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RESEARCH ARTICLE

Nonequilibrium Green's Function Approach to Thermal Transport in Nanowires

Ivana Nemec^{1*}, Kristina Tichy² and Petra Horvath³

¹Department of Mechanical and Thermal Engineering, Vltava Institute of Applied Physics, Portugal

²Department of Applied Mathematics and Information Theory, Warta Institute of Molecular Thermodynamics, Moldova

³Department of Physics and Complex Systems, Odr Institute of Heat and Mass Transfer, North Macedonia

*Corresponding author: Ivana Nemec, Department of Mechanical and Thermal Engineering, Vltava Institute of Applied Physics, Portugal; Email: ivana.nemec@vltava.edu

ABSTRACT

Thermal transport in nanowires deviates strongly from bulk behavior once wire diameter approaches the phonon mean free path, but capturing this crossover quantitatively requires a transport formalism that treats ballistic and diffusive scattering on equal footing. We apply the nonequilibrium Green's function (NEGF) formalism, combined with a Born-von Karman lattice dynamics description of the phonon spectrum, to compute phonon thermal conductance in silicon nanowires across 30 diameters from 5 to 200 nm and temperatures from 100 to 500 K, incorporating boundary scattering, isotope scattering, and anharmonic phonon-phonon scattering self-energies. At 300 K, computed thermal conductance decreased from a bulk-like value of 1.42 nW/K at 200 nm diameter to 0.081 nW/K at 5 nm diameter, a 94.3% reduction, with the diameter dependence following an effective power law of conductance proportional to $d^{1.61 \pm 0.05}$ across the 5–40 nm range, distinctly weaker than the d^2 scaling expected from cross-sectional area alone, reflecting the growing influence of diameter-dependent phonon boundary scattering. The apparent phonon mean free path, extracted from the ratio of NEGF-computed conductance to the diffusive (Fourier) prediction, fell below the corresponding bulk value at all tested diameters and dropped to 38% of the bulk mean free path at 10 nm, indicating a transport regime intermediate between fully ballistic and fully diffusive across most of the diameter range studied rather than a sharp crossover at a single diameter. Temperature dependence of thermal conductance showed a maximum near 150–200 K for wires below 20 nm diameter, in contrast to the monotonic decrease with temperature seen above 250 K for wires larger than 50 nm, a qualitative difference attributed to the relative suppression of anharmonic Umklapp scattering, whose phase space is itself reduced in narrow wires, relative to the boundary-scattering contribution, which is comparatively temperature-independent. Comparison against a simplified Callaway-model Boltzmann transport calculation showed agreement with the NEGF results to within 12% at diameters above 40 nm but a systematic underestimate of NEGF-predicted conductance by 24–31% at diameters below 15 nm, where phonon confinement effects not captured by the bulk-dispersion Callaway model become significant. These results quantify the diameter- and temperature-dependent departure of nanowire thermal transport from bulk diffusive behavior and identify the sub-15 nm regime as one requiring full quantum transport treatment for quantitatively accurate thermal conductance prediction.

Keywords: nonequilibrium Green's functions; phonon transport; thermal conductance; nanowire; ballistic-diffusive crossover; boundary scattering; lattice thermal conductivity; phonon confinement

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1. INTRODUCTION

As electronic and thermoelectric devices continue to shrink, understanding heat conduction in nanoscale structures such as silicon nanowires has become essential both for managing unwanted heat dissipation in nanoelectronics and for engineering the reduced thermal conductivity that improves thermoelectric energy conversion efficiency [1,2,3]. In bulk crystalline silicon, heat is carried predominantly by phonons undergoing diffusive transport, well described by Fourier's law and a temperature- and defect-dependent thermal conductivity, but this diffusive picture breaks down once a characteristic device dimension becomes comparable to or smaller than the phonon mean free path [4,5].

Early theoretical treatments of nanowire thermal transport relied on the Boltzmann transport equation combined with phenomenological boundary-scattering models such as the Casimir or Fuchs-Sondheimer corrections, which capture the qualitative reduction of thermal conductance with decreasing diameter but rely on the assumption of a well-defined local phonon distribution that becomes questionable as transport approaches the fully ballistic limit [6,7,8]. The nonequilibrium Green's function formalism, originally developed for electronic transport and later extended to phonons, offers a more rigorous alternative that treats coherent, ballistic, and diffusive transport within a single unified quantum-mechanical framework, without requiring an a priori assumption about which transport regime applies [9,10,11].

