
Comparison of Radial and Axial Thermal Transport in Silicon Nanowires

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Introduction

- Silicon nanowires are the core building blocks of advanced nanosystems which can be organized into 3D structures for a plethora of applications
- One of the important applications of silicon nanowires in VLSI microelectronics is their use as central parts of advanced gate-all-around field-effect transistors (GAA-FETs)
- Nanometric GAA-FETs build the leading edge of modern VLSI semiconductor technology (2026 VLSI Symposium), and further variants of GAA-FETs with cylindrical vertical nanowires are candidates for next generations of semiconductor technologies
- In addition to outstanding electrical properties of silicon nanowires, their thermal properties are of great importance, as advanced electronic devices involve high energy densities and there is a need to dissipate the heat from active regions of these devices
- In this work, we compare the heat transport in two directions, radial and axial, from the hot cylindrical silicon nanowires to their cooler surrounding
- Different dependencies of thermal conductivity on nanowire sizes for radial and axial directions and a significant anisotropy of thermal conductivity in silicon nanowires were found

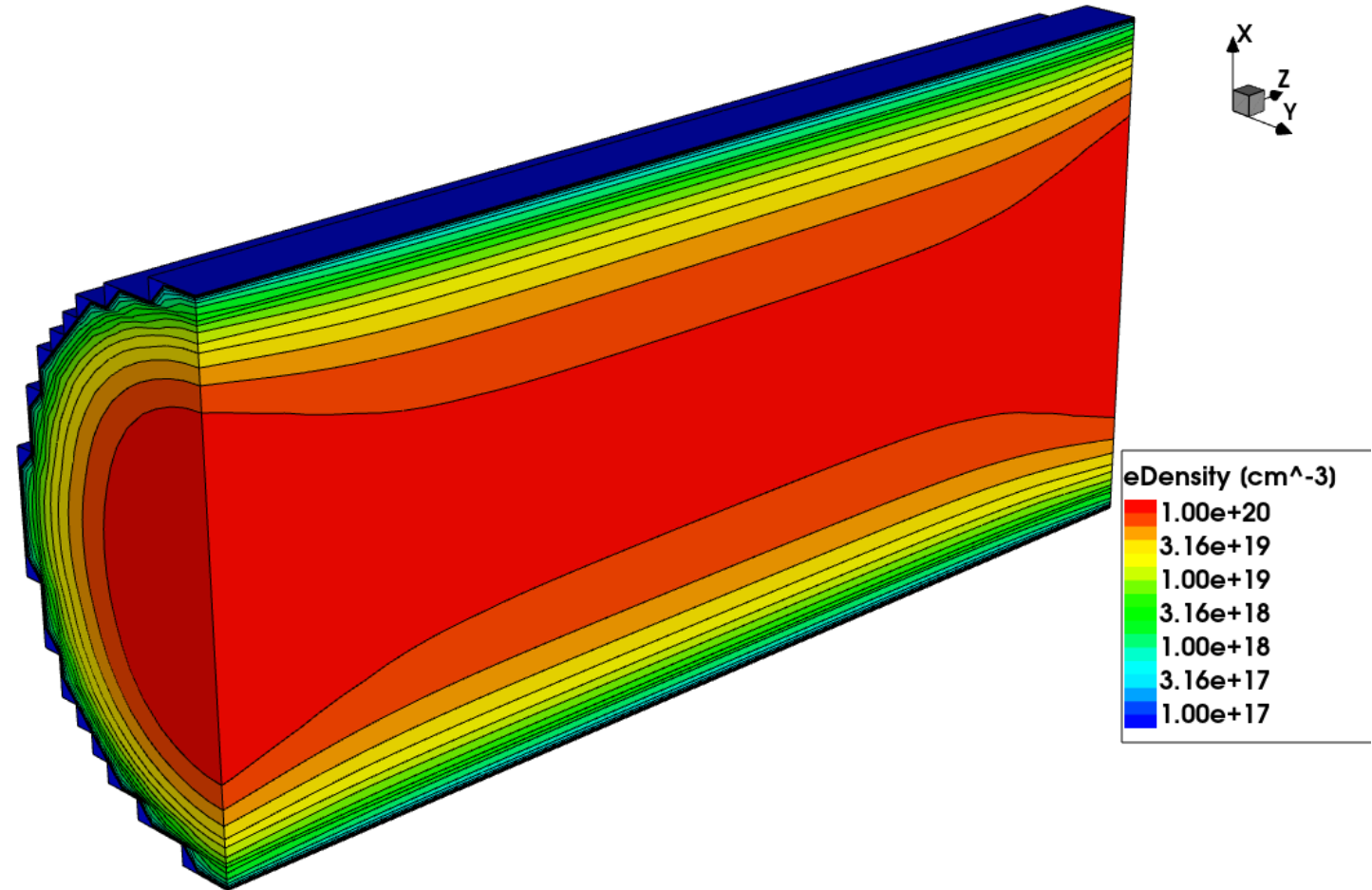
Background Work and Objective

- In our earlier work [1], we investigated thermal transport in radial direction from the heated cylindrical silicon nanowires
 - Dependences of thermal transport parameters in radial direction on nanowire length and radius were identified
 - Compact engineering models were formulated for efficient calculation of thermal transport in radial direction
- The objective of this work is: 1) to investigate thermal transport parameters for the axial thermal transport in nanowires, 2) to compare thermal properties of nanowires for axial thermal transport with corresponding properties for radial transport
- To establish a direct comparison with radial thermal transport, axial thermal transport was calculated for the same sizes of nanowires as it was done in [1].
- The size variations used in numerical calculations: Nanowire radius 1.2 to 2.6 nm, length 5 to 20 nm

[1] A. Burenkov, P. Pichler, "Radial thermal transport from heated silicon nanowires: Molecular dynamics simulations and compact engineering models," Case Studies in Thermal Engineering, vol. 69, p. 106056 (1-12), 2025.

