

IMPROVEMENT OF THERMOELECTRIC PROPERTIES IN  
NANOSTRUCTURES WITH CONSTRICTIONS

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*“All we have to decide is what to do with the time that is given us.”*

**J.R.R. Tolkien**

## ABSTRACT

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The results of a study into the development of novel Thermoelectric (TE) materials by engineering nanoscale constrictions are presented in this thesis. The aim of this investigation lies in the development of an enhanced TE material. To achieve this, the dependence of TE properties, specifically the TE figure of merit ( $ZT$ ) on the material properties has been considered. The enhancement of the  $ZT$  was achieved by reducing the thermal conductivity ( $k$ ) of the material. During this phase, the effects of different nanoscale modifications to the material structure on its electrical properties are contemplated to ensure that the TE  $ZT$  does not get vitiated.

Here, a novel nanostructure formed by the sintering of individual Silicon nanoparticles in a linear fashion has been used and is referred to as a Nanoparticle Chain (NPC) structure. The nanoparticle arrangement in an NPC structure causes nanoscale constrictions to be formed along the transport direction of the structure. This is seen to cause extremely low lattice  $k$  (reaching 0.614 W/mK) while preserving a considerable amount of crystallinity. The fabrication procedure of the NPC structure has also been considered through this study thereby ensuring that results can be translated to real-world applications using existing technologies. During the investigation, an interesting competing effect between two, phonon transport aspects has been observed to cause a nonmonotonic trend in the  $k$  of the structure, while a variation in the phonon density of states along the transport direction was identified to cause a  $k$  reduction to values lower than those attained with comparably sized nanowires.

Further variations of the structure are obtained by expanding the zero-dimensional constriction of NPC structures to a one-dimensional form referred to as Nanowire Chain (NWC) structures. Subsequently, the electrical properties of the structures in consideration are evaluated, and a three-order of magnitude enhancement in the TE  $ZT$  is observed in comparison to the bulk material. Thus, it is shown that nanoscale constrictions can be engineered to enhance the TE performance of materials.

**Keywords:** *Nanoparticles, Thermoelectric, Phonon transport, Electron transport, Ab-initio modelling, Constriction engineering*

### Journal Articles

- P. Henadeera, N. Samaraweera, C. Ranasinghe, and A. Wijewardane, “Ultra-low thermal conductivity of nanoparticle chains: A nanoparticle based structure for thermoelectric applications,” *J. Appl. Phys.*, vol. 130, no. 6, p. 064301, Aug. 2021.
- P. Henadeera, N. Samaraweera, C. Ranasinghe, and A. Wijewardane, “Surface and constriction engineering of nanoparticle based structures towards ultra-low thermal conductivity as thermoelectric materials,” *Nanoscale and Microscale Thermophysical Engineering.*, Minor revisions pending.
- P. Henadeera, N. Samaraweera, C. Ranasinghe, and A. Wijewardane, “Notable thermoelectric performance of laterally arranged Si nanowires: Constriction engineering as a promising pathway.” Submitted.

### Conference Articles

- P. Henadeera, N. Samaraweera, C. Ranasinghe, and A. Wijewardane, “Ultra-low Thermal Conductivity Through Nano-Constriction Engineering,” *13th Multidisciplinary International Student Workshop (MISW2022), Tokyo Institute of Technology*, p 43, 2022.

*This thesis is dedicated to my wife and my parents.*

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## DECLARATION

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I declare that this is my own work, and this thesis does not incorporate without acknowledgement any material previously published or submitted for a degree or diploma in any other university or institute of higher learning and to the best of my knowledge and belief it does not contain any material previously published or written by another person except where the acknowledgement is made in the text.

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## NOMENCLATURE

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### Abbreviations

|         |   |
|---------|---|
| 0D      | Zero Dimensional  |
| 1D      | One Dimensional   |
| 2D      | Two Dimensional   |
| BTE     | Boltzmann Transport Equation  |
| CBM     | Conduction Band Minimum   |
| COMPASS | Condensed-phase Optimized Molecular Potentials for Atomistic Simulation Studies |
| CUDA    | Compute Unified Device Architecture   |
| DFT     | Density Functional Theory   |
| DMT     | Derjaguin Müller Toporov  |
| DoS     | Phonon Density of States  |
| DP      | Deformation Potential   |
| DZP     | Double Zeta Polarized   |
| EMD     | Equilibrium Molecular Dynamics  |
| GGA     | Generalized Gradient Approximation  |
| GK      | Green Kubo  |
| GPU     | Graphics Processing Unit  |
| GULP    | General Utility Lattice Program   |
| HCAF    | Heat Current Autocorrelation Function   |
| JKR     | Johnson Kendall Roberts   |
| LAMMPS  | Large Scale Atomic/Molecular Massively Parallel Simulator                       |
| LD      | Lattice Dynamics  |
| LDA     | Local Density Approximation   |
| LJ      | Lennard Jones   |
| MCSN    | Modulated Core Shell Nanowires  |
| MD      | Classical Molecular Dynamics  |
| MEMS    | Micro Electro-Mechanical Systems  |
| MFP     | Mean Free Path  |
| NEMD    | Non-Equilibrium Molecular Dynamics  |

|       |                                  |
|-------|----------------------------------|
| NPB   | Nanoparticle Packed Bed          |
| NPC   | Nano Particle Chain              |
| NPM   | Nano Particle Mesh               |
| NWC   | Nano Wire Chain                  |
| Ovito | Open Visualization Tool          |
| PGEC  | Phonon Glass/ Electron Crystal   |
| PW    | Plane-Wave                       |
| SA    | Shell Alloyed                    |
| SA-1  | Type-1 SA                        |
| SA-2  | Type-2 SA                        |
| SED   | Spectral Energy Density          |
| SEM   | Scanning Electron Microscopy     |
| SW    | Stillinger Weber                 |
| TE    | Thermoelectric                   |
| TEG   | Thermoelectric Generator         |
| TEM   | Transmission Electron Microscopy |
| VBM   | Valance Band Maximum             |

