Thermal Conductivity of Silicon Nanostructures Using Molecular Dynamics

ALEXANDER ROBILLARD, RALF MEYER

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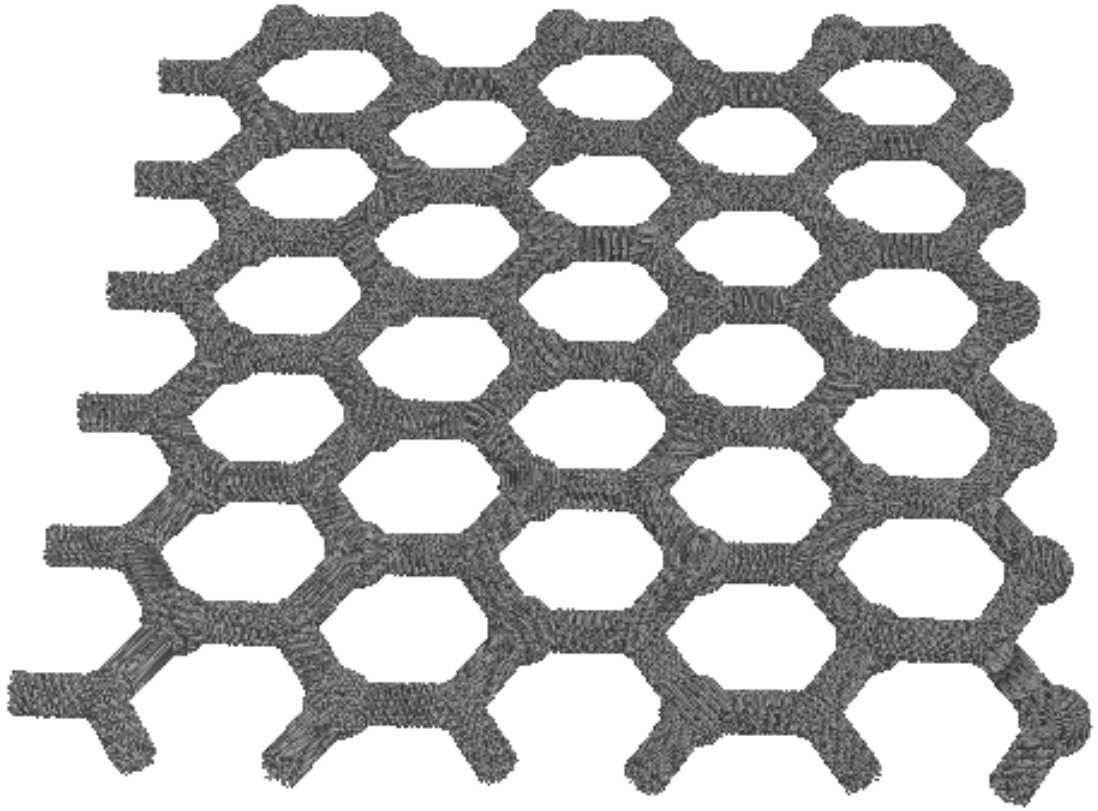
LaurentianUniversity
UniversitéLaurentienne

Introduction



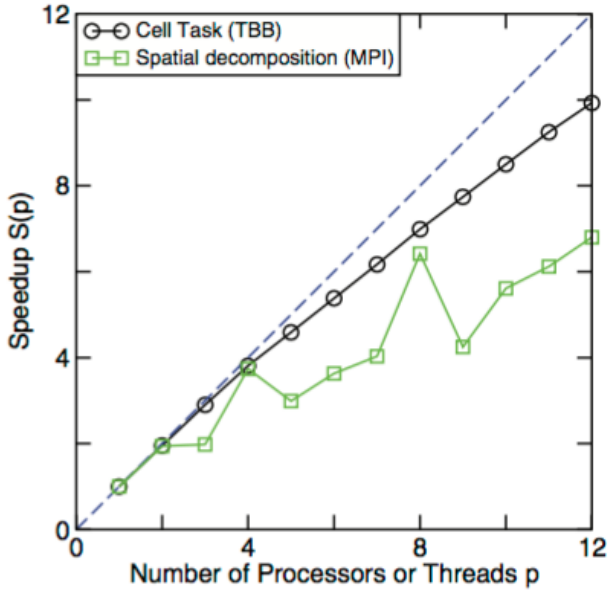
- Thermal properties of nanostructures vary greatly from bulk values
- Silicon nanowires are candidates for the construction of silicon phononic crystals (PCs) [3]
- The PC used here has 2.70 million Si atoms [6]
- Thermal conductivity can be calculated using Reverse Non-Equilibrium Molecular Dynamics (RNEMD) [7]
- $J = -\kappa \nabla T$

