WITHDRAWN:
Effect of temperature factors on the heat conduction properties of carbon nanotubes

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Research Article

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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The full text of this preprint has been withdrawn by the authors while they make corrections to the work.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

The effect of temperature on the thermal conductivity of carbon nanotubes was studied theoretically to understand the heat transport phenomena occurring in the nanostructured materials. The thermal conductivity of macroscopic carbon nanotubes was determined by employing the nonequilibrium molecular dynamics method. The effects of different temperature factors on the heat conduction properties were investigated to evaluate the roles of phonon scattering and defects in the thermal conductivity of the nanostructured materials. The results indicated that macroscopic carbon nanotubes can conduct heat very efficiently, depending on a variety of temperature factors. The structure and allotropes play fundamentally important roles in determining the heat conduction properties of carbon nanotube-based materials. Macroscopic materials formed by single-walled carbon nanotubes typically possess high heat conduction properties. The phonon scattering and defects negatively affect the heat conduction properties because of the low degree of the mean free path of phonons. Carbon nanotube-based materials give rise to a power-law dependence of thermal conductivity with respect to temperature. The lattice thermal conductivity of carbon nanotube-based materials first increases and then decreases with the temperature. Low levels of defects can compensate for the adverse effect of strong phonon scattering on lattice thermal conductivity. A maximum thermal conductivity is achieved at low temperatures, but Umklapp scattering occurs. The thermal conductivity of graphene is significantly higher than that of carbon nanotube-based materials because of the increased degree of ballistic thermal conductance.

1. Introduction

Reduction of interfacial thermal resistance remains a major challenge in the thermal management of many heat-generating engineered components and systems, including the chip-package interface of semiconductor devices, for example, a power integrated circuit and a heat sink or substrate [1, 2]. Thermal contact resistance exists at interfaces because of imperfections caused by microscopic asperities between contacting surfaces. Thermal interface materials, such as solders, thermal greases, oils, gels and pastes, phase change materials, and sheet-type solid materials, have been developed to reduce contact resistance [3, 4]. Thermal interface materials are generally more compliant than the contacting surfaces themselves, and tend to displace air gaps under the application of pressure to increase the extent of contact, thereby increasing thermal contact conductance [5, 6]. Some thermal interface materials have achieved very low interfacial resistances.

With flowable thermal interface materials, high thermal interface conductance is often achieved through enhanced spread ability and elasticity to fill the microscopic gaps between the interface surfaces [7, 8]. As a result of thermal fluctuations, during which the viscosity of a flowable thermal interface material decreases with increasing temperature, nonuniform thermal expansion and deformation of the interface surfaces under a given thermal load can cause pumping out of the thermal interface material from the outer edges of the interface [9, 10]. This phenomenon eventually causes part of the interface to dry out and results in dramatically increased thermal contact resistance.

In addition to those noted above, carbon fiber-based thermal interface composites have also been proposed, notable examples of which include thermal interface materials containing carbon nanotubes [11, 12]. Carbon nanotubes are in the form of cylindrical carbon molecules with diameters less than one micrometer, and can be formed by various processes including chemical vapor deposition on fine particles of a transition metal, particularly nickel or iron, that serve as a catalyst [13, 14]. Theory and experiments indicate that individual single-walled carbon nanotubes and multi-walled carbon nanotubes exhibit extremely high phonon-dominated thermal conductivities at room temperature [15, 16]. The extremely high thermal conductivity of carbon nanotubes suggests many applications in various engineering fields, including electronics packaging [17, 18]. High thermal conductivity composite materials containing aligned carbon nanotubes for heat-spreading devices, have also been proposed [19, 20]. While carbon nanotubes exhibit extremely high thermal conductivity, the interplay of temperature factors and heat conduction properties is poorly understood.

This study relates to the heat conduction properties of carbon nanotube-based materials. Heat conduction in carbon nanotube-based materials was modeled, and the nonequilibrium molecular dynamics method was employed to determine the thermal conductivity of carbon nanotubes. The effect of temperature on the thermal conductivity of carbon nanotube-based materials was investigated to understand the characteristics of thermal transport in the nanostructured materials. The effects of different temperature factors on the heat conduction properties of carbon nanotubes were investigated to evaluate the roles of phonon scattering and defects in the thermal conductivity of the nanostructured materials. The objective is to gain insight into the fundamental characteristics of thermal transport in carbon nanotubes. Particular emphasis is placed on the dependence of thermal conductivity on carbon nanotube structure and allotropes, with an attempt to improve the heat conduction properties for carbon nanotube-based materials.

