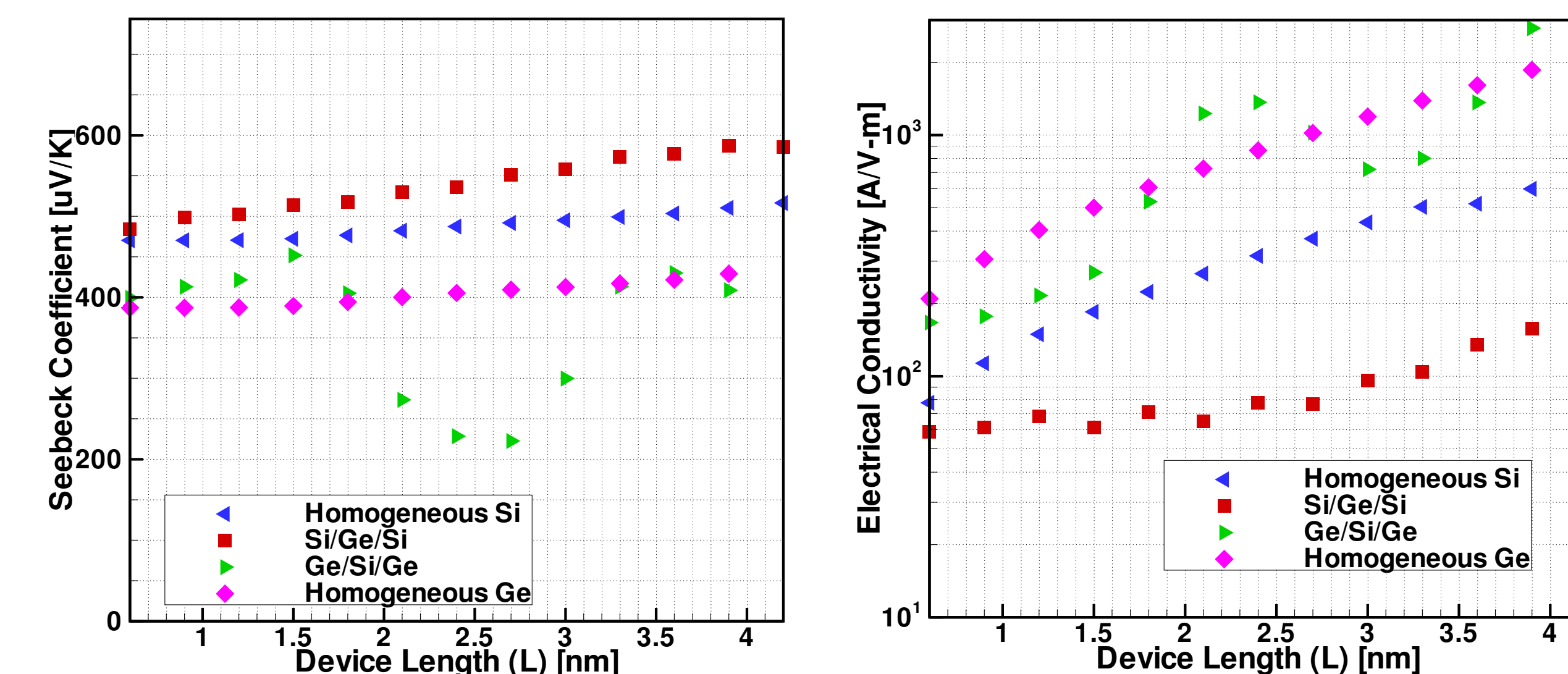
- Evolve 1D NEGF -> 2D NEGF
- Geometry Simplification
- Reflective Boundary Condition
- Material – Silicon, Germanium



