WITHDRAWN:
Effects of different physical factors on the heat conduction properties of carbon nanotubes on an atomic scale using molecular dynamics

Junjie Chen

cjjmmm@163.com

Department of Energy and Power Engineering, School of Mechanical and Power Engineering, Henan Polytechnic University, Jiaozuo, Henan, P.R. China

Research Article

Keywords: Physical factors, Atomic-scale computations, Heat conduction, Thermal properties, Carbon nanotubes, Phonon scattering

Posted Date: June 17th, 2022

DOI: https://doi.org/10.21203/rs.3.rs-1768287/v1

EDITORIAL NOTE:

The full text of this preprint has been withdrawn by the authors while they make corrections to the work. Therefore, the authors do not wish this work to be cited as a reference. Questions should be directed to the corresponding author.

Abstract

Atomic-scale computations were carried out to investigate the properties of nanoscale thermal transport in single-walled carbon nanotubes. The effects of crystal length, atom number, and temperature on the thermal conductivity of single-walled carbon nanotubes were evaluated. The thermal conductivity of single-walled carbon nanotubes was determined to understand the characteristics of thermal transport in the nanostructured materials. The objective is to gain insight into the fundamental characteristics of thermal transport in single-walled carbon nanotubes. Particular emphasis is placed on the dependence of crystal length, atom number, and temperature on the thermal conductivity of single-walled carbon nanotubes, with an attempt to improve the heat conduction properties for carbon-based nanostructured materials. The results indicated that phonons are derived from the crystal lattice. The crystal length and temperature are the primary factors affecting the thermal conductivity of single-walled carbon nanotubes. The atom number has little effect on the thermal conductivity. The difference in thermal conductivity is insignificant between single-walled zigzag and armchair carbon nanotubes. However, the thermal conductivity of single-walled carbon nanotubes depends strongly upon the crystal length. There is a significant effect of crystal length on the thermal conductivity. Phonon-boundary scattering instead of phonon-phonon Umklapp scattering is the dominant scattering mechanism. The thermal conductivity of single-walled carbon nanotubes is approximately constant at high temperatures. At low temperatures well below the Debye temperature, thermal conductivity of single-walled carbon nanotubes decreases, as does the heat capacity.

1. Introduction

A carbon nanotube is a tube made of carbon with diameters typically measured in nanometers. Single-walled carbon nanotubes are one of the allotropes of carbon, intermediate between fullerene cages and flat graphene, with diameters in the range of one nanometer. Although not made this way, single-walled carbon nanotubes can be idealized as cutouts from a two-dimensional hexagonal lattice of carbon atoms rolled up along one of the Bravais lattice vectors of the hexagonal lattice to form a hollow cylinder. In this construction, periodic boundary conditions are imposed over the length of this roll-up vector to yield a helical lattice of seamlessly bonded carbon atoms on the cylinder surface [1]. Multi-walled carbon nanotubes consisting of nested single-walled carbon nanotubes weakly bound together by van der Waals interactions in a tree ring-like structure. If not identical, these nanotubes are very similar to Oberlin, Endo, and Koyama's long straight and parallel carbon layers cylindrically arranged around a hollow nanotube [2]. Multi-walled carbon nanotubes are also sometimes used to refer to double-walled and triple-walled carbon nanotubes. Carbon nanotubes can exhibit remarkable electrical conductivity [3, 4], while others are semiconductors [5, 6]. They also have exceptional thermal conductivity [7, 8] and tensile strength [9, 10] because of their nanostructure and strength of the bonds between carbon atoms. In addition, they can be chemically modified [11, 12]. These properties are expected to be valuable in many areas of technology, such as electronics, optics, composite materials, nanotechnology, and other applications of materials science.

Within the last twenty years, as the properties of carbon nanotubes have been better understood, interests in carbon nanotubes have greatly increased within and outside of the research community [13, 14]. One key to making use of these properties is the synthesis of carbon nanotubes in sufficient quantities for them to be used industrially [15, 16]. For example, large quantities of carbon nanotubes may be needed if they are to be used as high strength components of carbon nanotubes in macroscale three-dimensional structures [17, 18]. Carbon nanotubes are known to have extraordinary tensile strength, including high strain to failure and relatively high tensile modulus [19, 20]. Carbon nanotubes may also be highly electrically and thermally conductive while being resistant to fatigue, radiation damage, and heat [21, 22]. For example, carbon nanotubes can be good thermal conductors along the nanotube, where each individual carbon nanotube can have thermal conductivities potentially in excess of 2000 W/(m·K) [23, 24]. However, this thermal conductivity is anisotropic, exhibiting properties with different values when measured in different directions and is dramatically reduced when a large ensemble of carbon nanotubes is used in a sheet or mat [25, 26]. Accordingly, it would be desirable to provide a material that can take advantage of the characteristics and properties of carbon nanotubes, so that efficient and light-weight devices, such as shielding and thermal insulators, can be manufactured in a cost-effective manner.

Because of a remarkable combination of their properties, carbon nanotubes are being considered as prime candidate materials for nano-scale device applications [27, 28]. Consequently, considerable effort has been invested in characterizing properties of carbon nanotubes, particularly their electronic and mechanical properties [29, 30]. Surprisingly, despite the importance of thermal management in nano-scale devices, there has been relatively little progress in characterizing thermal conductivity of carbon nanotubes. This is partly due to challenges associated with nano-scale experimental measurements, but it is also a result of technological difficulties of synthesizing high-quality, well-ordered carbon nanotubes [31, 32]. Consequently, theoretical computations of thermal conductivity of carbon nanotubes are presently very essential. Theoretical computations of thermal conductivity of materials can be classified as two main approaches: first principles based atomistic simulations and continuum computations based on transport theories. The atomistic approach is particularly useful for nano-scale devices where the experimental determination of the thermal conductivity is quite challenging [33, 34]. The main advantage of the continuum approach is that it enables an analysis of relatively large systems [35, 36]. However, the approach entails the knowledge of certain parameters such as phonon relaxation time and phonon density of states which must be determined using either experimental measurements or by theoretical computations. An addition shortcoming of the continuum approach is that solving the governing differential transport equation may be quite difficult in some cases. Because of the aforementioned limitations of the continuum approach, the first principles based atomistic simulations are increasingly getting more attention as a means of predicting thermal properties [37, 38]. Besides not requiring the prior knowledge of the model parameters, atomic-scale computations enable quantification of the effect of microstructure on thermal properties [39, 40]. Furthermore, atomistic simulations can be used to determine the parameters for the continuum models discussed above and, therefore, help bridge gap between atomistic-scale and continuum-level computations [41, 42]. While single-walled carbon

nanotubes exhibit extremely high thermal conductivity, the effects of different factors on the heat conduction properties of the carbon-based nanostructured material are poorly understood.