2. Numerical Methods

Fourier's law can be stated as follows:

$$\frac{Q}{\Delta t} = -kA\frac{\Delta T}{\Delta x}$$

1

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wherein Q is the amount of heat, Δt is the time interval during which the amount of heat flows through a cross-section of the material, k is the thermal conductivity of the material, ΔT is the temperature difference between the ends, and Δx is the distance between the ends. 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. Although commonly expressed as a scalar, the most general form of thermal conductivity is a second-rank tensor. However, the tensorial description only becomes necessary in materials which are

anisotropic. Newton's law of cooling is a discrete analogue of Fourier's law, while Ohm's law is the electrical analogue of Fourier's law and Fick's laws of diffusion is its chemical analogue.

The lattice thermal conductivity is expressed as

$$k_l = \frac{1}{3}\tau_c v^2 C_V$$

2

,

wherein k_l is the lattice thermal conductivity, τ_c is the combined relaxation time, v is the phonon velocity, and C_V is the volumetric heat capacity. Heat capacity or thermal capacity is a physical property of matter, defined as the amount of heat to be supplied to an object to produce a unit change in its temperature. Heat capacity is an extensive property. The corresponding intensive property is the specific heat capacity, found by dividing the heat capacity of an object by its mass. Dividing the heat capacity by the amount of substance in moles yields its molar heat capacity. The volumetric heat capacity measures the heat capacity per volume. In architecture and civil engineering, the heat capacity of a building is often referred to as its thermal mass.

The mean free path of phonons is given by

$$\Lambda = v\tau_c$$

3

,

wherein Λ is the mean free path of phonons. In physics, mean free path is the average distance over which a moving particle travels before substantially changing its direction or energy, typically as a result of one or more successive collisions with other particles. The mean free path of a particle can be described as the average length that the particle can travel freely, i.e., before a collision, which could change its momentum. The mean free path can be increased by reducing the number of impurities in a crystal or by lowering its temperature. Ballistic transport is observed when the mean free path of the particle is longer than the dimension of the medium through which the particle travels.

Metals are usually good conductors of thermal energy. This is due to the way that metals bond chemically: metallic bonds have free-moving electrons that transfer thermal energy rapidly through the metal. The electron fluid of a conductive metallic solid conducts most of the heat flux through the solid. Phonon flux is still present but carries less of the energy. Electrons also conduct electric current through conductive solids, and the thermal and electrical conductivities of most metals have about the same ratio. A good electrical conductor, such as copper, also conducts heat well. Thermoelectricity is caused by the interaction of heat flux and electric current. Heat conduction within a solid is directly analogous to diffusion of particles within a fluid, in the situation where there are no fluid currents. The thermal

conductivity of a material is a measure of its ability to conduct heat. The lattice thermal conductivity can be written as follows:

$$k_l = \frac{1}{3} v \Lambda C_V$$

4

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In engineering practice, it is common to work in terms of quantities which are derivative to thermal conductivity and implicitly take into account design-specific features such as component dimensions. For instance, thermal conductance is defined as the quantity of heat that passes in unit time through a plate of particular area and thickness when its opposite faces differ in temperature by one kelvin. The relationship between thermal conductivity and conductance is analogous to the relationship between electrical conductivity and electrical conductance. Thermal resistance is the inverse of thermal conductance. It is a convenient measure to use in multicomponent design since thermal resistances are additive when occurring in series.

Equilibrium molecular dynamics simulations are performed and the Green-Kubo method is used. Single-walled carbon nanotubes are one of the allotropes of carbon, intermediate between fullerene cages and flat graphene, with diameters in the range of a nanometer. 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. The lattice thermal conductivity of single-walled carbon nanotubes can be written as follows:

$$k_l = \frac{1}{3V} \frac{1}{k_B T^2} \int_0^\infty \langle \mathbf{J}(t) \cdot \mathbf{J}(0) \rangle dt$$

5

,

wherein V is the volume, k_B is the Boltzmann constant, and $\mathbf{J}$ is the heat flux vector.

Heat flux or thermal flux, sometimes referred also to as heat flux density, heat-flow density, or heat flow rate intensity, is a flow of energy per unit of area per unit of time. The heat flux vector can be written as follows:

$$\mathbf{J}(t) = \frac{d}{dt} \sum_i \mathbf{r}_i \Delta e_i = \sum_i \mathbf{v}_i \Delta e_i - \sum_i \sum_j r_{ij} \left(f_{ij} \cdot \mathbf{v}_i \right)$$

6

,

$$\Delta e_i = e_i - \langle e \rangle$$

7

,

$$\mathbf{r}_{ij} = \mathbf{r}_j - \mathbf{r}_i$$

8

,

$$\mathbf{f}_{ij} = -\nabla_i u_j$$

9

,

wherein e_i is the energy of atom i, $\mathbf{r}_i$ is the position of atom i, $\mathbf{v}_i$ is the velocity of atom i, and u_i is the binding energy of atom i.