1. Apply ΔT to get V
2. Apply V to get $I=0 \rightarrow S = \Delta V / \Delta T$

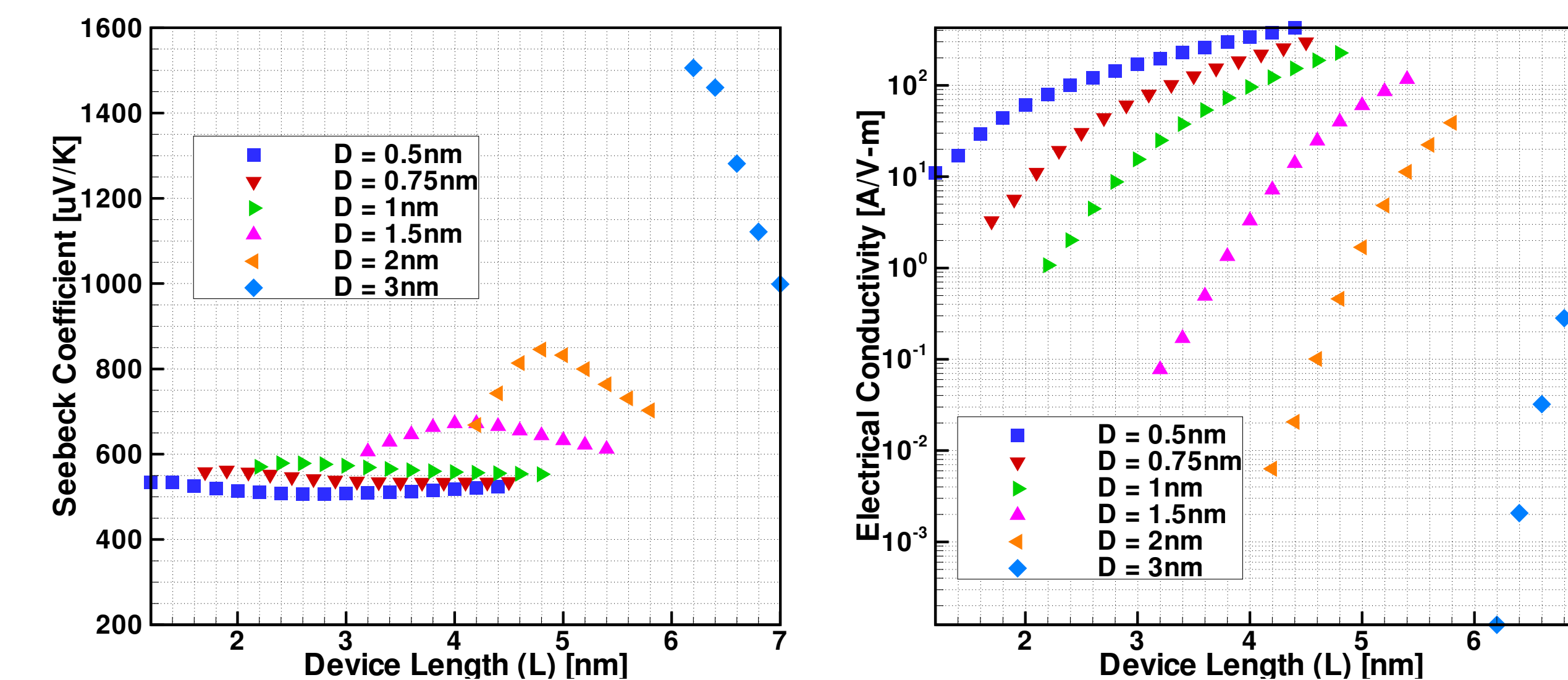


Matrix and Crystal Material



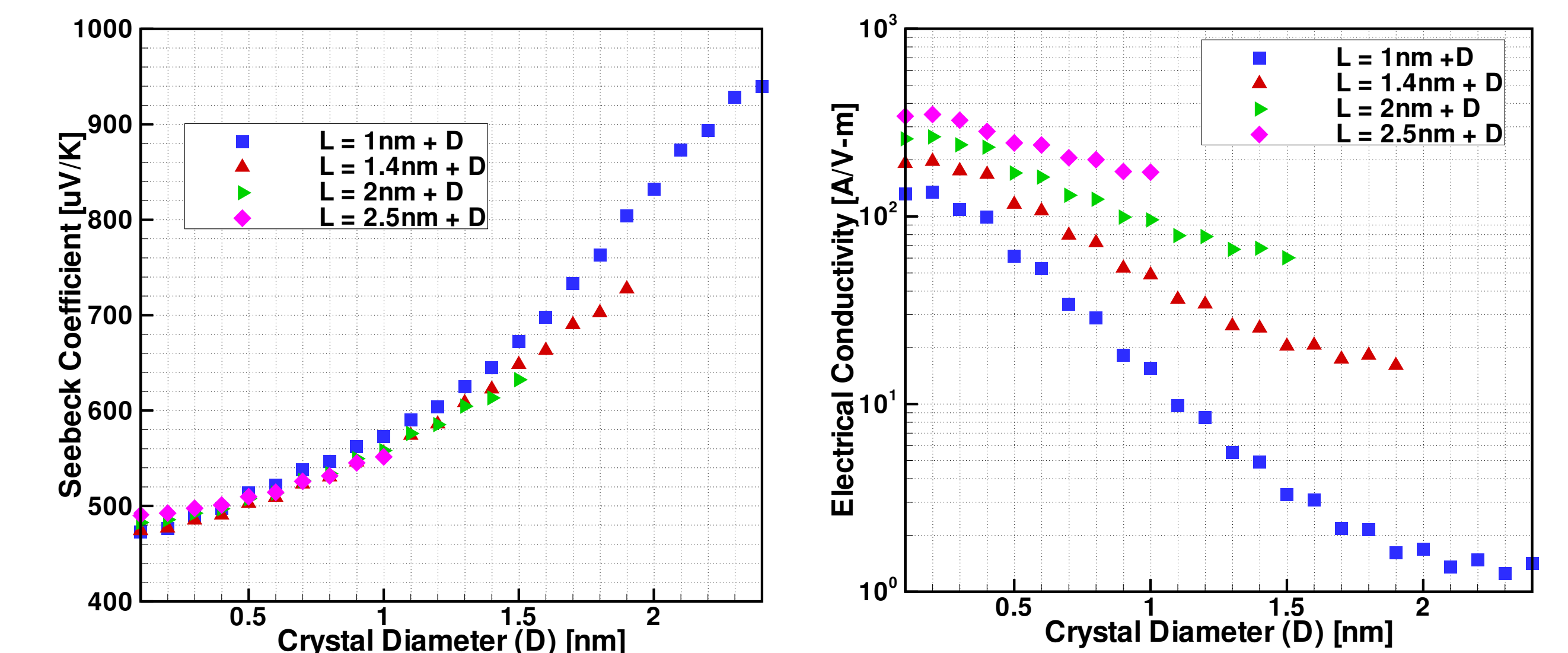
- Silicon Matrix, Germanium Crystal has greater Seebeck
- Straining of the Silicon crystal results in degeneracy and decreased Seebeck and increased Conductivity