This study relates to the heat conduction properties of single-walled carbon nanotubes. The effects of different factors on the heat conduction properties of single-walled carbon nanotubes were investigated by using the nonequilibrium molecular dynamics method. Computational simulations were performed using molecular dynamics to investigate the heat transport properties of single-walled carbon nanotubes. The intrinsic thermal conductivity of carbon nanotubes was determined to understand the characteristics of thermal transport in the nanostructured materials. The mechanism of phonon transport in carbon nanotubes was discussed. The physical factors limiting heat conduction in carbon nanotubes were provided. The objective is to gain insight into the fundamental characteristics of thermal transport in carbon nanotubes. Particular emphasis is placed on the dependence of different physical factors on the thermal conductivity of carbon nanotubes, with an attempt to improve the heat conduction properties for the carbon-based nanostructured material.

2. Numerical Methods

The heat transport characteristics of single-walled carbon nanotubes are investigated using molecular dynamics. The single-walled carbon nanotubes modeled in this study are depicted schematically in Fig. 1. The structures of single-walled carbon nanotubes are defined by either the chiral angle and diameter, or the chiral indices. The trajectories of atoms and molecules are determined by numerically solving Newton's equations of motion for the carbon-based nanostructured system of interacting particles, where forces between the particles and their potential energies are computed using interatomic potentials. Molecular dynamics is a computer simulation method for analyzing the physical movements of atoms and molecules.

The atomic structures of single-walled zigzag and armchair carbon nanotubes are illustrated schematically in Fig. 2. Because the molecular system consists of a vast number of particles, it is impossible to determine the properties of such a complex system analytically. Molecular dynamics simulation circumvents this problem by using numerical methods. However, long molecular dynamics simulations generate cumulative errors in numerical integration that can be minimized with proper selection of algorithms and parameters, but not eliminated entirely. Ab initio quantum mechanical and chemical methods are used to compute the potential energy of a system on the fly, as needed for conformations in a trajectory. This computation is usually made in the close neighborhood of the reaction coordinate. Although various approximations are used, these are based on theoretical considerations, not on empirical fitting.

The atomic structure of an individual single-walled carbon nanotube is divided into specific regions by defining hot and cold slabs. Heat is continually being transferred from the hot slab to the cold slabs so as to equalize the temperature. The temperature gradient can be determined in the direction of heat flow, since the total energy is conserved in the heat conduction process. Accordingly, the thermal conductivity

can be determined from the temperature gradient obtained and the heat flux imposed. The law of heat conduction, also known as Fourier's law, states that the rate of heat transfer through a material is proportional to the negative gradient in the temperature and to the area, at right angles to that gradient, through which the heat flows. The local heat flux density is equal to the product of thermal conductivity and the negative local temperature gradient. The heat flux density is the amount of energy that flows through a unit area per unit time. The ratio of heat flux to the slope of the temperature profile is proportional to the thermal conductivity of the single-walled carbon nanotube.

Atomistic simulations are performed using a classical molecular dynamic code LAMMPS [43]. Since the carbon-based nanostructured system doesn't satisfy equilibrium conditions, reverse non-equilibrium molecular dynamics are used. The Müller-Plathe algorithm [44] is used to exchange kinetic energy between two atoms in different regions of the single-walled carbon nanotube. This induces a temperature gradient in the system, thereby enabling the thermal conductivity of the single-walled carbon nanotube to be computed. The atomistic interactions in the single-walled carbon nanotube are treated with the AIREBO potential in its second-generation form [45]. This potential function can be used to describe the intermolecular interactions in condensed-phase hydrocarbon systems [46]. In the microcanonical ensemble, the carbon-based nanostructured system is isolated from changes in moles, volume, and energy. It corresponds to an adiabatic process with no heat exchange.

Molecular dynamics simulations are carried out in a microcanonical ensemble on the relaxed structure, with the velocity-Verlet integrator and a time step of 0.5 fs. After the system reaches a steady state finally, it will continue to carry out molecular dynamics simulations up to 2 ns to ensure reliable statistics for the heat transfer process. Parallel algorithms allow the load to be distributed among central processing units. The spatial and force decomposition algorithms are used. All pair-wise electrostatic and van der Waals interactions are accounted for explicitly.

3. Results And Discussion

3.1. Temperature profiles

Steady-state temperature profiles obtained for single-walled carbon nanotubes are presented in Fig. 3. The length of single-walled carbon nanotubes is assumed to be 80 nm. Energy flow due to thermal conduction is classified as heat. According to the second law of thermodynamics, heat flows from high to low temperature. Therefore, it is reasonable to postulate that energy flow due to thermal conduction is proportional to the gradient of the temperature field. The constant of proportionality is the thermal conductivity. This is called Fourier's law of heat conduction. The constant thermal conductivity itself usually depends on the temperature field and thereby implicitly on space and time. The temperature has a nonlinear dependence on the distance from the given reference point in the direction of heat flow. More specifically, in the vicinity of the hot and cold regions, there exists a nonlinear dependence of the temperature with respect to the distance. This nonlinear dependence is caused by the finite-size effect arising from single-walled carbon nanotubes, given the fact that the characteristic length scale of single-

walled carbon nanotubes is much smaller than the mean free path of phonons. In the regions between the hot slab and the cold slabs, the temperature has a more or less linear dependence on the distance, and therefore the thermal conductivity of single-walled carbon nanotubes can be determined by the temperature gradient.

3.2. Thermal conductivity

The thermal properties of single-walled carbon nanotubes with different lengths are investigated to determine the structure factors limiting the heat transfer process. The thermal conductivity of single-walled carbon nanotubes can conveniently be determined by the temperature gradient in the direction of heat flow. The effect of crystal length on the thermal conductivity of single-walled carbon nanotubes is illustrated in Fig. 4. The thermal conductivity of single-walled carbon nanotubes depends strongly upon the crystal length. More specifically, the thermal conductivity of single-walled carbon nanotubes increases with increasing crystal length due to the reduced probability of phonon scattering from grain boundaries. Phonons can scatter through several mechanisms as they travel through the material. These scattering mechanisms are: Umklapp phonon-phonon scattering, phonon-impurity scattering, phonon-electron scattering, and phonon-boundary scattering. Each scattering mechanism can be characterized by a relaxation rate, which is the inverse of the corresponding relaxation time. All scattering processes can be taken into account using Matthiessen's rule. Thermal transport in single-walled carbon nanotubes is usually considered to be governed by the three-phonon scattering process, and the role of four-phonon and higher-order scattering processes is believed to be negligible. Therefore, the less significant the scattering, the higher is the thermal conductivity. This is because the mean free path of phonons in single-walled carbon nanotubes is very large compared to the dimensions of the crystal. As a result, the length of single-walled carbon nanotubes is vital in determining the thermal conductivity. Consequently, the crystal length is an important factor affecting the thermal properties, and must be taken into account so as to provide more accurate predictions about the thermal conductivity of single-walled carbon nanotubes. On the other hand, the atomic structure has little effect on the thermal properties of single-walled carbon nanotubes. The thermal conductivity of single-walled zigzag carbon nanotubes is comparable to that of single-walled armchair carbon nanotubes under the conditions studied here.