The internal energy, which is the total vibrational energy, can be obtained by summing over all normal modes, approximating the lattice as a continuum but with a maximum frequency

$$U = \sum_p \int_0^{\omega_{max}} E(\omega) g_{ph}(\omega) \, d\omega$$

10

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wherein U is the internal energy, p is the index of phonon branches, ω is the angular frequency, ω_{max} is the maximum angular frequency, E is the energy of a linear lattice vibration, and g_{ph} is the phonon density of states. In physics, angular frequency, also referred to by the terms angular speed, radial frequency, circular frequency, orbital frequency, and radian frequency, is a scalar measure of rotation rate. Angular frequency is the magnitude of the vector quantity angular velocity. In solid state physics and condensed matter physics, the density of states of a system describes the proportion of states that are to be occupied by the system at each energy.

The lattice thermal conductivity can be written as follows:

$$k_l = \lim_{\mathbf{F}_e \to 0} \lim_{t \to \infty} \langle \mathbf{J}(\mathbf{F}_e, t) \rangle (\mathbf{F}_e T V)^{-1}$$

11

,

wherein $\mathbf{F}_e$ is the thermal force.

In the approach by Nosé and Hoover, an extra degree of freedom is introduced in the Hamiltonian. The heat bath is considered as an integral part of the system

$$\Delta \mathbf{F}_i = \Delta e_i \mathbf{F}_e - \sum_j \mathbf{f}_{ij} \left(\mathbf{r}_{ij} \cdot \mathbf{F}_e \right) + \frac{1}{N} \sum_j \sum_k \mathbf{f}_{jk} \left(\mathbf{r}_{jk} \cdot \mathbf{F}_e \right) - \alpha \mathbf{p}_i$$

12

,

$$\alpha = (T - T_{eq}) \cdot \beta^{-1}$$

13

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wherein α is the Nosé-Hoover thermostat multiplier, $\mathbf{p}_i$ the momentum of atom i, T_{eq} is the equilibrium temperature, and β is the thermal inertia. Thermodynamic equilibrium is an axiomatic concept of thermodynamics. It is an internal state of a single thermodynamic system, or a relation between several thermodynamic systems connected by more or less permeable or impermeable walls. In thermodynamic equilibrium there are no net macroscopic flows of matter or of energy, within a system or between systems. In a system that is in its own state of internal thermodynamic equilibrium, no macroscopic change occurs. A thermodynamic system in a state of internal thermodynamic equilibrium has a spatially uniform temperature. Its intensive properties, other than temperature, may be driven to spatial inhomogeneity by an unchanging long-range force field imposed on it by its surroundings. Thermal inertia is a term commonly used for modeling heat transfers. It is a bulk material property related to thermal conductivity and volumetric heat capacity. For example, "this material has a high thermal inertia", or "thermal inertia plays an important role in this system", mean that dynamic effects are prevalent in a model, so that a steady-state analysis will yield inaccurate results.

3. Results And Discussion

The nonequilibrium molecular dynamics simulations are performed for carbon nanotubes. Molecular dynamics is a computer simulation method for analyzing the physical movements of atoms and molecules. The results obtained for different times are presented in Fig. 1, in which the heat flux vector is plotted against the time at a temperature of 80 K. The time varies from 0 to 8 picoseconds. The heat flux vector first increases with time and then levels off. The heat flux has both a direction and a magnitude, and so it is a vector quantity. For carbon nanotubes, heat is transported mainly by conduction and the heat flux is adequately described by Fourier's law. In practice, the measurement of heat flux can be performed in a few different manners. A commonly known, but often impractical, method is performed by measuring a temperature difference over a piece of carbon nanotubes with known thermal conductivity. This method is analogous to a standard way to measure an electric current, where one measures the

voltage drop over a known resistor. Usually, this method is difficult to perform since the thermal resistance of the carbon nanotubes being tested is often not known. Accurate values for the carbon nanotube's thickness and thermal conductivity would be required in order to determine thermal resistance. Using the thermal resistance, along with temperature measurements on either side of the carbon nanotubes, heat flux can then be indirectly determined.