Objectives

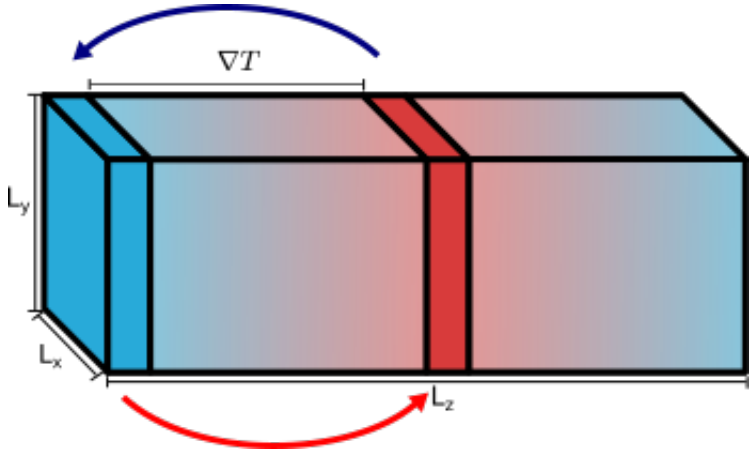
- Assess the size dependence of the thermal conductance of silicon nanowires for a generic data set
- Assess the size dependence of wires that constitute the described PC
- Compare the thermal conductance of the PC with that of very large nanowires (with similar atom numbers)
- Examine the impact of the methodology, mainly regarding the frequency of energy interchange

Computing Methods

- Custom multi-threaded software (C/C++)
- Implements Intel Threading Building Blocks (TBB)
- Uses the *cell task method* [5]
- Left: Cell Task method speedup vs. MPI for copper nanoparticle



Methods



Schematic of RNEMD procedure for a block with periodic boundaries along the z-axis

- Use RNEMD with Modified Embedded Atom Method Potential (MEAM) [2]
- Interchange kinetic energies every so many steps
- Calculate conductance, $C = \kappa \frac{A}{dz}$
- (easier to compare geometries vs. conductivity)
- Two methods:
  A. Use slabs where interchange of E occurs:

$$C = \frac{q}{t_s \Delta T}$$

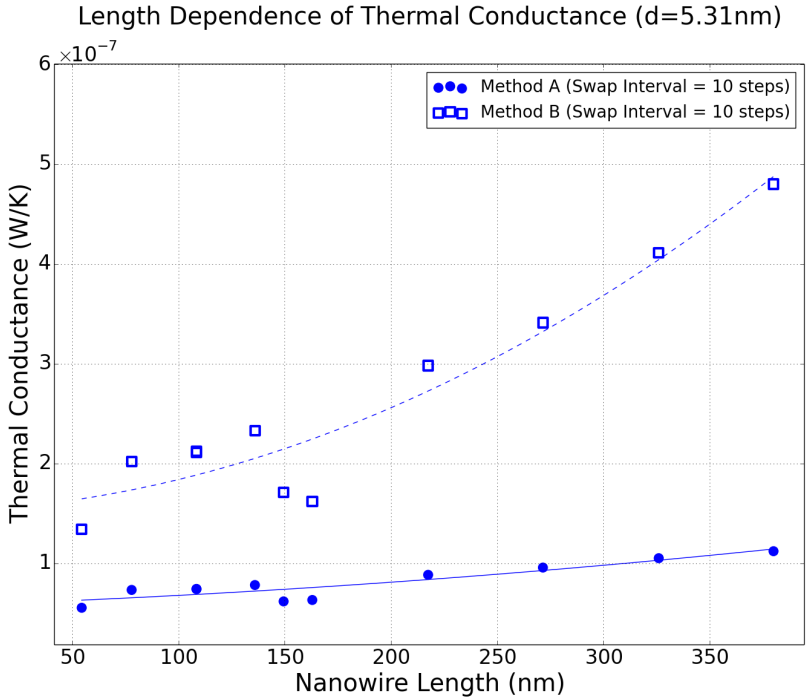
  B. Exclude slabs where interchange occurs, average subsections obtained:

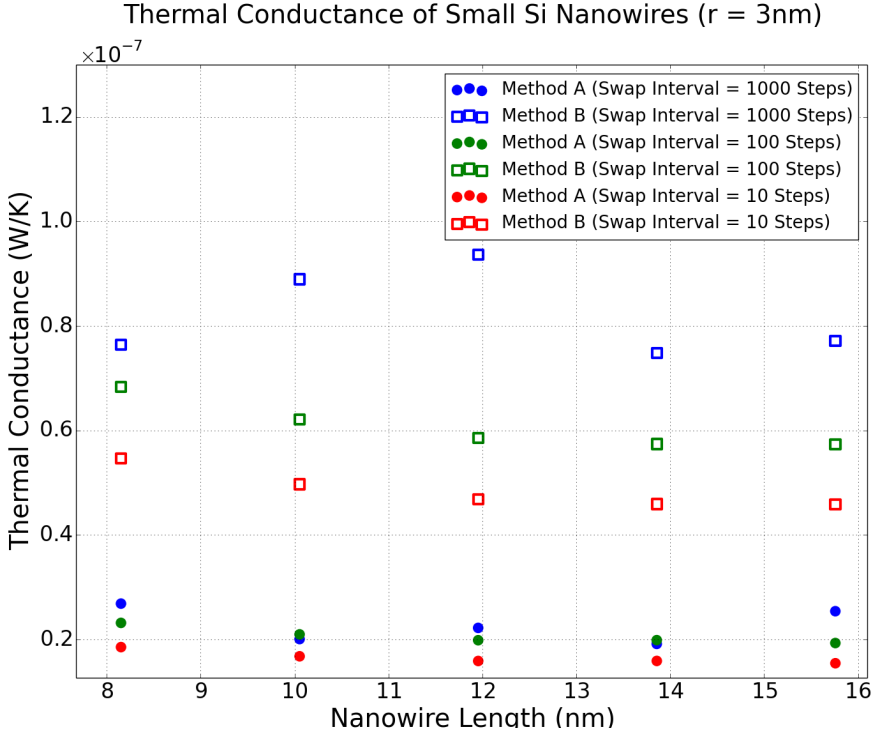
$$C = \frac{1}{2}\frac{q}{t_s}\left(\frac{1}{\Delta T_1} + \frac{1}{\Delta T_2}\right)$$