3.3. Effect of atom number

The thermal properties of single-walled carbon nanotubes with different numbers of atoms are investigated to determine the critical factors limiting the heat transfer process. The effect of the number of atoms on the thermal conductivity of single-walled carbon nanotubes is illustrated in Fig. 5. The thermal conductivity of single-walled carbon nanotubes depends strongly slightly the number of atoms. More specifically, the thermal conductivity of single-walled carbon nanotubes increases with increasing the number of atoms due to the reduced probability of phonon scattering from grain boundaries. Computations are performed for single-walled carbon nanotubes with varying numbers of atoms to determine the optimum number of atoms that would give the desired accuracy and minimize computation time. As the number of atoms increases, there is a convergence of the solution. The

minimum number, consisting of 280 atoms in total, fails to accurately capture the thermal conductivity of single-walled carbon nanotubes. Solutions obtained with single-walled carbon nanotubes consisting of a few thousand atoms are reasonably accurate. Larger dimensions of single-walled carbon nanotubes, up to 8000 atoms, yield no obvious advantage.

3.4. Effect of temperature

The thermal properties of single-walled carbon nanotubes at different temperatures are investigated to determine the critical factors limiting the heat transfer process. The effect of temperature on the thermal conductivity of single-walled carbon nanotubes is illustrated in Fig. 6. The thermal conductivity of single-walled carbon nanotubes depends heavily upon temperature. More specifically, the thermal conductivity of single-walled carbon nanotubes first increases and then decreases with increasing temperature. At the lowest temperature explored, the thermal conductivity of single-walled carbon nanotubes increases with an increase in temperature. In the upper portion of the temperature range examined, however, the thermal conductivity of single-walled carbon nanotubes decreases with an increase in temperature. This finding suggests that, at lower temperatures, the thermal conductivity of single-walled carbon nanotubes is dominated by acoustic phonons. At higher temperatures, phonon-phonon Umklapp scattering causes the thermal conductivity of single-walled carbon nanotubes to decrease with an increase in temperature. The effect of temperature on thermal conductivity is identical for single-walled zigzag and armchair carbon nanotubes. Heat conductivity in single-walled carbon nanotubes is mainly due to lattice vibrations or phonons [47, 48]. Except for high-quality single-walled carbon nanotubes at low temperatures, the mean free path of phonons is not reduced significantly at higher temperatures. Therefore, the thermal conductivity of single-walled carbon nanotubes is approximately constant at high temperatures. At low temperatures well below the Debye temperature, thermal conductivity of single-walled carbon nanotubes decreases, as does the heat capacity, due to carrier scattering from defects.

4. Conclusions

This study relates to the heat conduction properties of single-walled carbon nanotubes. Computational simulations were performed using molecular dynamics to investigate the heat transport properties of single-walled carbon nanotubes. The intrinsic thermal conductivity of single-walled carbon nanotubes was determined to understand the characteristics of thermal transport in the nanostructured materials. The effects of different factors on the heat conduction properties of single-walled carbon nanotubes were investigated. The mechanism of phonon transport in single-walled carbon nanotubes was discussed. The physical factors limiting heat conduction in single-walled carbon nanotubes were provided.

The results indicated that the thermal properties of single-walled carbon nanotubes are directly related to its unique structure. The crystal length and temperature are the primary factors affecting the thermal conductivity of single-walled carbon nanotubes. Single-walled carbon nanotubes generally have very high thermal conductivity, but the presence of impurities reduces the degree of the mean free path of phonons, thereby degrading the thermal performance. The number of atoms has little effect on the thermal

conductivity, since there is little difference in the thermal conductivity of single-walled carbon nanotubes with 280 and 8000 atoms. The difference in thermal conductivity is insignificant between single-walled zigzag and armchair carbon nanotubes. However, the thermal conductivity of single-walled carbon nanotubes depends strongly upon the crystal length. There is a significant effect of crystal length on the thermal conductivity. Phonon-boundary scattering instead of phonon-phonon Umklapp scattering is the dominant scattering mechanism. Phonon scattering by grain boundaries reduces the efficiency of thermal transport in single-walled carbon nanotubes. The thermal conductivity of single-walled carbon nanotubes is approximately constant at high temperatures. At low temperatures well below the Debye temperature, thermal conductivity of single-walled carbon nanotubes decreases, as does the heat capacity.

Declarations

Declaration of competing interest

The authors declare that there is no conflict of interest.

References

1. S. Iijima. Helical microtubules of graphitic carbon. Nature, Volume 354, Issue 6348, 1991, Pages 56–58.
2. A. Oberlin, M. Endo, and T. Koyama. Filamentous growth of carbon through benzene decomposition. Journal of Crystal Growth, Volume 32, Issue 3, 1976, Pages 335–349.
3. J.W. Mintmire, B.I. Dunlap, and C.T. White. Are fullerene tubules metallic? Physical Review Letters, Volume 68, Issue 5, 1992, Pages 631–634.
4. S.J. Tans, M.H. Devoret, H. Dai, A. Thess, R.E. Smalley, L.J. Geerligs, and C. Dekker. Individual single-wall carbon nanotubes as quantum wires. Nature, Volume 386, Issue 6624, 1997, Pages 474–477.
5. N. Hamada, S.-I. Sawada, and A. Oshiyama. New one-dimensional conductors: Graphitic microtubules. Physical Review Letters, Volume 68, Issue 10, 1992, Pages 1579–1581.
6. J.W.G. Wilder, L.C. Venema, A.G. Rinzler, R.E. Smalley, and C. Dekker. Electronic structure of atomically resolved carbon nanotubes. Nature, Volume 391, Issue 6662, 1998, Pages 59–62.
7. S. Berber, Y.-K. Kwon, and D. Tománek. Unusually high thermal conductivity of carbon nanotubes. Physical Review Letters, Volume 84, Issue 20, 2000, Pages 4613–4616.
8. M. Grujicic, G. Cao, and B. Gersten. Atomic-scale computations of the lattice contribution to thermal conductivity of single-walled carbon nanotubes. Materials Science and Engineering: B, Volume 107, Issue 2, 2004, Pages 204–216.
9. M. Yu, O. Lourie, M.J. Dyer, K. Moloni, T.F. Kelly, and R.S. Ruoff. Strength and breaking mechanism of multiwalled carbon nanotubes under tensile load. Science, Volume 287, Issue 5453, 2000, Pages 637–640.