The results obtained at a temperature of 200 K are presented in Fig. 2, in which the heat flux vector is plotted against the time. The time also varies from 0 to 8 picoseconds. The heat flux vector also first increases with time and then levels off. However, the heat flux vector obtained at a temperature of 200 K is much higher than that obtained at a temperature of 80 K. In practice, the measurement of heat flux can be performed by using a heat flux sensor [21, 22] or heat flux transducer [23, 24]. A heat flux sensor can be used to directly measure the amount of heat being transferred from the surface of carbon nanotubes that the heat flux sensor is mounted to. The most common type of heat flux sensor is a differential temperature thermopile which operates on essentially the same principle as the first measurement method that is mentioned except it has the advantage in that the thermal conductivity of carbon nanotubes does not need to be a known parameter. Heat transport in single-walled carbon nanotubes is by way of elastic vibrations of the lattice, i.e., phonons. This transport mechanism is theorized to be limited by the elastic scattering of acoustic phonons at lattice defects. The phonon mean free path is associated directly with the effective relaxation length for processes without directional correlation. Regarding the dependence of wave velocity on wavelength or frequency, low-frequency phonons of long wavelength will be limited in relaxation length by elastic Rayleigh scattering. This type of light scattering from small particles is proportional to the fourth power of the frequency. For higher frequencies, the power of the frequency will decrease until at highest frequencies scattering is almost frequency independent.

The results obtained for the time dependence are presented in Fig. 3, in which the heat flux vector divided by the temperature is plotted against the time. The time also varies from 0 to 8 picoseconds. The heat flux vector divided by the temperature also first increases with time and then levels off. The mean heat flux vector divided by the temperature is proportional to the lattice thermal conductivity. Phonons in the acoustical branch dominate the phonon heat conduction within carbon nanotubes as they have greater energy dispersion and therefore a greater distribution of phonon velocities. Additional optical modes could also be caused by the presence of internal structure at a lattice point; it is implied that the group velocity of these modes is low and therefore their contribution to the lattice thermal conductivity of carbon nanotubes is small. Conduction is mediated by the combination of propagation and collisions of phonons. The inter-molecular transfer of energy is primarily by phonon vibration in carbon nanotubes. The heat flux is carried almost entirely by phonon vibrations. Due to the connections between atoms, the displacement of one or more atoms from their equilibrium positions gives rise to a set of vibration waves propagating through the lattice. For carbon nanotubes, the dispersion relations exhibit two types of phonons, namely optical and acoustic modes. Acoustic phonons are coherent movements of atoms of the lattice out of their equilibrium positions. Optical phonons are out-of-phase movements of the atoms

in the lattice, one atom moving to the left, and its neighbor to the right. This occurs if the lattice basis consists of two or more atoms.

The results obtained for the dependence of thermal force are presented in Fig. 4, in which the lattice thermal conductivity of carbon nanotubes is plotted at a temperature of 80 K. The lattice thermal conductivity first decreases with the thermal force. The lattice thermal conductivity of carbon nanotubes at a temperature of 80 K is significantly higher than that of a highly conductive metal such as copper. Describing anharmonic effects is complicated because an exact treatment as in the harmonic case is not possible, and phonons are no longer exact eigen solutions to the equations of motion. Even if the state of motion of the crystal could be described with a plane wave at a particular time, its accuracy would deteriorate progressively with time. Time development would have to be described by introducing a spectrum of other phonons, which is known as the phonon decay. The two most important anharmonic effects are the thermal expansion and the phonon thermal conductivity.

The results obtained for the dependence of temperature are presented in Fig. 5, in which the lattice thermal conductivity is plotted for single-walled carbon nanotubes. The temperature varies from 80 to 600 K. The lattice thermal conductivity first increases and then decreases with the temperature. Single-walled carbon nanotubes are very good thermal conductors along the tube, exhibiting a property known as "ballistic conduction", but good insulators lateral to the tube axis. An individual single-walled carbon nanotube has a room-temperature thermal conductivity along its axis of about 3000 $\mathrm{W} \cdot \mathrm{m}^{-1} \cdot \mathrm{K}^{-1}$. Compare this to copper, a metal well known for its good thermal conductivity, which transmits 380 $\mathrm{W} \cdot \mathrm{m}^{-1} \cdot \mathrm{K}^{-1}$. The effect of temperature on thermal conductivity is different for metals and single-walled carbon nanotubes. In metals, heat conductivity is primarily due to free electrons [25, 26]. Following the Wiedemann-Franz law, thermal conductivity of metals is approximately proportional to the absolute temperature times electrical conductivity. In pure metals, the electrical conductivity decreases with increasing temperature and therefore the product of the two, the thermal conductivity, stays approximately constant. However, as temperatures approach absolute zero, the thermal conductivity of single-walled carbon nanotubes decreases sharply. In alloys the change in electrical conductivity is usually smaller and therefore thermal conductivity increases with temperature, often proportionally to temperature. Single-walled carbon nanotubes have a peak thermal conductivity between 100 K and 200 K. Heat conductivity in carbon nanotubes is mainly due to lattice vibrations, namely phonons [27, 28]. Except for high-quality crystals at low temperatures, the phonon mean free path is not reduced significantly at higher temperatures. Therefore, the thermal conductivity of single-walled carbon nanotubes is approximately constant at very high temperatures. At low temperatures well below the Debye temperature, thermal conductivity decreases, as does the heat capacity, due to carrier scattering from defects. A maximum thermal conductivity is achieved at low temperatures, but Umklapp scattering occurs.