Motivation for the Choice of Nanowires with Small Radius

- In GAA-FETs with silicon nanowire diameters of a few nanometers, a volume inversion effect of the charge carriers can be established
- This effect allows the on-state current to be maximized while minimizing the leakage current of GAA-FETs
- Figure illustrates the volume inversion effect in a GAA-FET with a 5 nm diameter silicon nanowire (numerical simulation using Synopsys TCAD)
- Electron density is not near the surface, but fills the volume of the active area

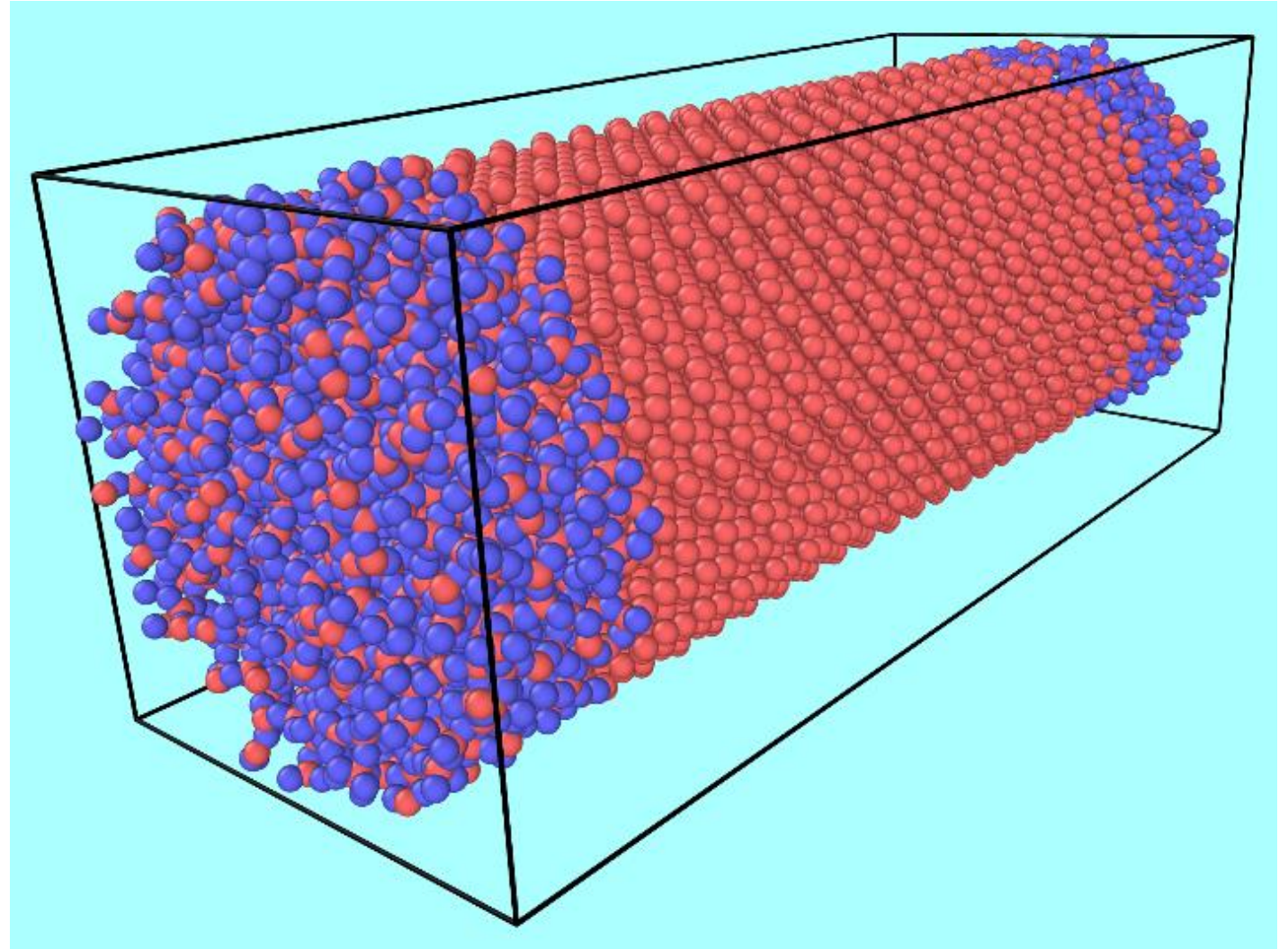


Electron density distribution in a GAA-FET
Gate voltage: 0.7 V. Drain voltage: 0.05 V

Methodology: Molecular Dynamics Simulations (1)

Simulation samples for MD simulations to study axial thermal transport

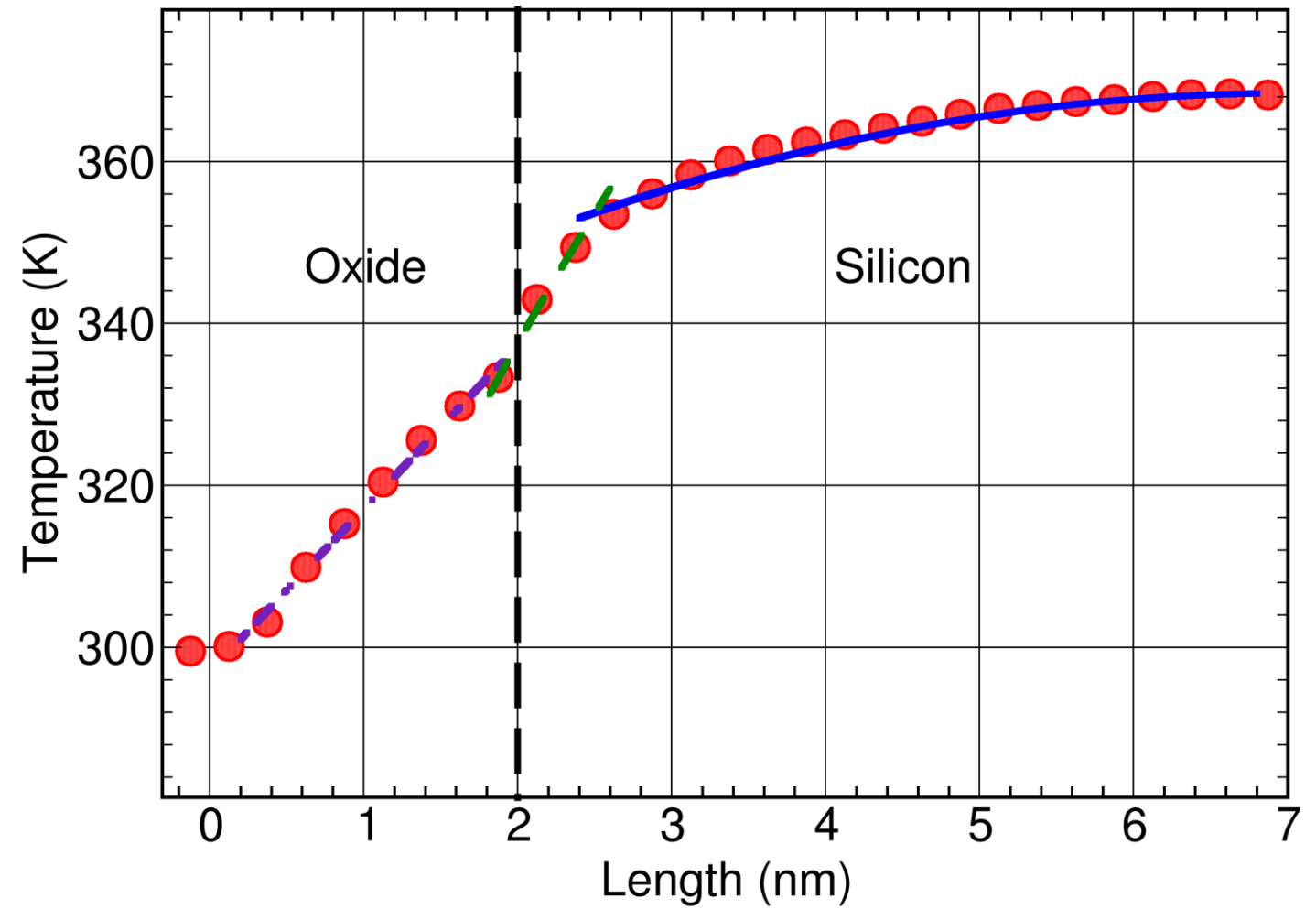
- Atomic arrangement in a simulation sample of a cylindrical silicon nanowire, radius: 2.6 nm, length; 10 nm
- Silicon atoms: Red; Oxygen: Blue
- Crystalline silicon wire is cupped with SiO₂ oxide lids that are kept at room temperature at external sides
- Silicon nanowire is heated by a uniformly distributed heat source
- MD simulation calculates thermal vibrations of the atoms and outputs temperature distribution in the sample