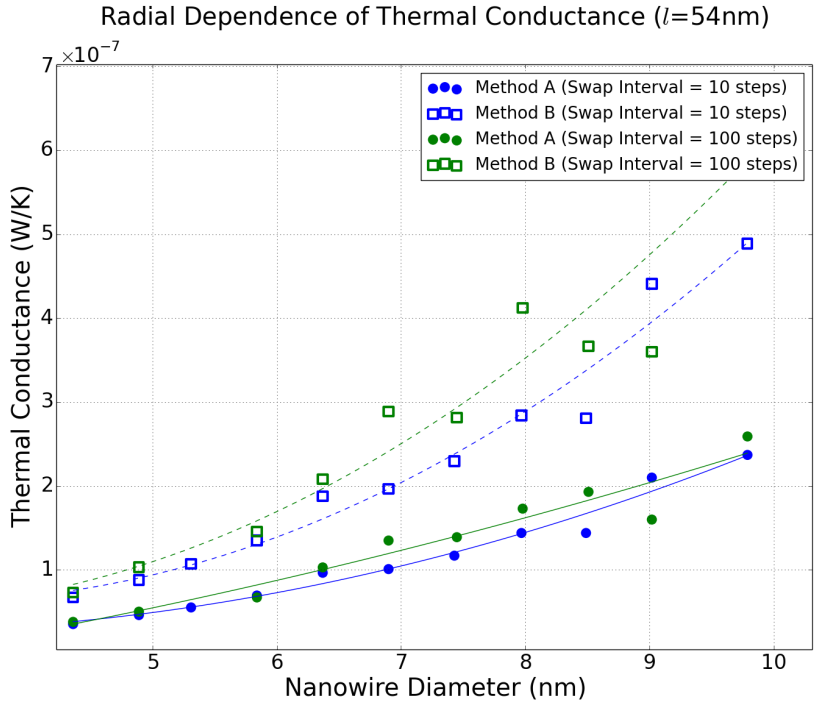
q : exchanged energy, t_s: time between exchanges, ΔT: temperature difference

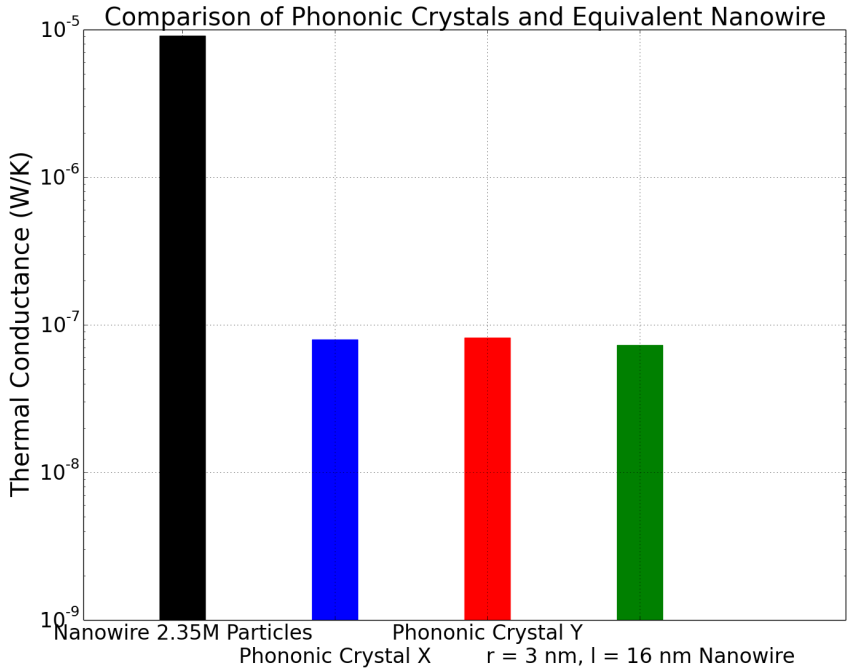
Results

- Curves are second order polynomial fits
- Length dependence: conductance increases with method B (smaller ΔT)
- Radial behaviour: quadratic more pronounced at low swap rate
- Small wires: method B and higher swap rates behave more stably
- Phononic crystal (150 nm length, 2.7M atoms) conductance is much smaller than a nanowire (150nm length, 93.5nm radius, 2.35M atoms) with similar number of particles
- Similar to the conductance of constituent wires



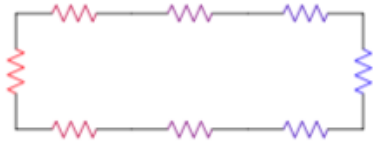






Conclusions

- Thermal conductances vary greatly from macroscopic value
- The phononic crystal model has thermal properties dominated by its smaller constituents rather than its overall size
- Methodological choices can artificially modify the simulation results.
  - Temperature variation of κ is a factor [1,4]
- Forthcoming research: methodology examination of RNEMD, temperature profile assessment, alternative calculation methods (e.g. resistance model)



Resistance Model

References

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Acknowledgements

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