Comparisons of lattice thermal conductivity are made between different carbon-based materials. The results are presented in Fig. 6, in which the lattice thermal conductivity is plotted for single-walled carbon nanotubes, graphite, and graphene. The temperature varies from 200 to 600 K. The lattice thermal

conductivity decreases with the temperature. Thermal transport in graphene is an active area of research, which has attracted attention because of the potential for thermal management applications. Suspended graphene has an exceptionally large thermal conductivity up to about 9000 $\mathrm{W} \cdot \mathrm{m}^{-1} \cdot \mathrm{K}^{-1}$, compared with the thermal conductivity of graphite of approximately 200 $\mathrm{W} \cdot \mathrm{m}^{-1} \cdot \mathrm{K}^{-1}$ at room temperature. For single-walled carbon nanotubes and graphite, the thermal conductivity differs from each other by at least one order of magnitude due to the weak binding forces between basal planes as well as the larger lattice spacing. The thermal conductivity of graphene is significantly higher than that of single-walled carbon nanotubes. The ballistic thermal conductance of graphene gives the lower limit of the ballistic thermal conductance, per unit circumference, length of carbon nanotubes. The ballistic thermal conductance of graphene is isotropic. Crystallographic defects strongly affect the single-walled carbon nanotube's thermal properties. Such defects lead to phonon scattering, which in turn increases the relaxation rate of the phonons. This reduces the mean free path and reduces the thermal conductivity of single-walled carbon nanotube structures. Substitutional defects will primarily lead to scattering of high-frequency optical phonons. However, larger-scale defects such as Stone-Wales defects cause phonon scattering over a wide range of frequencies, leading to a greater reduction in thermal conductivity.

4. Conclusions

Heat conduction in carbon nanotube-based materials was modeled, and the nonequilibrium molecular dynamics method was employed to determine the thermal conductivity of carbon nanotubes. The effect of temperature on the heat conduction properties of carbon nanotube-based materials were investigated to understand the characteristics of thermal transport in the nanostructured materials.

The results indicated that macroscopic materials formed by single-walled carbon nanotubes generally have very high thermal conductivity. The presence of phonon scattering and defects reduces the degree of the mean free path of phonons, thereby increasing the thermal resistance and degrading the thermal performance. The thermal conductivity presents a power-law dependence with respect to temperature or has a linear relationship with temperature. The lattice thermal conductivity of carbon nanotube-based materials first increases and then decreases with the temperature. Low levels of defects can compensate for the adverse effect of strong phonon scattering on lattice thermal conductivity. A maximum thermal conductivity is achieved at low temperatures, but Umklapp scattering occurs. The thermal conductivity of graphene is significantly higher than that of carbon nanotube-based materials. The improved thermal properties are caused by the increased degree of ballistic thermal conductance. Macroscopic materials formed by single-walled carbon nanotubes can conduct heat very efficiently due to the increased degree of the mean free path of phonons.

Declarations

Declaration of competing interest

The authors declare that there is no conflict of interest.