Methodology: Molecular Dynamics Simulations (2)

Temperature distribution along the axis of the MD simulation sample

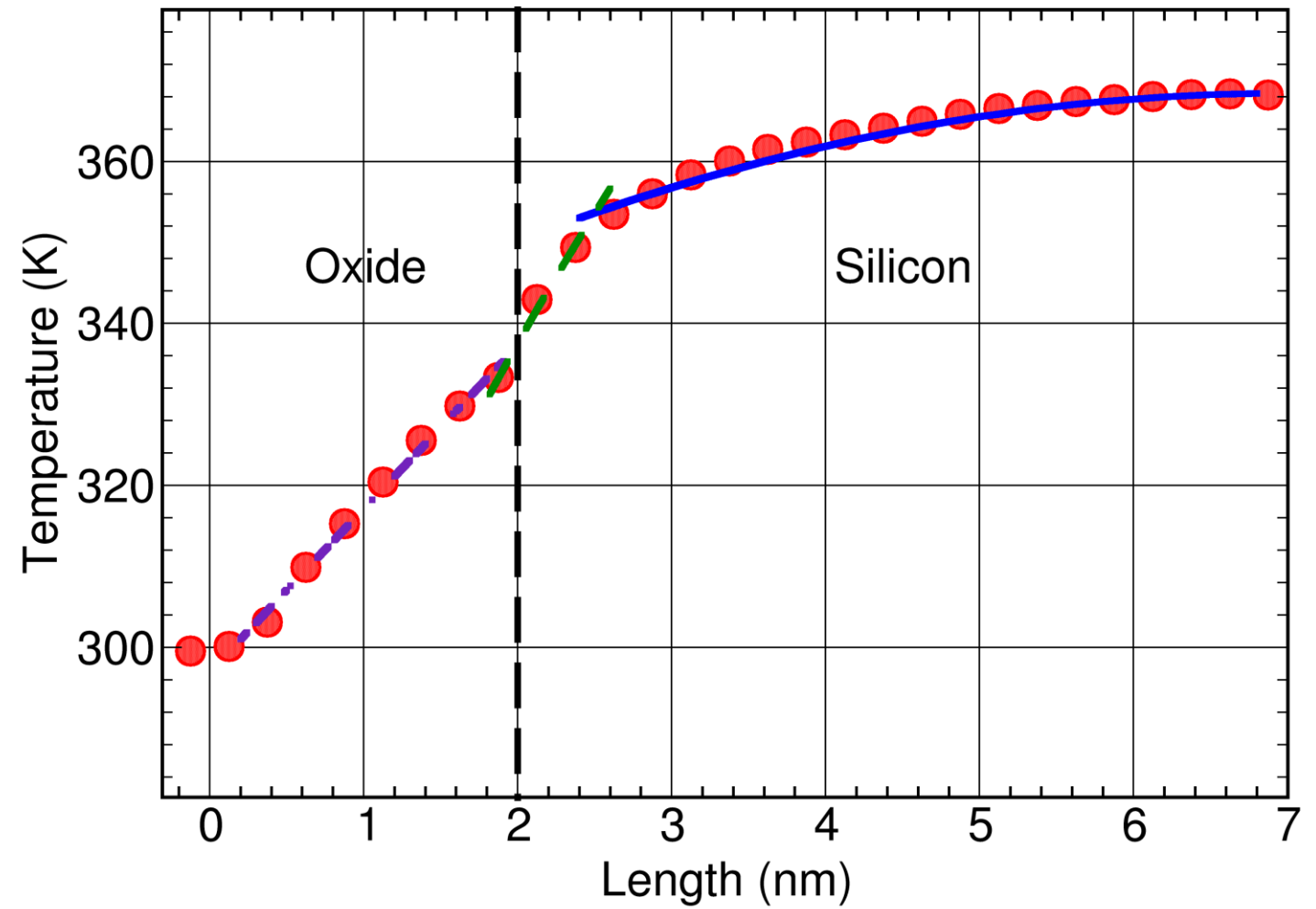
- Temperature distribution for a silicon nanowire (radius: 2 nm, length: 10 nm) shown in the Figure →
- Red dots: MD simulation, lines: approximations used for extraction of thermal parameters
- MD simulations were performed for a physical time of 12 ns using 12 Mio timesteps
- A stationary temperature distribution was observed after 0.1 ns of physical simulation time



Methodology: Molecular Dynamics Simulations (3)

Temperature distribution along the axis of the MD simulation sample

- There are four distinct areas in the temperature distribution
 1. There is room temperature at the external surface of oxide lid at Length=0
 2. About linearly increasing temperature in oxide
 3. A rapidly increased temperature in silicon at the interface to SiO_2
 4. A slowly increased temperature reaching its maximum in the middle of the nanowire



Methodology: Molecular Dynamics Simulations (4)

Power density of the heat source for the study of the axial heat transport in silicon nanowires

- The heating power density in MD simulations was chosen to establish an equal heat outflux for each simulation sample
- For this purpose, the heating power density was taken inversely proportional to the nanowire length as shown in the table below
- Such choice of power density resulted in similar maximum temperatures inside of all studied samples