10. A. Takakura, K. Beppu, T. Nishihara, A. Fukui, T. Kozeki, T. Namazu, Y. Miyauchi, and K. Itami. Strength of carbon nanotubes depends on their chemical structures. *Nature Communications*, Volume 10, 2019, Article Number: 3040.
11. N. Karousis, N. Tagmatarchis, and D. Tasis. Current progress on the chemical modification of carbon nanotubes. *Chemical Reviews*, Volume 110, Issue 9, 2010, Pages 5366–5397.
12. D. Tasis, N. Tagmatarchis, A. Bianco, and M. Prato. Chemistry of carbon nanotubes. *Chemical Reviews*, Volume 106, Issue 3, 2006, Pages 1105–1136.
13. S. Rathinavel, K. Priyadharshini, and D. Panda. A review on carbon nanotube: An overview of synthesis, properties, functionalization, characterization, and the application. *Materials Science and Engineering: B*, Volume 268, 2021, Article Number: 115095.
14. Y.R. Poudel and W. Li. Synthesis, properties, and applications of carbon nanotubes filled with foreign materials: A review. Materials Today Physics, Volume 7, 2018, Pages 7–34.
15. M.S. Dresselhaus, G. Dresselhaus, and R. Saito. Physics of carbon nanotubes. Carbon, Volume 33, Issue 7, 1995, Pages 883–891.
16. A.N. Khlobystov, D.A. Britz, and G.A.D. Briggs. Molecules in carbon nanotubes. Accounts of Chemical Research, Volume 38, Issue 12, 2005, Pages 901–909.
17. M. Jagannatham, P. Chandran, S. Sankaran, P. Haridoss, N. Nayan, and S.R. Bakshi. Tensile properties of carbon nanotubes reinforced aluminum matrix composites: A review. Carbon, Volume 160, 2020, Pages 14–44.
18. M. Monthioux, E. Flahaut, and J.P. Cleuziou. Hybrid carbon nanotubes: Strategy, progress, and perspectives. Journal of Materials Research, Volume 21, Issue 11, 2006, Pages 2774–2793.
19. B. Peng, M. Locascio, P. Zapol, S.Y. Li, S.L. Mielke, G.C. Schatz, and H.D. Espinosa. Measurements of near-ultimate strength for multiwalled carbon nanotubes and irradiation-induced crosslinking improvements. Nature Nanotechnology, Volume 3, 2008, Pages 626–631.
20. M.M.J. Treacy, T.W. Ebbesen, and J.M. Gibson. Exceptionally high Young's modulus observed for individual carbon nanotubes. Nature, Volume 381, Issue 6584, 1996, Pages 678–680.
21. C. Guerret-Piécourt, Y.L. Bouar, A. Lolseau, and H. Pascard. Relation between metal electronic structure and morphology of metal compounds inside carbon nanotubes. Nature, Volume 372, Issue 6508, 1994, Pages 761–765.
22. P. Kim, L. Shi, A. Majumdar, and P.L. McEuen. Thermal transport measurements of individual multiwalled nanotubes. Physical Review Letters, Volume 84, Issue 20, 2000, Pages 4613–4616.
23. E. Pop, D. Mann, Q. Wang, K. Goodson, and H. Dai. Thermal conductance of an individual single-wall carbon nanotube above room temperature. Nano Letters, Volume 6, Issue 1, 2006, Pages 96–100.
24. B. Kumanek and D. Janas. Thermal conductivity of carbon nanotube networks: A review. Journal of Materials Research, Volume 54, Issue 10, 2019, Pages 7397–7427.
25. Z. Han and A. Fina. Thermal conductivity of carbon nanotubes and their polymer nanocomposites: A review. Progress in Polymer Science, Volume 36, Issue 7, 2011, Pages 914–944.

26. T. Ji, Y. Feng, M. Qin, and W. Feng. Thermal conducting properties of aligned carbon nanotubes and their polymer composites. *Composites Part A: Applied Science and Manufacturing*, Volume 91, Part 1, 2016, Pages 351–369.
27. Y. Ando, X. Zhao, T. Sugai, and M. Kumar. Growing carbon nanotubes. Materials Today, Volume 7, Issue 10, 2004, Pages 22–29.
28. T.W. Ebbesen. Carbon nanotubes. Materials Today, Volume 49, Issue 6, 1996, Pages 26–32.
29. E.A. Laird, F. Kuemmeth, G.A. Steele, K. Grove-Rasmussen, J. Nygård, K. Flensberg, and L.P. Kouwenhoven. Quantum transport in carbon nanotubes. Reviews of Modern Physics, Volume 87, Issue 3, 2015, Pages 703–764.
30. M.B. Nardelli, B.I. Yakobson, and J. Bernholc. Mechanism of strain release in carbon nanotubes. Physical Review B, Volume 57, Issue 8, 1998, Pages R4277-R4280.
31. J. Hone, M. Whitney, C. Piskoti, and A. Zettl. Thermal conductivity of single-walled carbon nanotubes. Physical Review B, Volume 59, Issue 4, 1999, Pages R2514-R2516.
32. A.M. Marconnet, M.A. Panzer, and K.E. Goodson. Thermal conduction phenomena in carbon nanotubes and related nanostructured materials. Reviews of Modern Physics, Volume 85, Issue 3, 2013, Pages 1295–1326.
33. D. Macgowan and D.J. Evans. A comparison of NEMD algorithms for thermal conductivity. Physics Letters A, Volume 117, Issue 8, 1986, Pages 414–416.
34. D.J. Evans. Homogeneous NEMD algorithm for thermal conductivity-Application of non-canonical linear response theory. Physics Letters A, Volume 91, Issue 9, 1982, Pages 457–460.
35. S.G. Volz and G. Chen. Molecular dynamics simulation of thermal conductivity of silicon nanowires. Applied Physics Letters, Volume 75, Issue 14, 1999, Pages 2056–2058.
36. A. Balandin and K.L. Wang. Significant decrease of the lattice thermal conductivity due to phonon confinement in a free-standing semiconductor quantum well. Physical Review B, Volume 58, Issue 3, 1998, Pages 1544–1549.
37. Z. Yao, J.-S. Wang, B. Li, and G.-R. Liu. Thermal conduction of carbon nanotubes using molecular dynamics. *Physical Review B*, Volume 71, Issue 8, 2005, Article Number: 085417.
38. Y. Chalopin, S. Volz, and N. Mingo. Upper bound to the thermal conductivity of carbon nanotube pellets. *Journal of Applied Physics*, Volume 105, Issue 8, 2009, Article Number: 084301.
39. A.N. Volkov and L.V. Zhigilei. Heat conduction in carbon nanotube materials: Strong effect of intrinsic thermal conductivity of carbon nanotubes. *Applied Physics Letters*, Volume 101, Issue 4, 2012, Article Number: 043113.
40. W.J. Evans, M. Shen, and P. Keblinski. Inter-tube thermal conductance in carbon nanotubes arrays and bundles: Effects of contact area and pressure. *Applied Physics Letters*, Volume 100, Issue 26, 2012, Article Number: 261908.
41. A.N. Volkov and L.V. Zhigilei. Scaling laws and mesoscopic modeling of thermal conductivity in carbon nanotube materials. *Physical Review Letters*, Volume 104, Issue 21, 2010, Article Number:

215902.