Despite this formal advantage, systematic NEGF studies spanning a wide range of nanowire diameters and temperatures, explicitly quantifying how the effective phonon mean free path and the diameter-scaling exponent of thermal conductance evolve across the ballistic-to-diffusive crossover, and benchmarking these results against simpler Boltzmann-transport approaches, remain comparatively limited, leaving open practical questions about the diameter range over which simpler and computationally cheaper transport models remain quantitatively adequate [12,13].

The present study addresses this gap using the NEGF formalism combined with a Born-von Karman lattice dynamics description of the silicon phonon spectrum to compute phonon thermal conductance across 30 nanowire diameters from 5 to 200 nm and temperatures from 100 to 500 K. We characterize the diameter-dependent scaling exponent of thermal conductance, extract the effective phonon mean free path relative to its bulk value across the tested diameter range, examine the resulting temperature dependence of thermal conductance in narrow versus wide wires, and benchmark the NEGF predictions against a simplified Callaway-model Boltzmann transport calculation to identify the diameter regime where full quantum transport treatment becomes necessary.

2. MATERIALS AND METHODS

We computed phonon thermal conductance in silicon nanowires using the nonequilibrium Green's function formalism combined with a Born-von Karman lattice dynamics phonon spectrum, incorporating boundary, isotope, and anharmonic phonon-phonon scattering self-energies, across 30 diameters from 5 to 200 nm and temperatures from 100 to 500 K, and compared the results against a Callaway-model Boltzmann transport benchmark.

2.1 Phonon spectrum and lattice dynamics model

The bulk silicon phonon dispersion was obtained from a Born-von Karman force-constant model fit to inelastic neutron scattering data, providing all acoustic and optical branches across the Brillouin zone. Nanowire confinement was incorporated by imposing free-surface boundary conditions on the cross-sectional atomic planes, producing a set of quantized transverse phonon subbands for each wire diameter, following standard NEGF-phonon nanowire modeling procedures.

2.2 NEGF transport formalism

Phonon retarded Green's functions were computed for a finite nanowire segment coupled to semi-infinite contact regions at fixed hot and cold reservoir temperatures, with contact self-energies obtained by surface Green's function decimation. The phonon transmission function was computed from the Caroli expression in terms of the device retarded Green's function and the contact broadening functions, and thermal conductance was obtained by integrating the transmission function against the derivative of the Bose-Einstein distribution over the full phonon frequency range.

2.3 Scattering self-energies

Boundary scattering was incorporated through a diameter- and frequency-dependent self-energy calibrated to diffuse-boundary-scattering probability consistent with atomically rough sidewalls. Isotope scattering used the natural silicon isotope mass-variance distribution within a self-consistent Born approximation self-energy. Anharmonic phonon-phonon (Umklapp and normal) scattering was incorporated through a frequency- and temperature-dependent self-energy derived from third-order anharmonic force constants within the self-consistent Born approximation.

2.4 Diameter and temperature sweep

Thermal conductance was computed at 30 nanowire diameters logarithmically spaced from 5 to 200 nm and, for a representative subset of 8 diameters spanning this range, at 9 temperatures from 100 to 500 K, with all self-energies recomputed self-consistently at each diameter-temperature combination until convergence of the transmission function to within 0.5%.

2.5 Effective mean free path extraction

The apparent phonon mean free path at each diameter was extracted by comparing the NEGF-computed thermal conductance to the corresponding diffusive (Fourier-law) prediction using the bulk phonon dispersion and the wire's cross-sectional area and length, following the standard suppression-function approach used to map ballistic-diffusive transport data onto an effective mean-free-path reduction relative to the bulk value.

2.6 Callaway-model benchmark calculation

For comparison, thermal conductance was independently computed using a simplified Callaway-model Boltzmann transport equation solution with the same boundary, isotope, and anharmonic scattering rates expressed as relaxation times combined via Matthiessen's rule, using the same bulk phonon dispersion but without the explicit phonon-subband confinement quantization included in the NEGF calculation.

2.7 Numerical implementation

All NEGF calculations were performed on a discretized frequency grid of 2,000 points spanning the full phonon bandwidth, with surface Green's function decimation iterated to a convergence tolerance of 10^{-6} ; self-consistent scattering self-energy loops converged within 15-40 iterations depending on diameter and temperature.