Nanowire Length (nm)	5	10	15	20
Power Density (nW/nm ³)	7.54	3.77	2.51	1.89

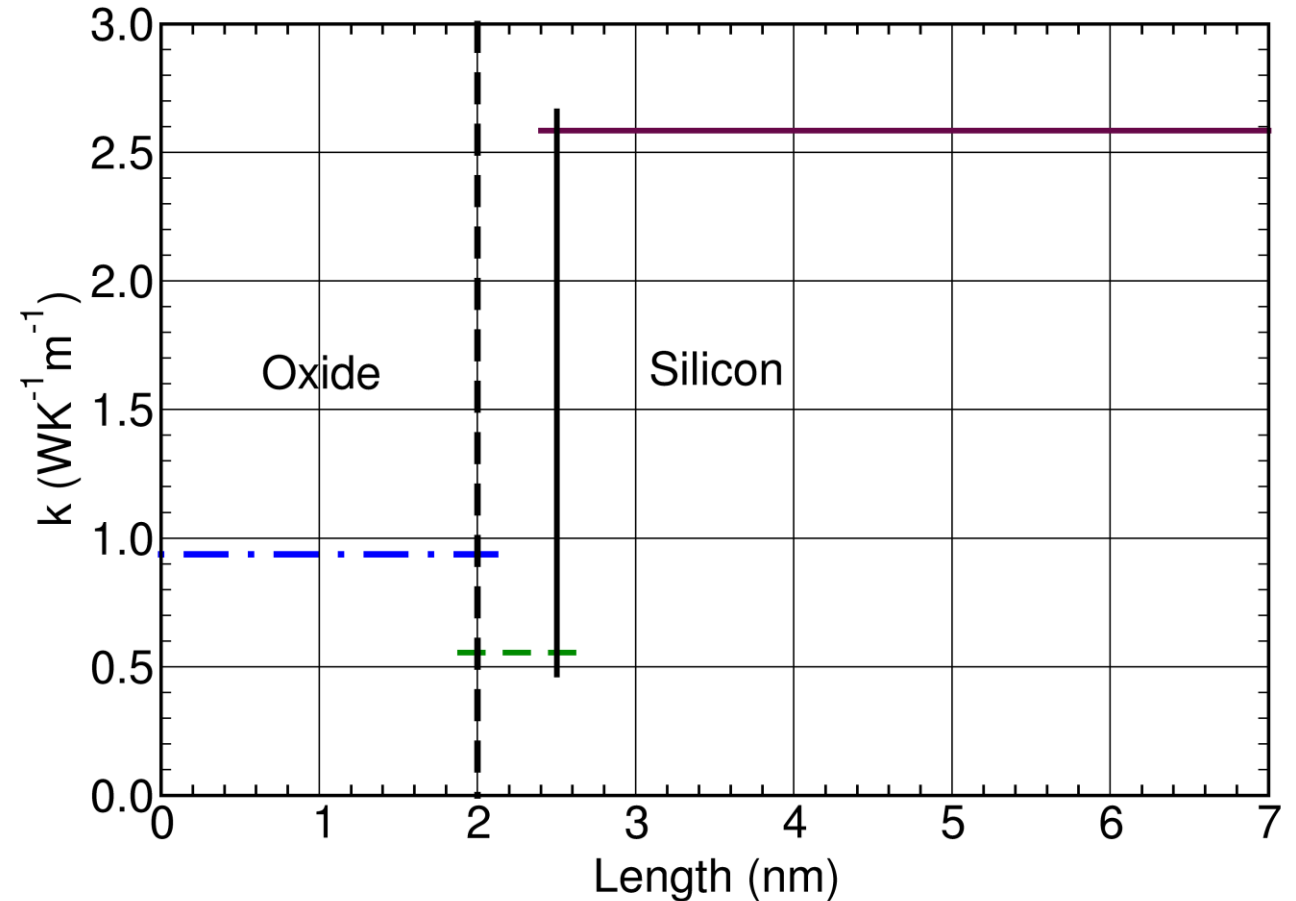
Methodology: Extraction of Thermal Conductivities and Resistances

- In standard MD simulations, temperature distributions exhibit significant statistical fluctuations which negatively impact the accuracy of thermal characterization
- To minimize statistical fluctuations, we performed MD simulations for longer physical simulation times using more than 10 Mio timesteps in each MD simulation
- Further, to minimize inaccuracies associated with numerical calculations of derivatives of temperature distributions, we approximated numerical results of MD with analytical functions that belong to the class of solutions of classical equations for thermal transport
- These measures allowed us to obtain reliable data on thermal conductivities and thermal resistances for nanowires of different sizes
- The nanowires with radius varied between 1.2 and 2.6 nm, and lengths between 5 and 20 nm were thermally characterized using MD simulations

Results: Effective Thermal Conductivity for the Axial Thermal Transport (1)

Thermal conductivity along the nanowire axis

- There are three distinct areas with a position-independent, but different values of thermal conductivity k
 1. Oxide layer with a relatively low k
 2. Near-surface layer of silicon with a thickness of about 0.5 nm with a low thermal conductivity
 3. A higher position-independent thermal conductivity inside of silicon nanowire