42. R.S. Prasher, X.J. Hu, Y. Chalopin, N. Mingo, K. Lofgreen, S. Volz, F. Cleri, and P. Keblinski. Turning carbon nanotubes from exceptional heat conductors into insulators. *Physical Review Letters*, Volume 102, Issue 10, 2009, Article Number: 105901.
43. S. Plimpton. Fast parallel algorithms for short-range molecular dynamics. Journal of Computational Physics, Volume 117, Issue 1, 1995, Pages 1–19.
44. F. Müller-Plathe. A simple nonequilibrium molecular dynamics method for calculating the thermal conductivity. The Journal of Chemical Physics, Volume 106, Issue 14, 1997, Pages 6082–6085.
45. S.J. Stuart, A.B. Tutein, and J.A. Harrison. A reactive potential for hydrocarbons with intermolecular interactions. The Journal of Chemical Physics, Volume 112, Issue 14, 2000, Pages 6472–6486.
46. G. Barbarino, C. Melis, and L. Colombo. Effect of hydrogenation on graphene thermal transport. Carbon, Volume 80, 2014, Pages 167–173.
47. X. Yang, J. Tiwari, and T. Feng. Reduced anharmonic phonon scattering cross-section slows the decrease of thermal conductivity with temperature. *Materials Today Physics*, Volume 24, 2022, Article Number: 100689.
48. Z.-G. Mei, Y.S. Kim, A.M. Yacout, J. Yang, X. Li, and Y. Cao. First-principles study of thermal conductivities of uranium aluminides. Materialia, Volume 4, 2018, Pages 449–456.

Figures

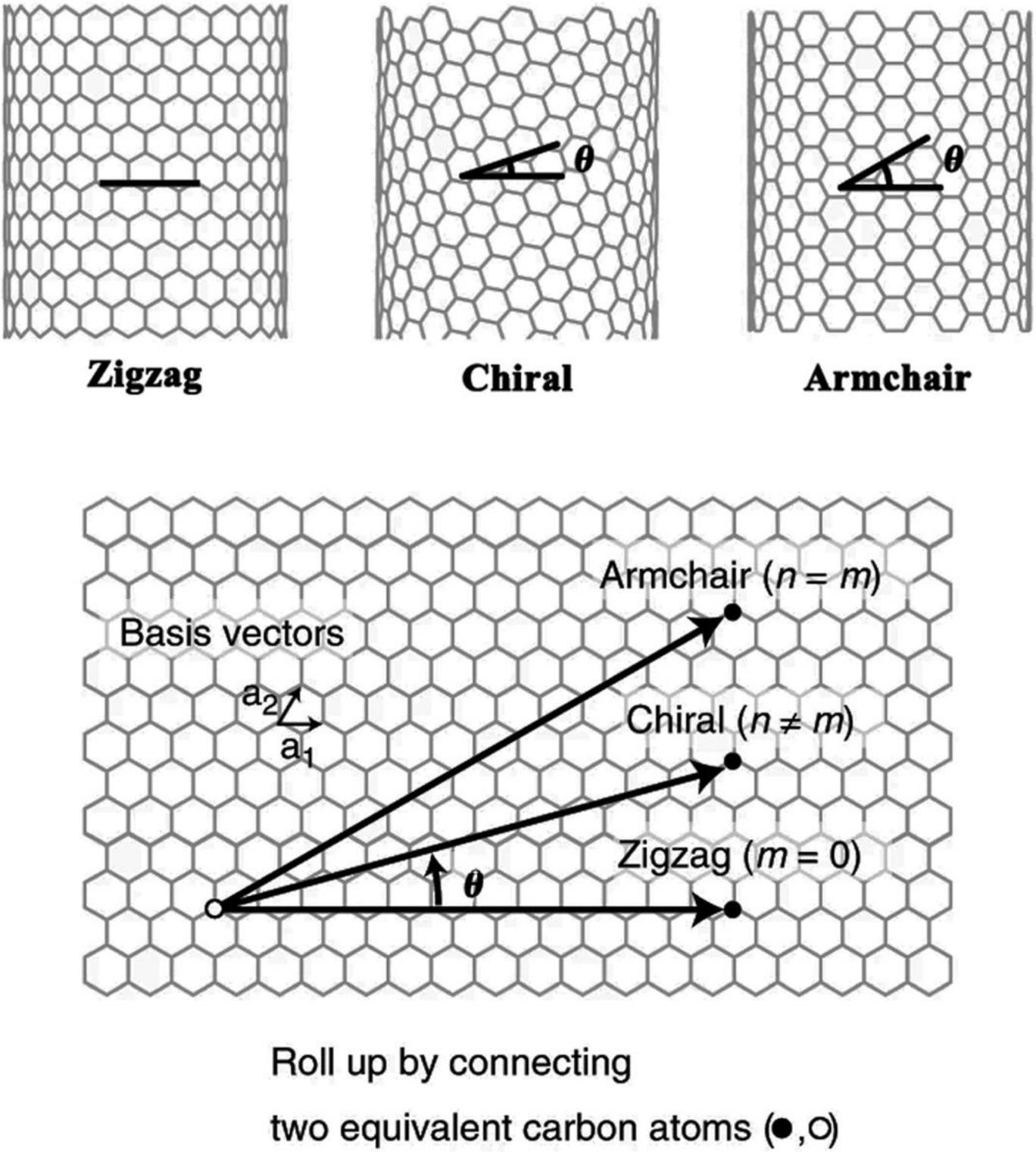

Figure 1

Schematic illustration of the single-walled carbon nanotubes modeled in this study. Single-walled carbon nanotubes can be classified by their chiral indices, or diameter and chiral angle. The chiral indices define the chiral vector that connects two equivalent carbon atoms in a graphene plane. The chiral angle is defined as the angle between the zigzag direction and circumference. Achiral carbon nanotubes are called zigzag and armchair carbon nanotubes, respectively.