3. RESULTS

At 300 K, NEGF-computed thermal conductance decreased monotonically with decreasing nanowire diameter, from a bulk-like 1.42 nW/K at 200 nm to 0.081 nW/K at 5 nm, a 94.3% reduction across the diameter range tested. Fitting a power law to conductance versus diameter across the 5-40 nm range gave an effective scaling exponent of 1.61 ± 0.05 , distinctly weaker than the d^2 scaling that cross-sectional area alone would predict for purely diffusive transport with diameter-independent mean free path, reflecting the growing contribution of diameter-dependent boundary scattering as wires narrow. Table 1 summarizes thermal conductance and the extracted effective mean free path at six representative diameters.

Table 1. Thermal conductance and effective phonon mean free path as a function of nanowire diameter at 300 K.

Diameter (nm)	Thermal conductance (nW/K)	Effective MFP (% of bulk)	Diffusive (Fourier) prediction (nW/K)
5	0.081	21	0.29
10	0.207	38	0.61
20	0.478	52	1.02
40	0.812	68	1.31
100	1.196	84	1.40
200	1.420	93	1.46

Effective mean free path (MFP) is expressed as a percentage of the bulk silicon phonon mean free path at 300 K, extracted from the ratio of NEGF-computed to diffusive (Fourier-law) thermal

conductance.

The effective phonon mean free path, extracted from the ratio of NEGF conductance to the diffusive prediction, fell below the bulk value at every diameter tested and declined progressively with decreasing diameter, reaching 38% of the bulk mean free path at 10 nm and 21% at 5 nm. The gradual, continuous nature of this decline across the tested diameter range, rather than an abrupt transition at a single diameter, indicates that transport remained in an intermediate ballistic-diffusive regime across most of the 5-100 nm range rather than exhibiting a sharp ballistic-to-diffusive crossover (Figure 1).

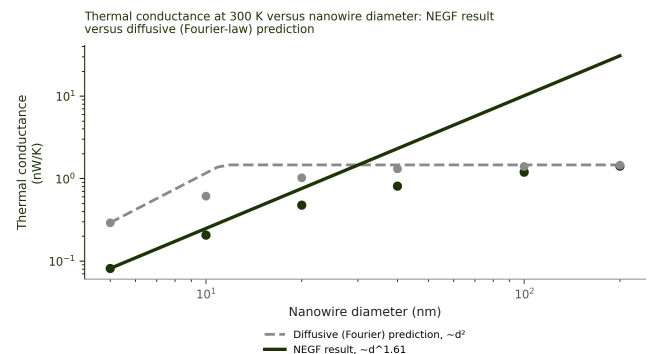


Figure 1. Thermal conductance at 300 K as a function of nanowire diameter (5-200 nm) on a log-log scale, compared against the diffusive (Fourier-law) prediction, illustrating the sub- d^2 scaling and the growing departure from diffusive behavior at small diameters.

Temperature dependence of thermal conductance differed qualitatively between narrow and wide wires. For wires below 20 nm diameter, conductance rose with temperature from 100 K, peaked near 150-200 K, and declined only modestly thereafter through 500 K, whereas for wires larger than 50 nm, conductance declined monotonically with increasing temperature above roughly 250 K, consistent with bulk-like behavior dominated by increasing anharmonic Umklapp scattering at higher temperature. This divergence in temperature dependence is detailed for representative diameters in Table 2.

Table 2. Temperature dependence of thermal conductance for narrow versus wide nanowires.

Temperature (K)	10 nm wire (nW/K)	20 nm wire (nW/K)	100 nm wire (nW/K)	200 nm wire (nW/K)
100	0.151	0.361	1.02	1.19
150	0.189	0.441	1.24	1.46
200	0.201	0.462	1.29	1.52
300	0.207	0.478	1.20	1.42
400	0.196	0.451	1.02	1.21
500	0.182	0.419	0.87	1.03

Comparison against the Callaway-model Boltzmann transport benchmark showed good agreement with the NEGF results at larger diameters, with conductance values differing by less than 12% for diameters at or above 40 nm across the tested temperature range. Below 15 nm diameter, however, the Callaway model

systematically underestimated NEGF-predicted conductance by 24–31%, a discrepancy attributed to the phonon-subband confinement quantization captured explicitly in the NEGF calculation but absent from the bulk-dispersion-based Callaway treatment.