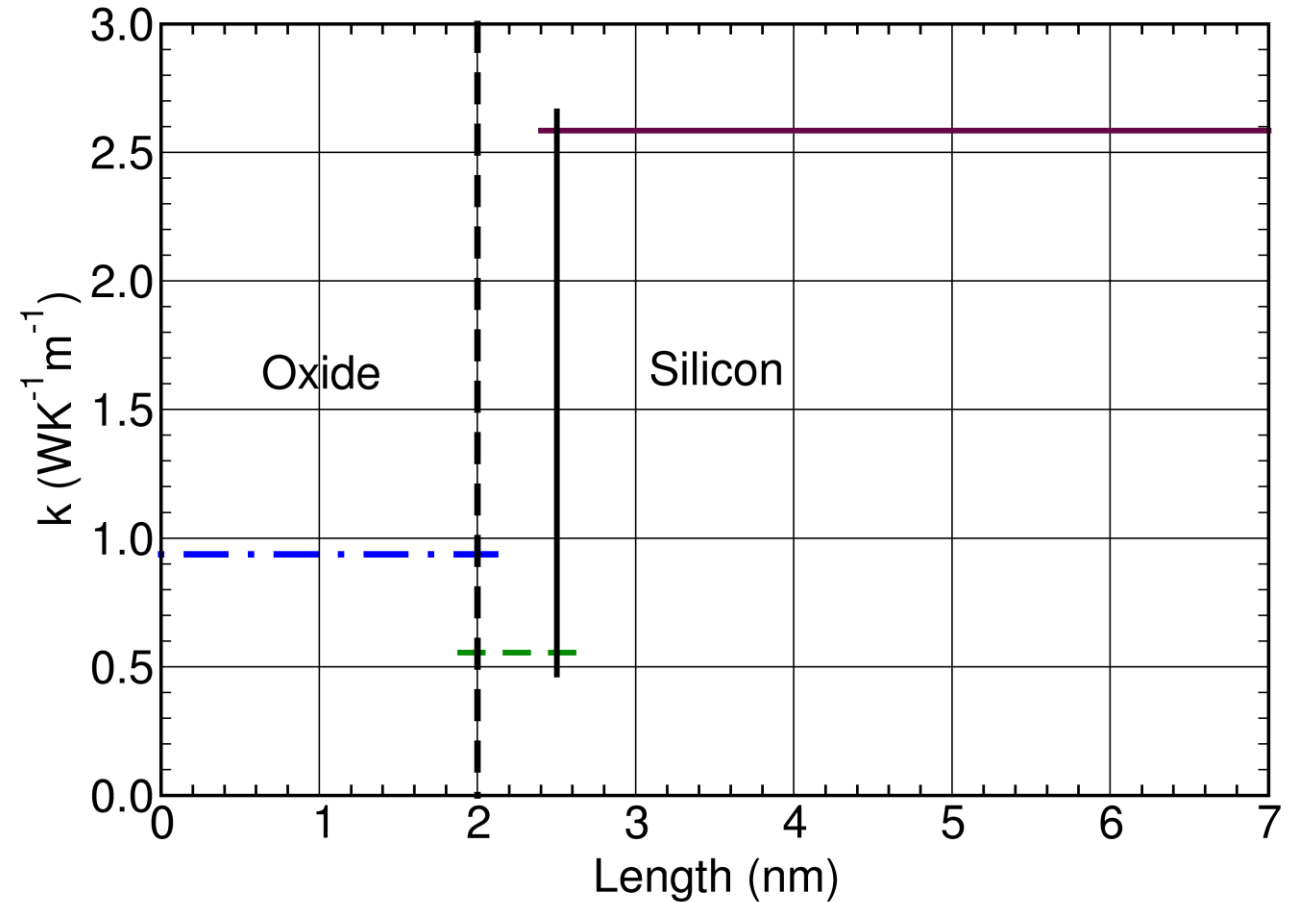


Effective thermal conductivity for the axial thermal transport in a silicon nanowire sample ($R_{\text{Si}}=2$ nm, $L_{\text{Si}}=10$ nm) as a function of position along the nanowire axis

Results: Effective Thermal Conductivity for the Axial Thermal Transport (2)

Physical meaning of thermal conductivity k in areas 1 to 3

1. Thermal conductivity in amorphous oxide layer, no size dependence expected and confirmed by MD
2. Low k in near-surface layer of silicon: Manifestation of thermal Kapitza-resistance at the Si/SiO₂ interface
3. Thermal conductivity for the axial thermal transport inside of silicon nanowire – depends on nanowire radius and length → subject of this study

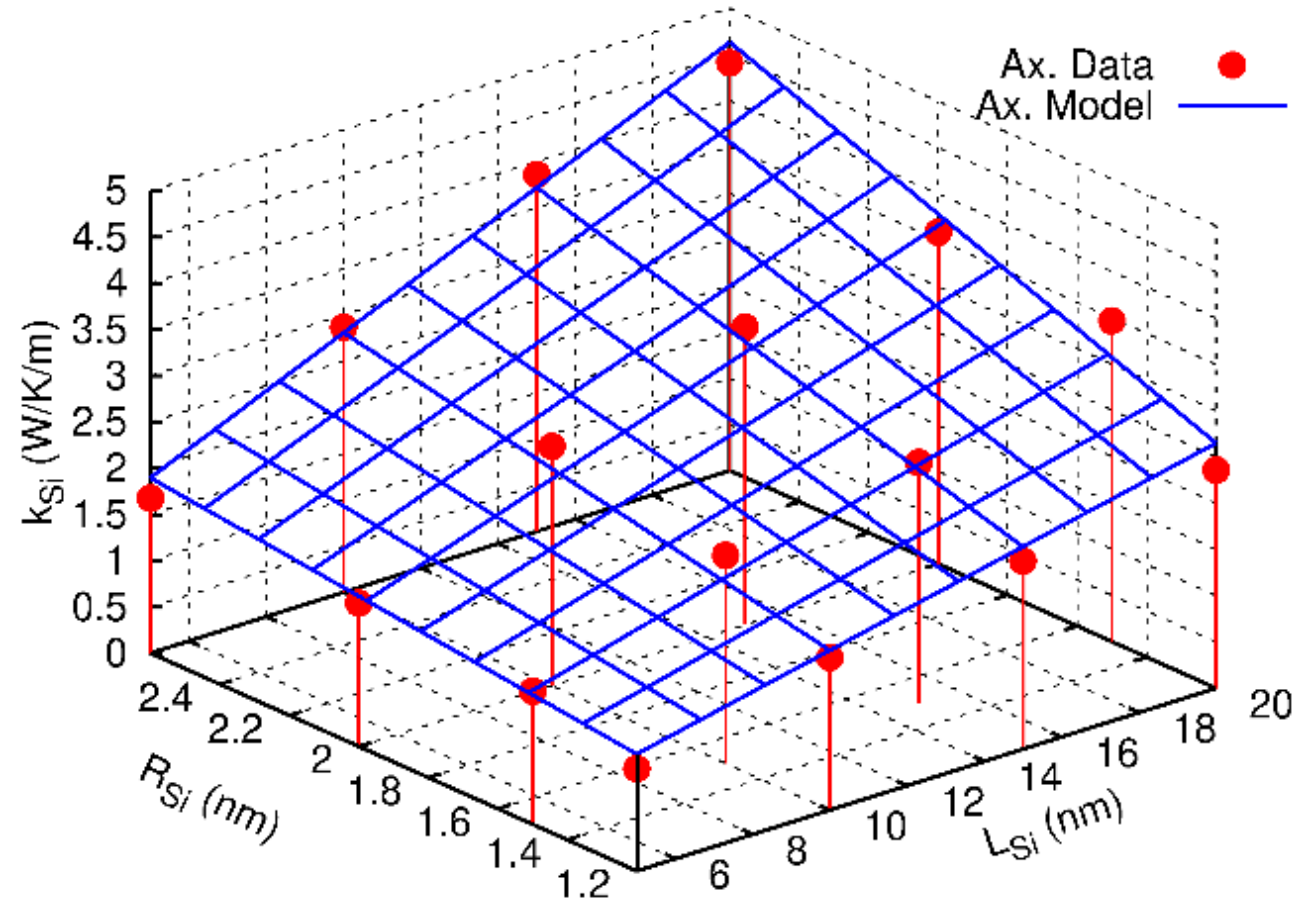


Effective thermal conductivity for the axial thermal transport in a silicon nanowire sample ($R_{\text{Si}}=2$ nm, $L_{\text{Si}}=10$ nm) as a function of position along the nanowire axis

Results: Effective Thermal Conductivity for the Axial Thermal Transport (3)

Dependence of the axial thermal conductivity in silicon nanowires on nanowire radius and length

- Thermal conductivity increases when radius or length of nanowires increases
- Analytical model assuming linear dependencies on R_{Si} and L_{Si} and a correlation term proportional to $R_{Si} * L_{Si}$ describes well the results of MD
- Such analytical model can be used in conventional TCAD tools for efficient engineering of electronic devices based on silicon nanowires