References

1. M.-J. Huang and P.-K. Tsai. The size effect on the interfacial thermal resistances of sandwich structures. *International Journal of Heat and Mass Transfer*, Volume 183, Part C, 2022, Article Number: 122217.
2. G. Feng, Y. Feng, L. Qiu, and X. Zhang. Pore scale simulation for melting of composite phase change materials considering interfacial thermal resistance. *Applied Thermal Engineering*, Volume 212, 2022, Article Number: 118624.
3. S. Avcıoğlu, P. Uyan, O. Yontar, and S. Çevik. Electrospray deposition of AlN-PVA composite coating as thermal interface material. *Materials Letters*, Volume 318, 2022, Article Number: 132235.
4. Q. Ma, Z. Wang, T. Liang, Y. Su, J. Li, Y. Yao, X. Zeng, Y. Pang, M. Han, X. Zeng, J. Xu, L. Ren, and R. Sun. Unveiling the role of filler surface energy in enhancing thermal conductivity and mechanical properties of thermal interface materials. *Composites Part A: Applied Science and Manufacturing*, Volume 157, 2022, Article Number: 106904.
5. L. Lv, W. Dai, J. Yu, N. Jiang, and C.-T. Lin. A mini review: application of graphene paper in thermal interface materials. New Carbon Materials, Volume 36, Issue 5, 2021, Pages 930–938.
6. J. Cai, L. Ding, J. Wang, and N. Jiang. Impact of thermal interface material on power cycling lifetime of IGBT module. *Microelectronics Reliability*, Volume 126, 2021, Article Number: 114272.
7. X. Hu, M. Huang, N. Kong, F. Han, R. Tan, and Q. Huang. Enhancing the electrical insulation of highly thermally conductive carbon fiber powders by SiC ceramic coating for efficient thermal interface materials. *Composites Part B: Engineering*, Volume 227, 2021, Article Number: 109398.
8. D. Shia and J. Yang. A Hertzian contact based model to estimate thermal resistance of thermal interface material for high-performance microprocessors. *Microelectronics Journal*, Volume 112, 2021, Article Number: 105058.
9. H. Zhang and X. Zhang. Peridynamic analysis of materials interface fracture with thermal effect. *Theoretical and Applied Fracture Mechanics*, Volume 120, 2022, Article Number: 103420.
10. M. Li, L. Li, X. Hou, Y. Qin, G. Song, X. Wei, X. Kong, Z. Zhang, H. Do, J.C. Greer, F. Han, T. Cai, W. Dai, C.-T. Lin, N. Jiang, and J. Yu. Synergistic effect of carbon fiber and graphite on reducing thermal resistance of thermal interface materials. Composites Science and Technology, Volume 212, 2021, Article Number: 108883.
11. X. Guo, S. Cheng, W. Cai, Y. Zhang, and X. Zhang. A review of carbon-based thermal interface materials: Mechanism, thermal measurements and thermal properties. Materials & Design, Volume 209, 2021, Article Number: 109936.
12. Q. Wu, W. Li, C. Liu, Y. Xu, G. Li, H. Zhang, J. Huang, and J. Miao. Carbon fiber reinforced elastomeric thermal interface materials for spacecraft. Carbon, Volume 187, 2022, Pages 432–438.
13. V. Sivamaran, V. Balasubramanian, M. Gopalakrishnan, V. Viswabaskaran, and A.G. Rao. Combined synthesis of carbon nanospheres and carbon nanotubes using thermal chemical vapor deposition process. *Chemical Physics Impact*, Volume 4, 2022, Article Number: 100072.

14. G.P. Gakis, S. Termine, A.-F.A. Trompeta, I.G. Aviziotis, and C.A. Charitidis. Unraveling the mechanisms of carbon nanotube growth by chemical vapor deposition. *Chemical Engineering Journal*, Volume 445, 2022, Article Number: 136807.
15. 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.
16. K.K. Koziol, D. Janas, E. Brown, and L. Hao. Thermal properties of continuously spun carbon nanotube fibres. Physica E: Low-dimensional Systems and Nanostructures, Volume 88, 2017, Pages 104–108.
17. B. Kumanek and D. Janas. Thermal conductivity of carbon nanotube networks: A review. Journal of Materials Science, Volume 54, 2019, Pages 7397–7427.
18. E.T. Thostenson, C. Li, and T.-W. Chou. Nanocomposites in context. *Composites Science and Technology*, Volume 65, Issues 3–4, 2005, Pages 491–516.
19. S.R. Mousavi, S. Estaji, H. Kiaei, M. Mansourian-Tabaei, S. Nouranian, S.H. Jafari, H. Ruckdäschel, M. Arjmand, and H.A. Khonakdar. A review of electrical and thermal conductivities of epoxy resin systems reinforced with carbon nanotubes and graphene-based nanoparticles. *Polymer Testing*, Volume 112, 2022, Article Number: 107645.
20. B. Liu, N. Vu-Bac, X. Zhuang, X. Fu, and T. Rabczuk. Stochastic integrated machine learning based multiscale approach for the prediction of the thermal conductivity in carbon nanotube reinforced polymeric composites. *Composites Science and Technology*, Volume 224, 2022, Article Number: 109425.
21. O. Hotra, S. Kovtun, and O. Dekusha. Analysis of the characteristics of bimetallic and semiconductor heat flux sensors for in-situ measurements of envelope element thermal resistance. *Measurement*, Volume 182, 2021, Article Number: 109713.
22. M. Akoshima. Developement of an apparatus for practical calibration of heat flux sensors. *Measurement: Sensors*, Volume 18, 2021, Article Number: 100343.
23. T. Perl, A. Bräuer, W. Weyland, and U. Braun. Application of heat flux transducers to determine perioperative heat exchange. *Thermochimica Acta*, Volume 422, Issues 1–2, 2004, Pages 35–40.
24. S.K. Manjhi and R. Kumar. Performance analysis of coaxial thermocouples for heat flux measurement of an aerodynamic model on shock tube facility. *Measurement*, Volume 166, 2020, Article Number: 108221.
25. E. Saavedra-Otero. On conduction heat transfer in metals. Physica B: Condensed Matter, Volume 415, 2013, Pages 23–27.
26. P.J. Catto and M. Grinneback. Electron heat conduction modifications due to long mean free path effects. Physics Letters A, Volume 277, Issue 6, 2000, Pages 323–330.
27. Z.P. Popović, M. Damnjanović, and I. Milošević. Phonon transport in helically coiled carbon nanotubes. Carbon, Volume 77, 2014, Pages 281–288.
28. A. Duzynska, M. Swiniarski, A. Wroblewska, A. Lapinska, K. Zeranska, J. Judek, and M. Zdrojek. Phonon properties in different types of single-walled carbon nanotube thin films probed by Raman