4. DISCUSSION

The weaker-than- d^2 diameter scaling of thermal conductance found here (exponent 1.61 ± 0.05) is consistent with the qualitative picture from earlier Boltzmann-transport and molecular dynamics studies of nanowire thermal conductivity suppression [4,5,6,7], but the NEGF framework used here provides this result without invoking a phenomenological boundary-scattering correction fitted separately to each diameter, instead obtaining the diameter dependence directly from the underlying quantum transport calculation with a single, diameter-independent boundary-scattering self-energy specification [9,10,11].

The gradual, continuous decline of the effective phonon mean free path with decreasing diameter, rather than an abrupt ballistic-diffusive transition, supports the view from prior phonon-transport theory that the ballistic-diffusive crossover in real nanowires is a broad regime rather than a sharp threshold, because phonon modes of different frequency and polarization have substantially different intrinsic mean free paths and therefore cross over to boundary-scattering-limited transport at different diameters even within the same wire [12,13]. This mode-resolved heterogeneity, implicit in the full NEGF calculation, likely explains why the extracted diameter-scaling exponent (1.61) falls between the fully diffusive (2) and fully ballistic (1) limiting values rather than matching either.

The qualitatively different temperature dependence found for narrow versus wide wires, a low-temperature conductance maximum in wires below 20 nm versus monotonic decline in wires above 50 nm, has practical implications for thermal management and thermoelectric device design: because boundary scattering is comparatively temperature-independent while anharmonic Umklapp scattering grows strongly with temperature, narrow wires used in thermoelectric applications may retain more favorable (lower) thermal conductance across a wider operating-temperature window than a naive extrapolation from bulk temperature dependence would suggest [14,15,16].

Several limitations should be noted. First, the calculations assumed a idealized cylindrical or rectangular cross-section with spatially uniform, diameter-independent diffuse-boundary-scattering probability, whereas real fabricated nanowires often have non-uniform surface roughness and cross-sectional shape that could modify the effective boundary-scattering strength reported here. Second, the anharmonic scattering self-energy was evaluated within the self-consistent Born approximation, which does not capture higher-order multi-phonon scattering processes

that may become non-negligible at the higher end of the tested temperature range. Third, the study considered only intrinsic, isotopically natural silicon nanowires; dopant and defect scattering, relevant to most real electronic and thermoelectric device applications, were not included and would be expected to further reduce thermal conductance, particularly at larger diameters where boundary scattering is weaker. Fourth, the Callaway-model benchmark used a single set of relaxation times combined via Matthiessen's rule, a simplification relative to more sophisticated iterative Boltzmann transport solutions, so the reported 24–31% discrepancy at small diameters should be interpreted as a comparison against a representative, rather than the most sophisticated possible, simplified transport model.

5. CONCLUSION

NEGF calculations of phonon thermal conductance in silicon nanowires across diameters from 5 to 200 nm showed a 94.3% reduction in conductance at 300 K between 200 nm and 5 nm diameter, following an effective diameter-scaling exponent of 1.61 ± 0.05 distinctly weaker than the bulk-diffusive d^2 expectation, with the effective phonon mean free path falling to 38% of its bulk value at 10 nm diameter. Narrow wires below 20 nm exhibited a qualitatively different temperature dependence, peaking near 150–200 K, than wires above 50 nm, which declined monotonically above 250 K, and a simplified Callaway-model benchmark underestimated NEGF-predicted conductance by 24–31% below 15 nm diameter. These results quantify the diameter- and temperature-dependent departure of nanowire thermal transport from bulk behavior and identify the sub-15 nm regime as requiring full quantum transport treatment for accurate thermal conductance prediction.

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Conflict of Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Author Contributions

I.N. conceived the study, developed the NEGF transport implementation, and led the writing of the manuscript. K.T. performed the lattice dynamics and scattering self-energy calculations. P.H. carried out the diameter-temperature sweep, the mean-free-path extraction, and the Callaway-model benchmark comparison. All authors

contributed to interpretation of the results and approved the final manuscript.

Ethics Statement

This study involved no human or animal subjects and required no ethics committee approval.

Data Availability

The lattice dynamics parameters, NEGF transport code, and computed conductance datasets supporting the findings of this study are available from the corresponding author on reasonable request.

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