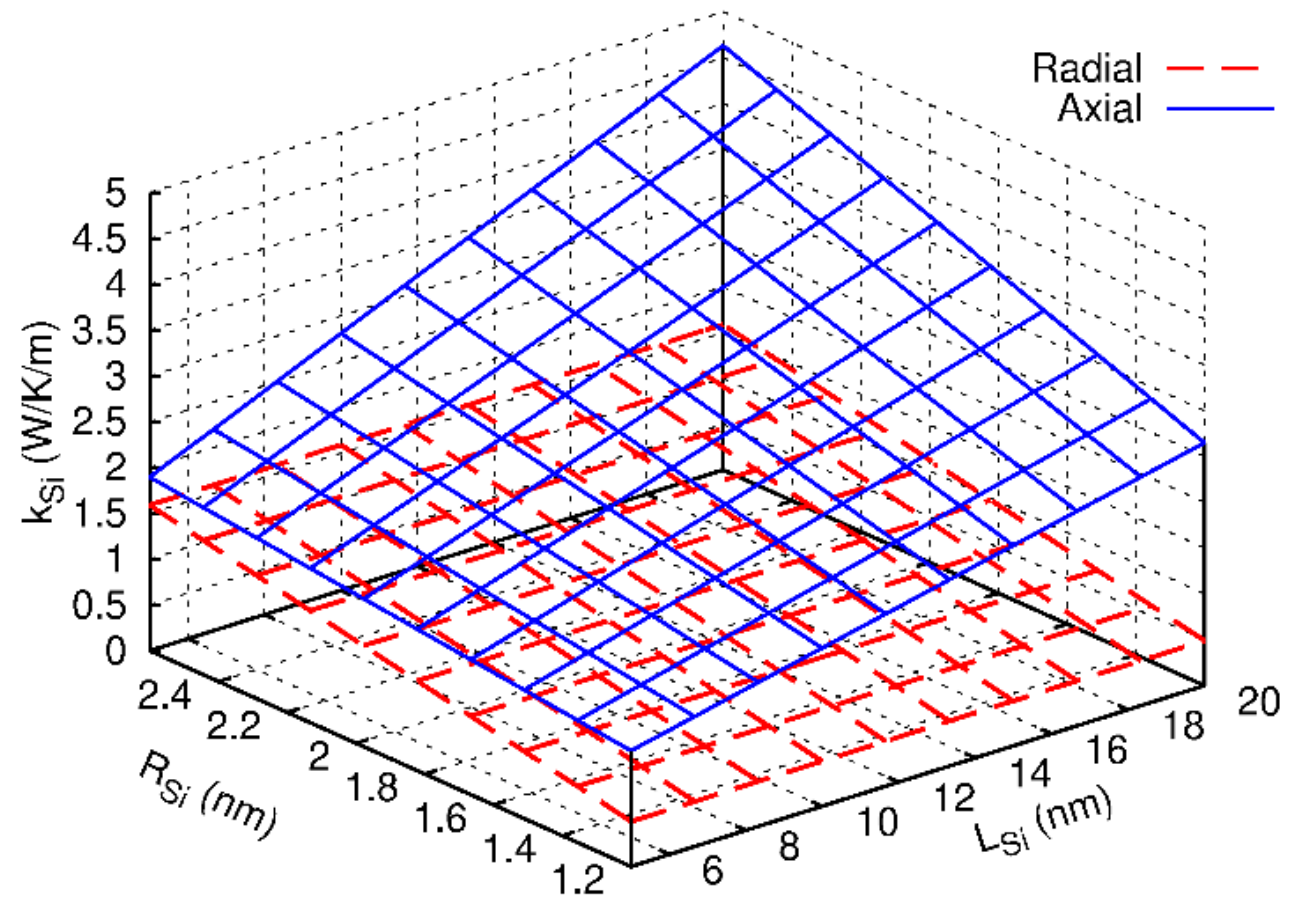


Thermal conductivity for the axial thermal transport in silicon nanowires with different radii R_{Si} , and lengths L_{Si}

Results: Comparison of Thermal Conductivity for the Axial vs Radial Thermal Transport (4)

Main properties of thermal conductivity in silicon nanowires for axial and radial thermal transport

- Thermal conductivity in axial direction is significantly higher than that in radial direction
- Both radial and axial thermal conductivities increase for larger nanowire radii
- Thermal conductivity in radial direction remains unchanged when length of nanowires increases
- In contrast, thermal conductivity in axial direction increases when length of nanowires increases