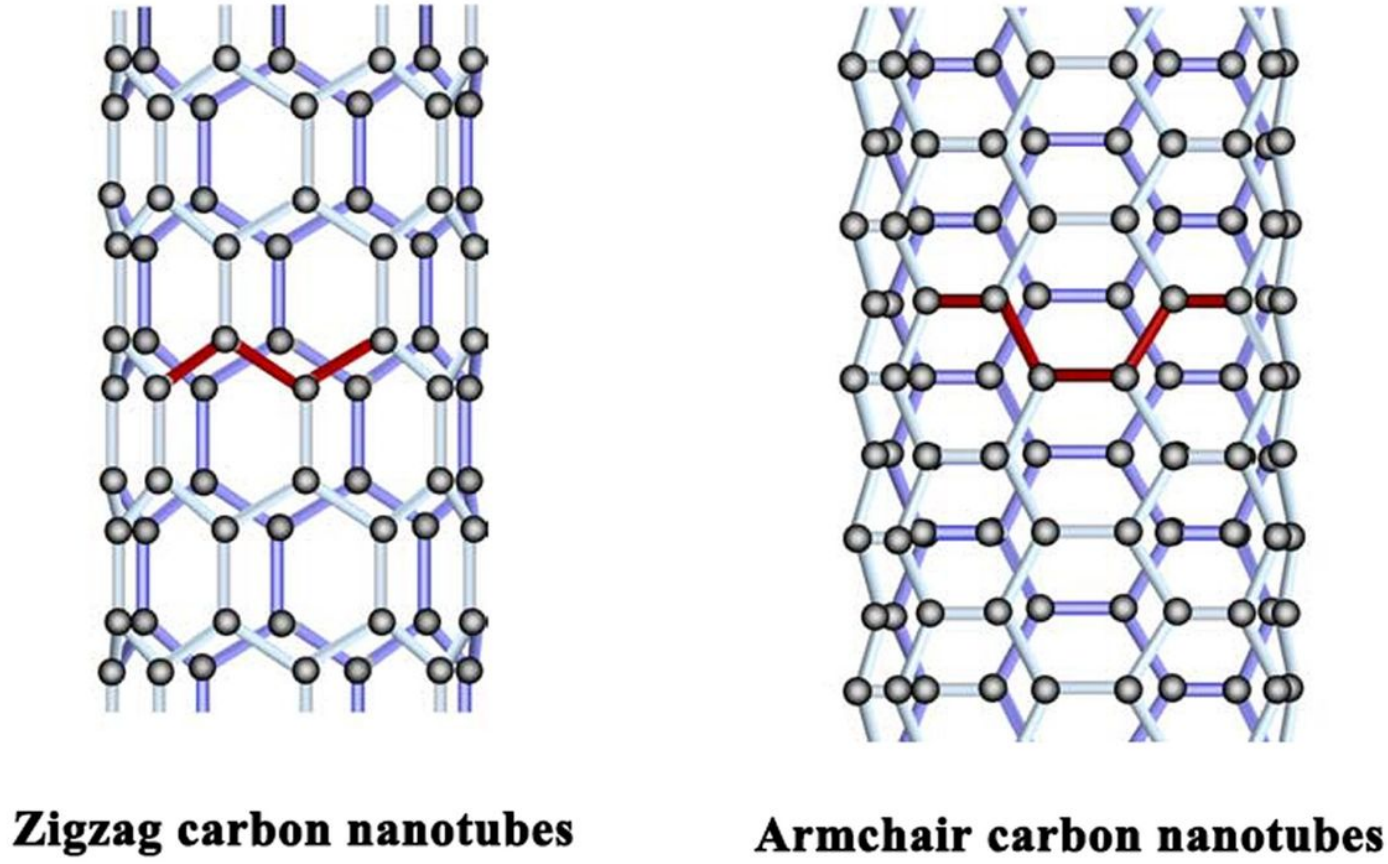

Figure 2

Schematic illustration of the atomic structures of single-walled zigzag and armchair carbon nanotubes. The atomic structures can be described in terms of the chirality or helicity.