spectroscopy. Carbon, Volume 105, 2016, Pages 377–386.

Figures

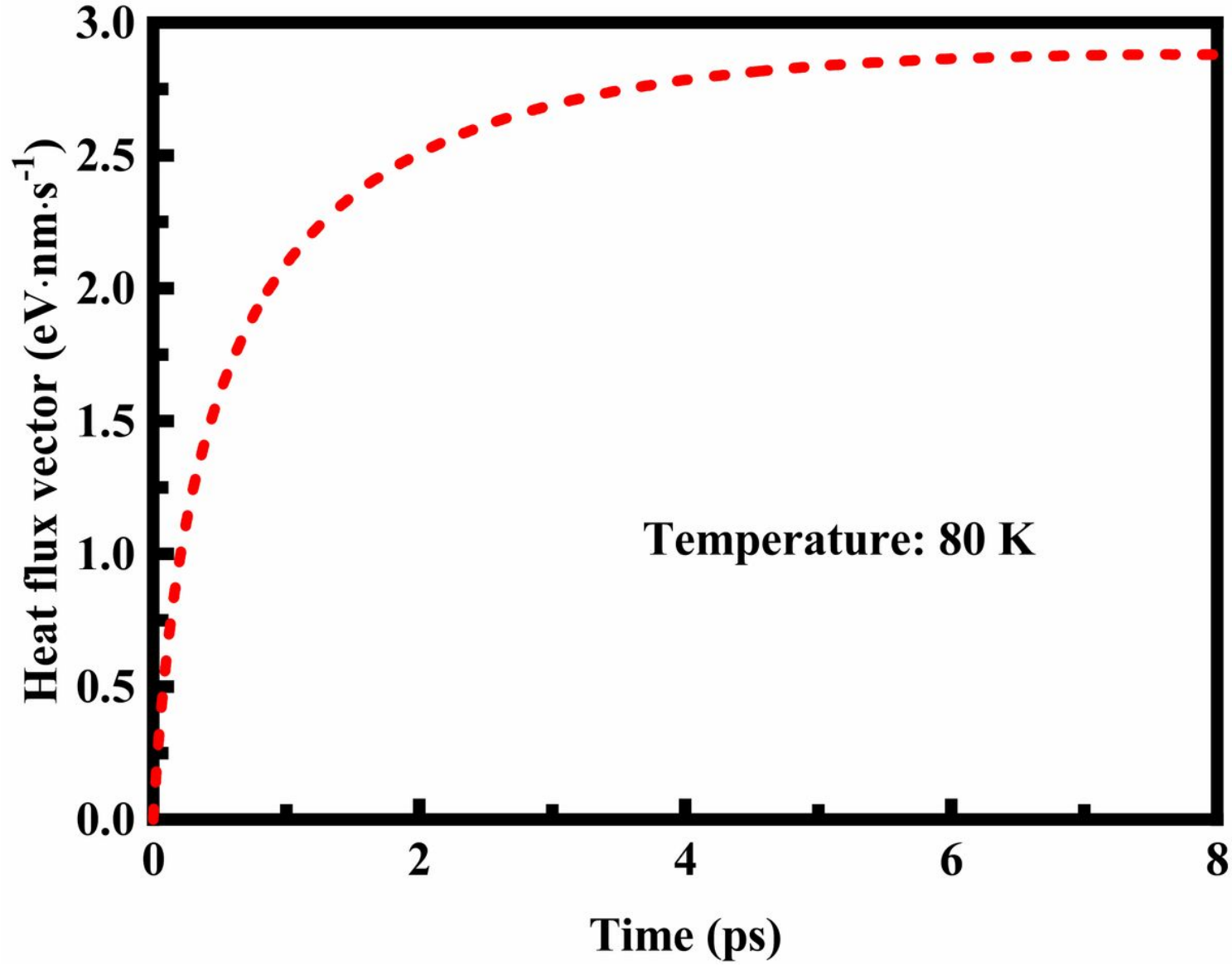

Figure 1

Heat flux vector along an individual single-walled carbon nanotube as a function of time at a temperature of 80 K.