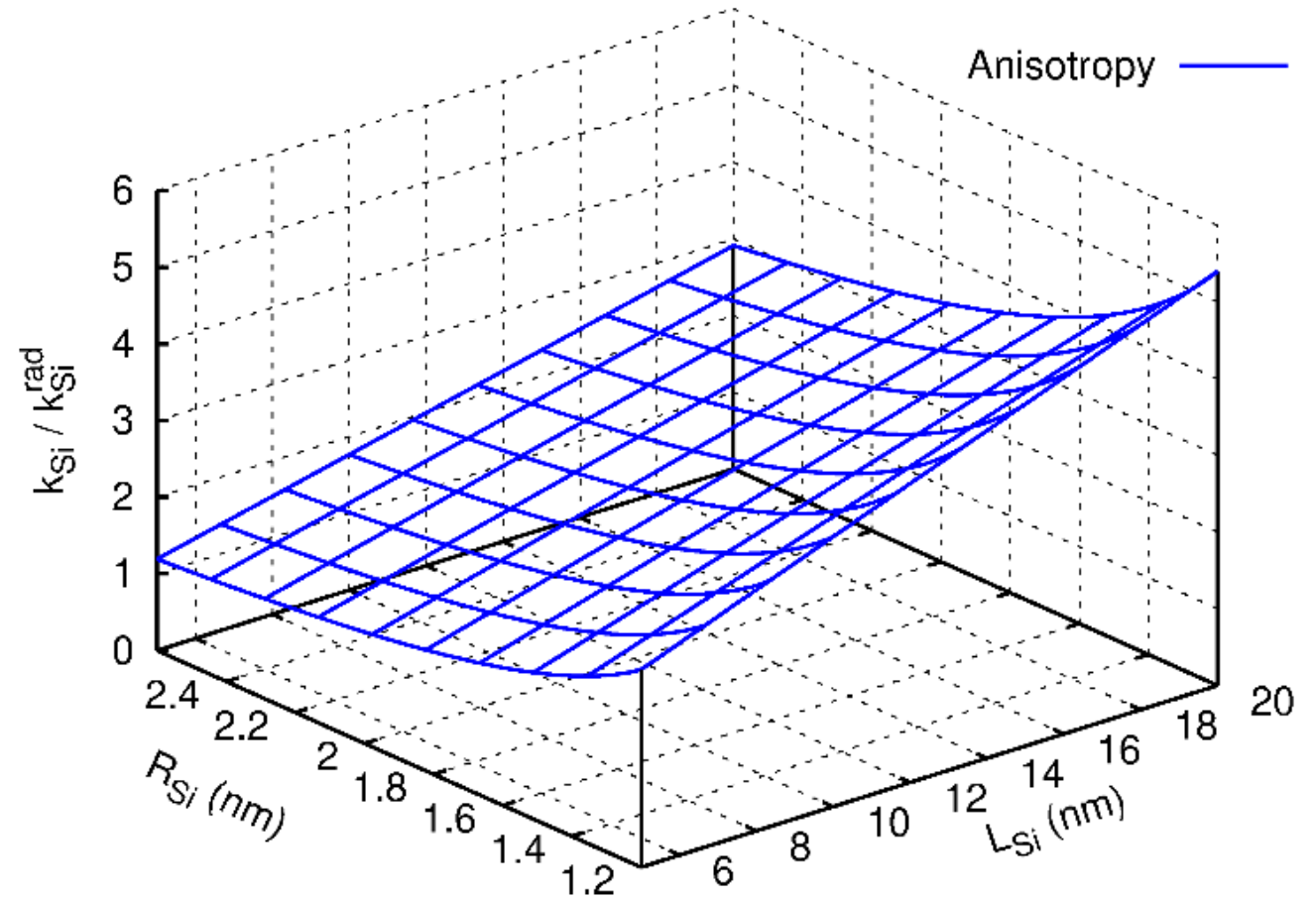


Comparison of thermal conductivity for the axial versus radial thermal transport in silicon nanowires with different radii R_{Si} , and lengths L_{Si}

Results: Comparison of Thermal Conductivity for the Axial vs Radial Thermal Transport (5)

Anisotropy of thermal conductivity in silicon nanowires

- Since thermal conductivity in axial direction is significantly higher than that in radial direction, there is an anisotropy of thermal conductivity in silicon nanowires
- We define the ratio of the axial thermal conductivity to the radial one as a measure of the anisotropy, see figure →
- The anisotropy factor increases for nanowires with larger lengths and smaller radii
- The anisotropy factor for nanowires with $R_{Si}=1.2$ nm and $L_{Si}=20$ nm exceeds 5



Anisotropy factor for thermal conductivity in silicon nanowires with different radii R_{Si} , and lengths L_{Si}

Results: Comparison of Thermal Resistances for the Axial and Radial Thermal Transport

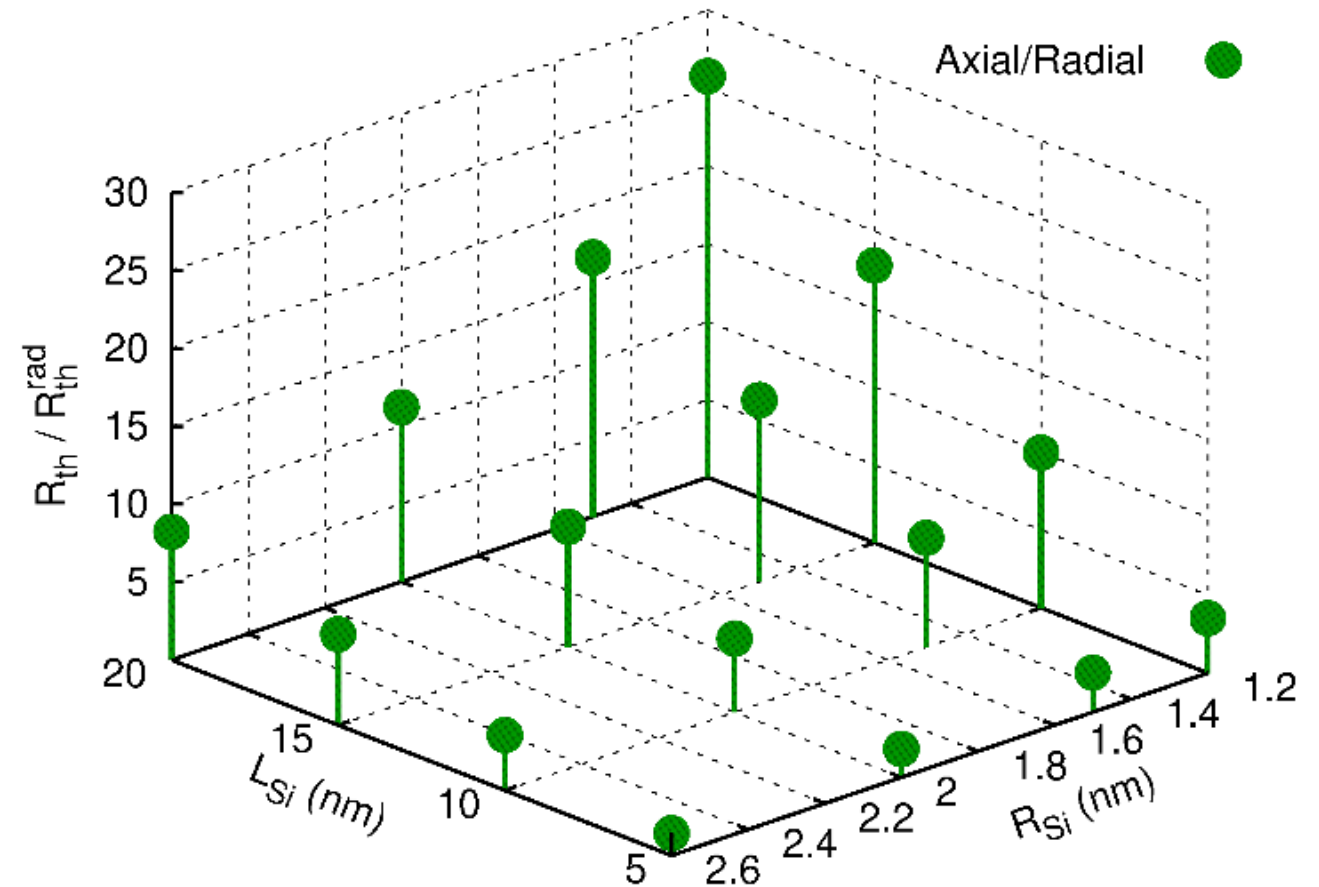
Ratio of thermal resistances as a function of nanowire sizes

- Thermal resistance of a nanowire is defined as

$$R_{th} = \frac{(T_{max} - T_{surf})}{P},$$

where T_{max} is the maximum temperature inside of nanowire, T_{surf} the temperature at the nanowire surface in contact to the heat drain, P is the heating power

- The thermal resistance for the axial heat transport exceeds that for the radial transport by a factor of about 25 for $R_{Si}=1.2$ nm and $L_{Si}=20$ nm