## Variables

### Greek letters

|  |   |
|--|---|
| $\sigma$   | Electrical conductivity   |
| $\eta$   | Efficiency  |
| $\Gamma_i$   | Per Atom Stress Tensor  |
| $\rho(\omega)$   | Phonon density of states at omega frequency   |
| $\omega$   | Frequency   |
| $\phi$   | Potential energy  |
| $\phi(x)$  | Potential energy between two neighbors at a distance $x$ from one another   |
| $\phi \left( \begin{smallmatrix} ij \\ ab \end{smallmatrix} \right)$ | Energy of interaction between the $i^{\text{th}}$ and $j^{\text{th}}$ atoms in the $a^{\text{th}}$ and $b^{\text{th}}$ unit-cells |

|   |   |
|---|---|
| $\omega_0$  | Center of the Lorentzian function   |
| $\Gamma$  | Full width at half maximum of Lorentz function                                  |
| $\tau$  | Relaxation time   |
| $\psi_i(r)$   | Wave function at location $r$   |
| $v_k$   | Velocity of electrons   |
| $\tau_e$  | Relaxation time of electrons  |
| $v_j(t)$  | Velocity of the $j^{\text{th}}$ atom at time $t$                                |
| $n$   | Phonon normal mode  |
| $\nu$   | Phonon branch   |
| $\phi_{Tot}$  | Total potential energy  |
| $\lambda^* \begin{pmatrix} K & i \\ n & \alpha \end{pmatrix}$ | Conjugate of the eigenvector of the $n^{\text{th}}$ mode at the wave vector $K$ |
| $\lambda_{i,n}$   | Eigen vector of the $i^{\text{th}}$ atom for the $n^{\text{th}}$ normal mode    |
| $\varepsilon_i$   | Eigen energy of electrons   |

### Roman letters

|                        |  |
|------------------------|--|
| $c$                    | Speed of light                         |
| $C$                    | Elastic constant                       |
| $d$                    | Dimensionality of the system           |
| $D$                    | Diffusion Coefficient                  |
| $\mathbf{D}$           | The dynamical matrix                   |
| $ \Delta(\text{DoS}) $ | Difference in Density of States        |
| $e$                    | Charge of an electron                  |
| $E$                    | Electric field                         |
| $E_1$                  | The potential of deformation           |
| $E_{atom}$             | Total energy of an atom in equilibrium |
| $E_{edge}$             | Energy of the band edge                |
| $E_{Lat}$              | Lattice energy                         |
| $E[n]$                 | Total energy of the system             |

|                |  |
|----------------|--|
| $E_{xc}$       | Exchange correlation energy                    |
| $\mathbf{F}$   | Force constant matrix                          |
| $f_k(r, t)$    | Distribution function                          |
| $\hbar$        | Reduced Planks constant                        |
| $H$            | Magnetic field                                 |
| $J_x(n)$       | Heat Flux in the $x$ Direction at Time $t = n$ |
| $k$            | Thermal conductivity                           |
| $k_B$          | Boltzmann Constant                             |
| $k_e$          | Electronic Thermal Conductivity                |
| $k_l$          | Lattice Thermal Conductivity                   |
| $k_x$          | The thermal conductivity in $x$ direction      |
| $K$            | Wave vector                                    |
| $\Delta l/l_0$ | Applied strain                                 |
| $L$            | Lorentz Number                                 |
| $m_e$          | Mass of electron                               |
| $m_i$          | Mass of the $i^{\text{th}}$ atom               |
| $N$            | Total Number of Atoms                          |
| $N_{cell}$     | Total number of cells                          |
| $P$            | Probability                                    |
| $PR$           | Participation Ratio                            |
| $q$            | Heat Flux                                      |
| $\mathbf{q}$   | Heat Flux vector                               |
| $\dot{Q}$      | Phonon normal mode coordinates                 |
| $\mathbf{r}$   | Displaced position of atom                     |
| $\mathbf{r}_0$ | Equilibrium position of atom                   |
| $S$            | Seebeck coefficient                            |
| $S_i$          | Per-atom stress tensor                         |
| $t$            | Time   |
| $T$            | Absolute Temperature                           |
| $T_0$          | Sampling time                                  |
| $T_c$          | Cold side temperature                          |

|   |   |
|---|---|
| $T_h$                                       | Hot side temperature  |
| $T[n]$                                      | Kinetic energy of the system  |
| $\mathbf{u}$                                | Small displacement  |
| $\tilde{u}$                                 | Amplitude of the phonon   |
| $u_a$                                       | displacement vector component of each atom in the $a^{\text{th}}$ unit cell   |
| $U_\alpha \left( \overset{a}{i}, t \right)$ | $\alpha^{\text{th}}$ component of the velocity of the $i^{\text{th}}$ atom in the $a^{\text{th}}$ unit cell at time $t$ |
| $V$   | Volume of the System  |
| $V_0$                                       | Unstrained volume   |
| $V_{eff}$                                   | Effective external potential  |
| $V_{inf}$                                   | Infinitesimal volume  |
| $V_{int}[n]$                                | Electron-electron interaction energy of the system  |
| $ZT$  | Figure of Merit   |

## LIST OF APPENDICES

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