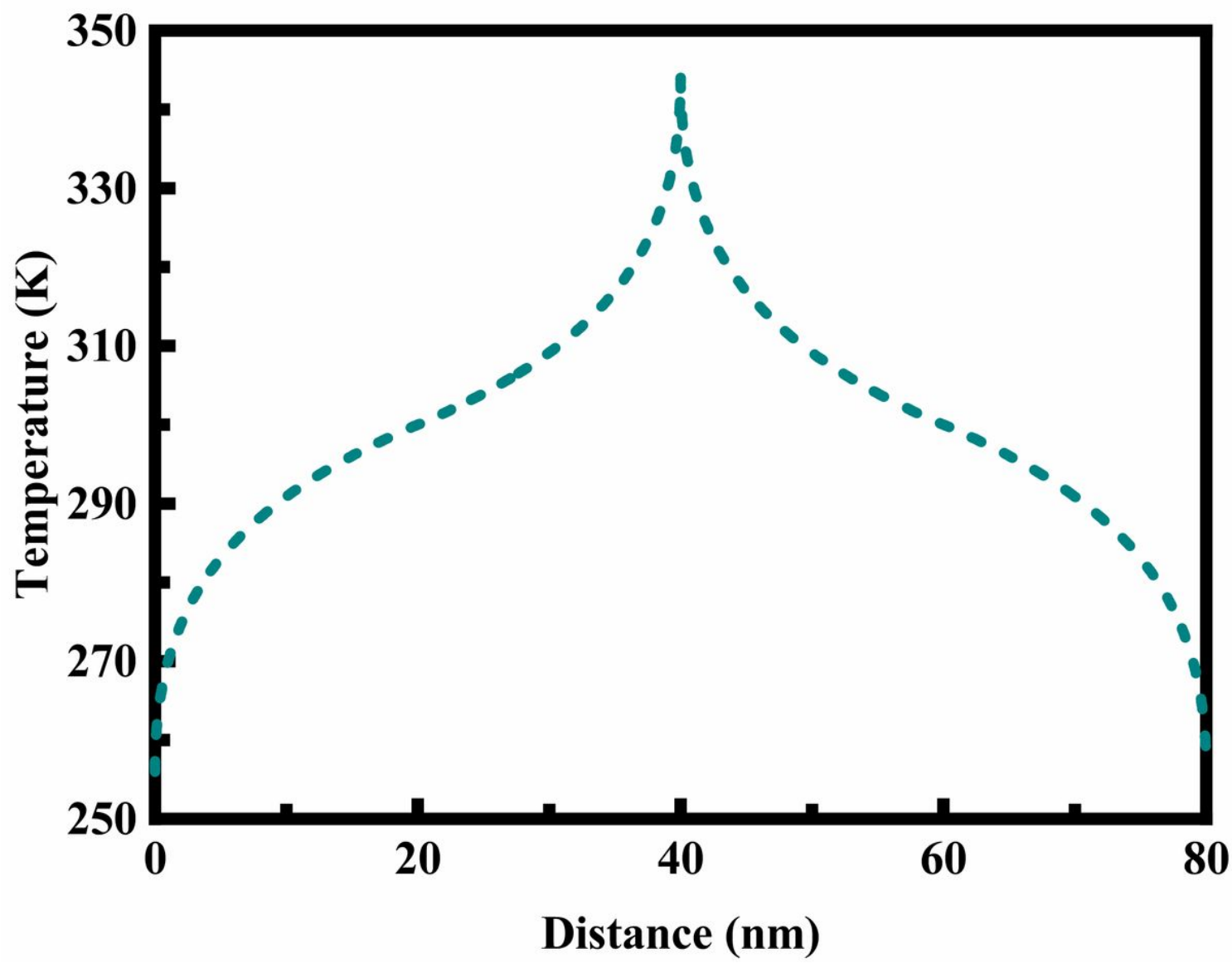

Figure 3

Steady-state temperature profiles obtained for single-walled carbon nanotubes. The length of the single-walled carbon nanotubes is 80 nm.

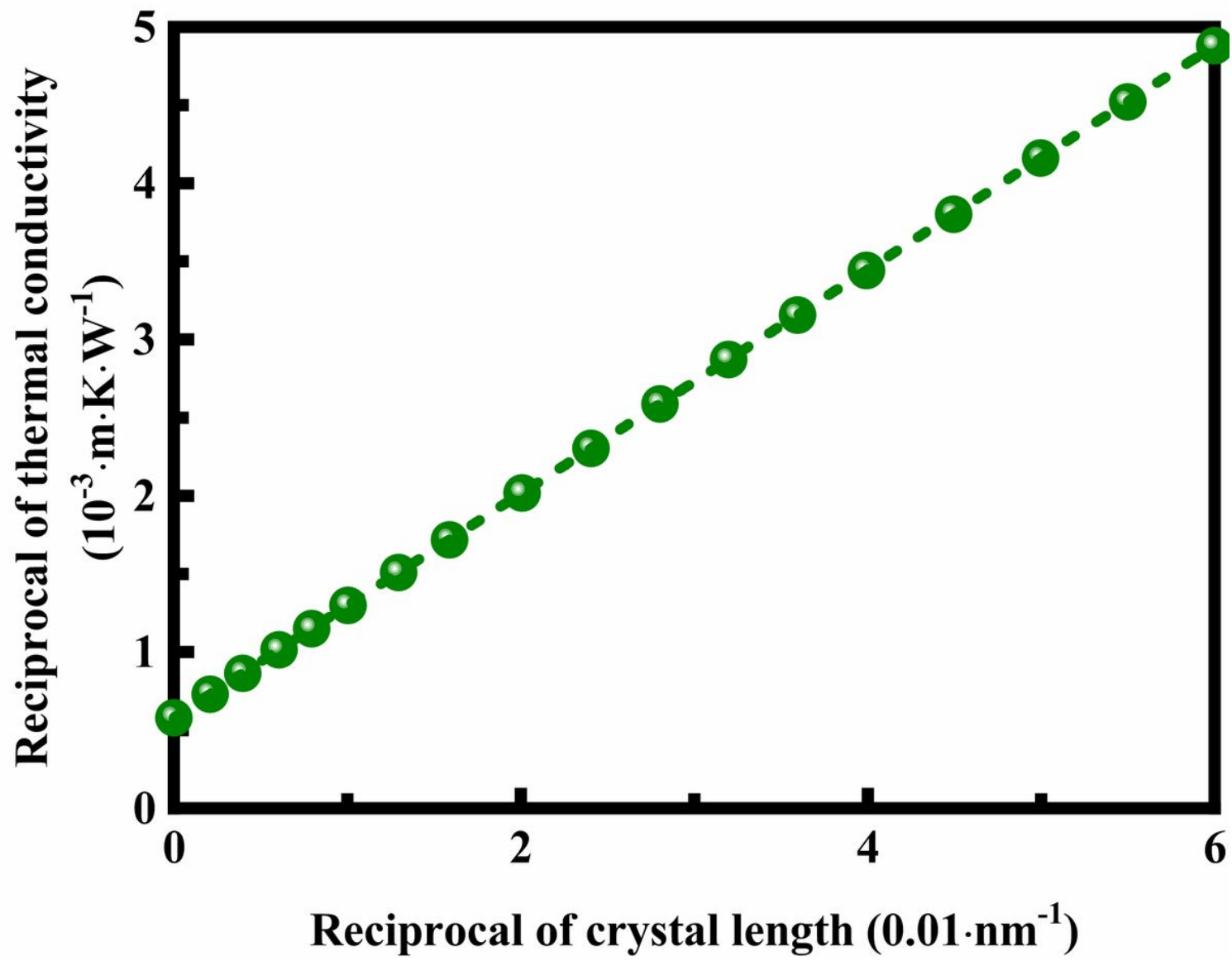

Figure 4

Effect of crystal length on the thermal conductivity of single-walled carbon nanotubes. The thermal conductivity of single-walled carbon nanotubes depends strongly upon the crystal length.