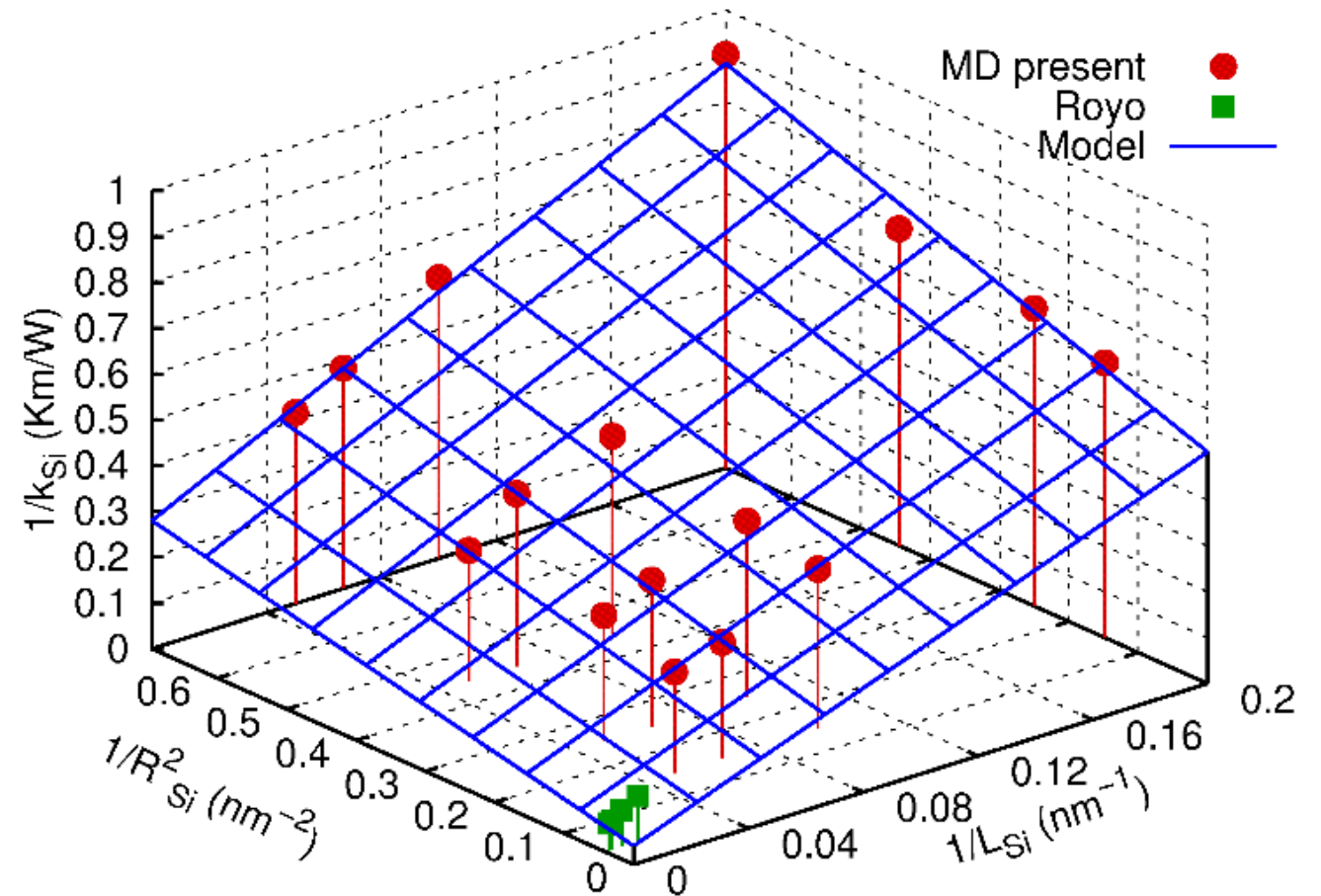


Ratio of thermal resistances for the axial thermal transport to thermal resistances for the radial thermal transport in silicon nanowires with different radii R_{Si} and lengths L_{Si}

Results: Extrapolation of Axial Thermal Conductivity to Larger Nanowire Sizes

Example of extrapolation of simulation results of this work to published results for larger nanowires

- Methods of interpolation/extrapolation of thermal parameters have been addressed in literature: $k_{Si}^{-1}(L_{Si})$ in axial direction of silicon nanowires linearly depends on L_{Si}^{-1} ; $k_{Si}^{-1}(R_{Si})$ is linearly dependent on R_{Si}^{-2}
- We take the results of Royo et al. for $R_{Si} = 5$ nm and L_{Si} between 90 and 900 nm as reference for comparison with extrapolation of our results
- Considering the largely different length ranges, the comparison can be considered good and the extrapolation successful



Extrapolation of the axial thermal conductivity to larger radii R_{Si} , and lengths L_{Si} .
Ref. M. Royo, R. Rurali, Phys. Chem. Chem. Phys., vol. 18, p. 26262, 2016

Discussion (1)

Physical reasons behind the observed phenomena and dependencies

- Thermal transport in crystalline silicon is determined by the phonon transport
- Wavelength spectrum of phonons covers the wavelengths from atomic size to the size of the sample
- In nanowires, phonons that move along the nanowire axis have a much wider wavelength spectrum than the phonons that move in radial direction → wider spectrum → more vibration modes → more heat energy transported → Anisotropy of heat transport in nanowires
- Longer nanowires have more phonon modes for the axial heat transport → Nanowire length dependence of k for the axial heat transport
- Thicker nanowires have more lateral phonon modes → Nanowire radius dependence of k for the radial heat transport
- The probability of surface scattering of phonons moving along the nanowire axis in thicker nanowires is lower → Radius dependence of k for the axial heat transport

Discussion (2)

Physical reasons behind the observed phenomena and dependencies

- Thermal transport in amorphous oxide is also determined by the transport of energy of atomic vibrations, but the properties of these vibrations in amorphous material differ from those of phonons in silicon
- The frequency spectrum of vibrations in amorphous oxide differs from that in crystalline silicon → reflection and scattering of phonons which carry heat from silicon to oxide on the Si/SiO₂ interface
➡ Additional thermal resistance at the Si/SiO₂ interface → Kapitza thermal resistance
- Because of wave nature of phonons, temperature at the interface does not jump but takes a certain space interval to change from one side to another side of interface. This interval can be characterized by a low value of thermal conductance
- The calculated value of Kapitza resistance for Si/SiO₂ interface does not depend on nanowire size

Conclusion

- We calculated axial thermal transport in cylindrical silicon nanowires of different sizes by means of molecular dynamics
- Several thermal transport parameters were extracted from these calculations
- The newly obtained parameters were compared to the corresponding data on radial thermal transport in silicon nanowires of the same shape and size range from our previous work
- An anisotropy of the thermal conductivity of silicon in nanowires was found, particularly strong for long nanowires
- The absolute thermal resistance in axial direction appears mostly larger than that in radial direction because of the longer mean distance for heat to travel to the periphery of the nanowires
- This fact indicates that cooling of hot nanowires via their sidewalls can be more efficient than cooling them via their ends
- Numerical data on thermal conductance and resistances of silicon nanowires are presented in form of analytical models in the corresponding full paper

Thank you for your attention