Crystal Spacing Effects



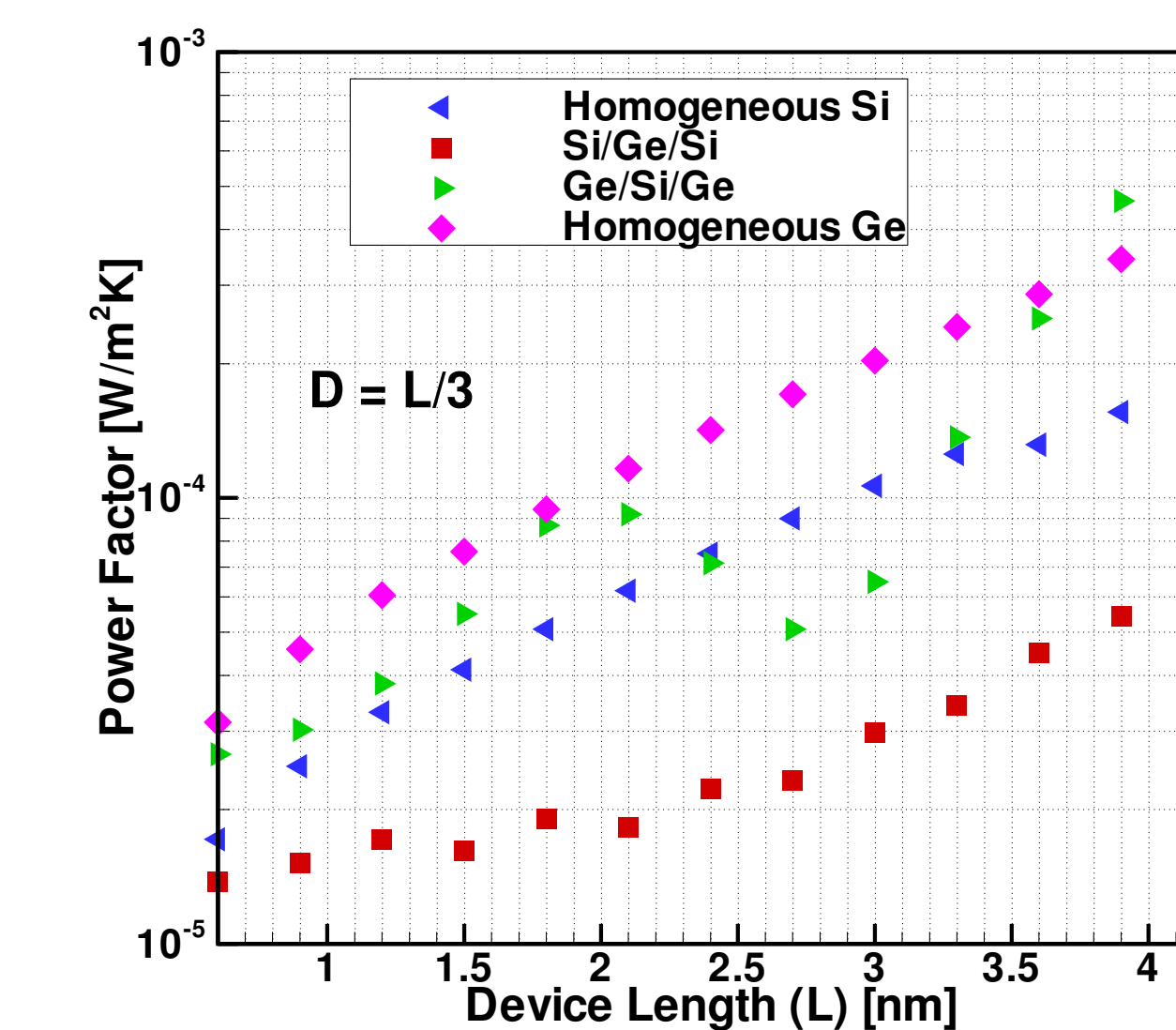
- Maximum in Seebeck is evident for larger crystals
- Locus of optimal crystal spacing evident

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.
 - Kim (2006) experimental research of NCCs showed that thermal conductivity is greater for homogeneous Si over NCC structures.

• W. Kim, J. Zide, A. Gossard, D. Klenov, S. Stemmer, A. Shakouri, A. Majumdar, "Thermal Conductivity Reduction and Thermoelectric Figure of Merit Increase by Embedding Nanoparticles in Crystalline Semiconductors," Physical Review Letters, Vol. 96, 045901 (2006)