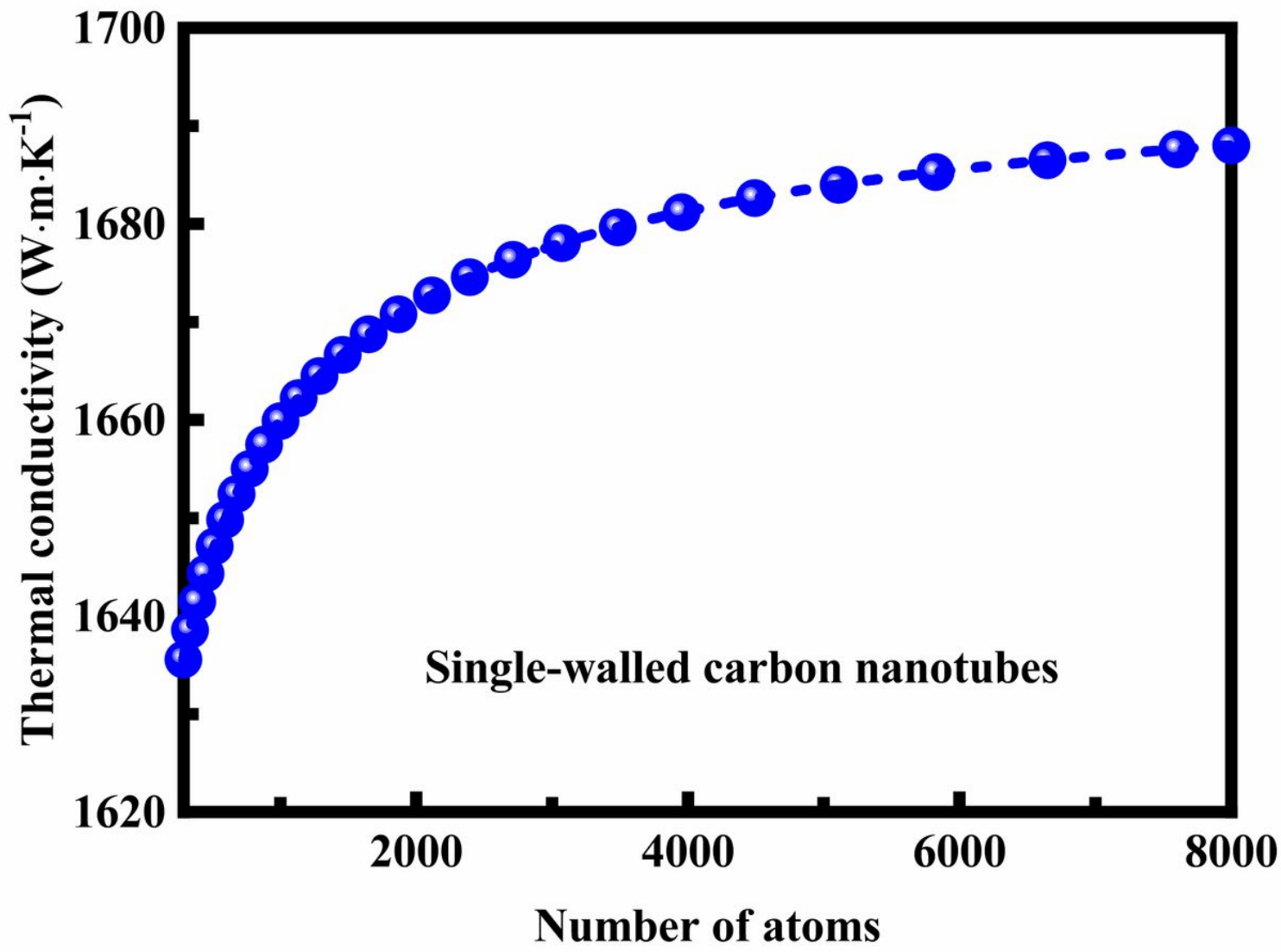

Figure 5

Effect of atom number on the thermal conductivity of single-walled carbon nanotubes. The thermal conductivity of single-walled carbon nanotubes depends slightly upon the number of atoms.

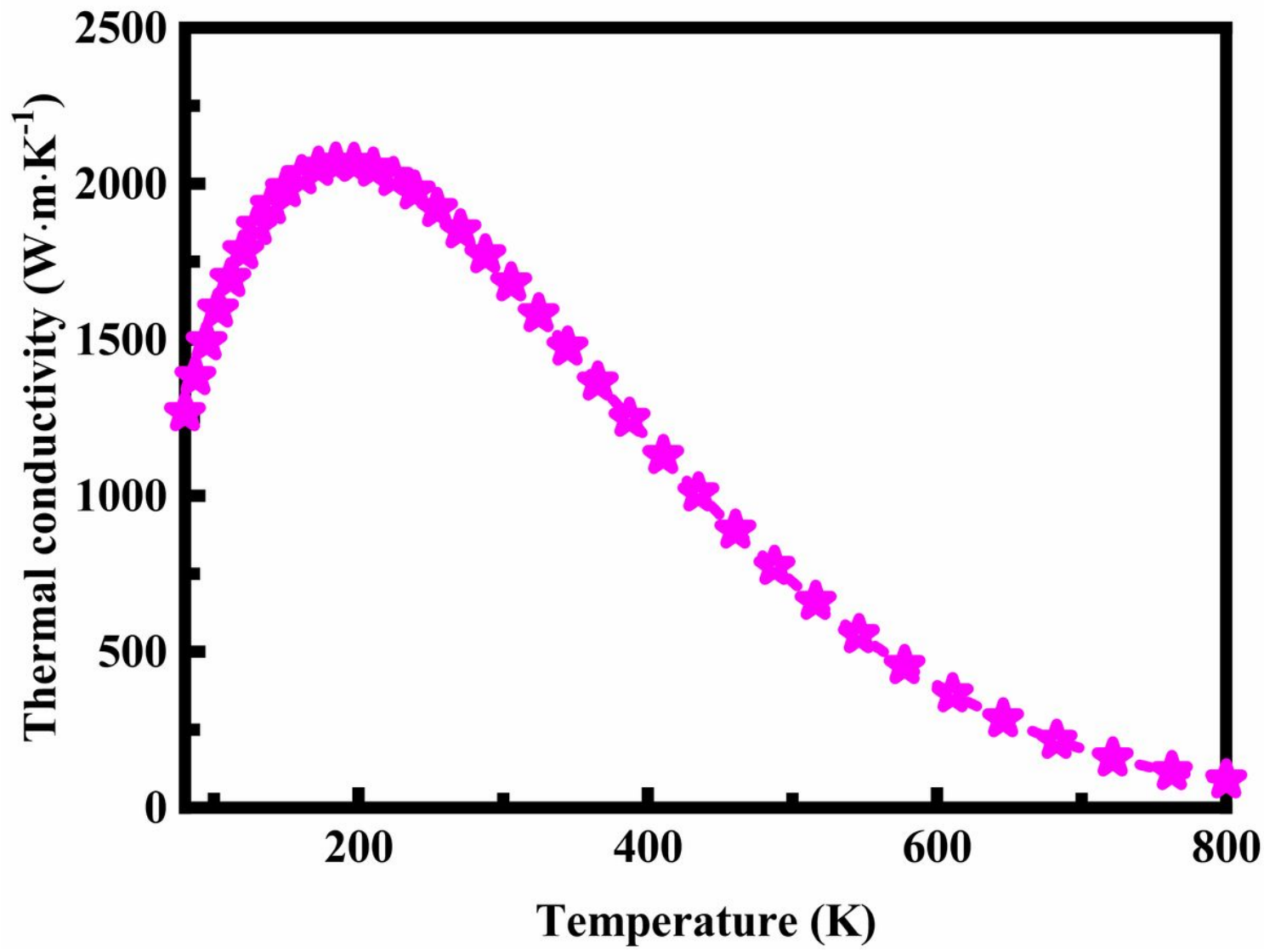

Figure 6

Effect of temperature on the thermal conductivity of single-walled carbon nanotubes. The thermal conductivity of single-walled carbon nanotubes depends heavily upon temperature.