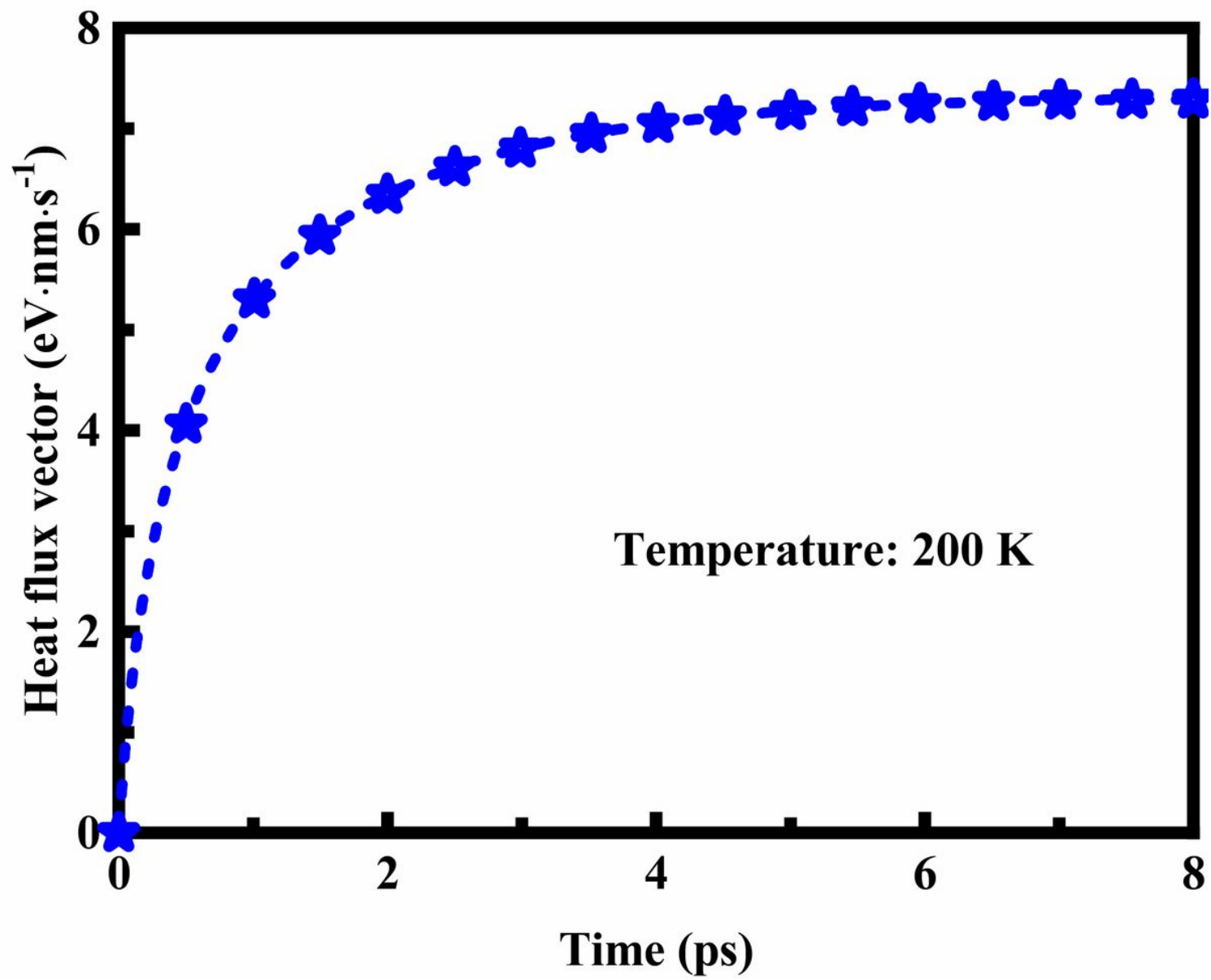

Figure 2

Heat flux vector along an individual single-walled carbon nanotube as a function of time at a temperature of 200 K.

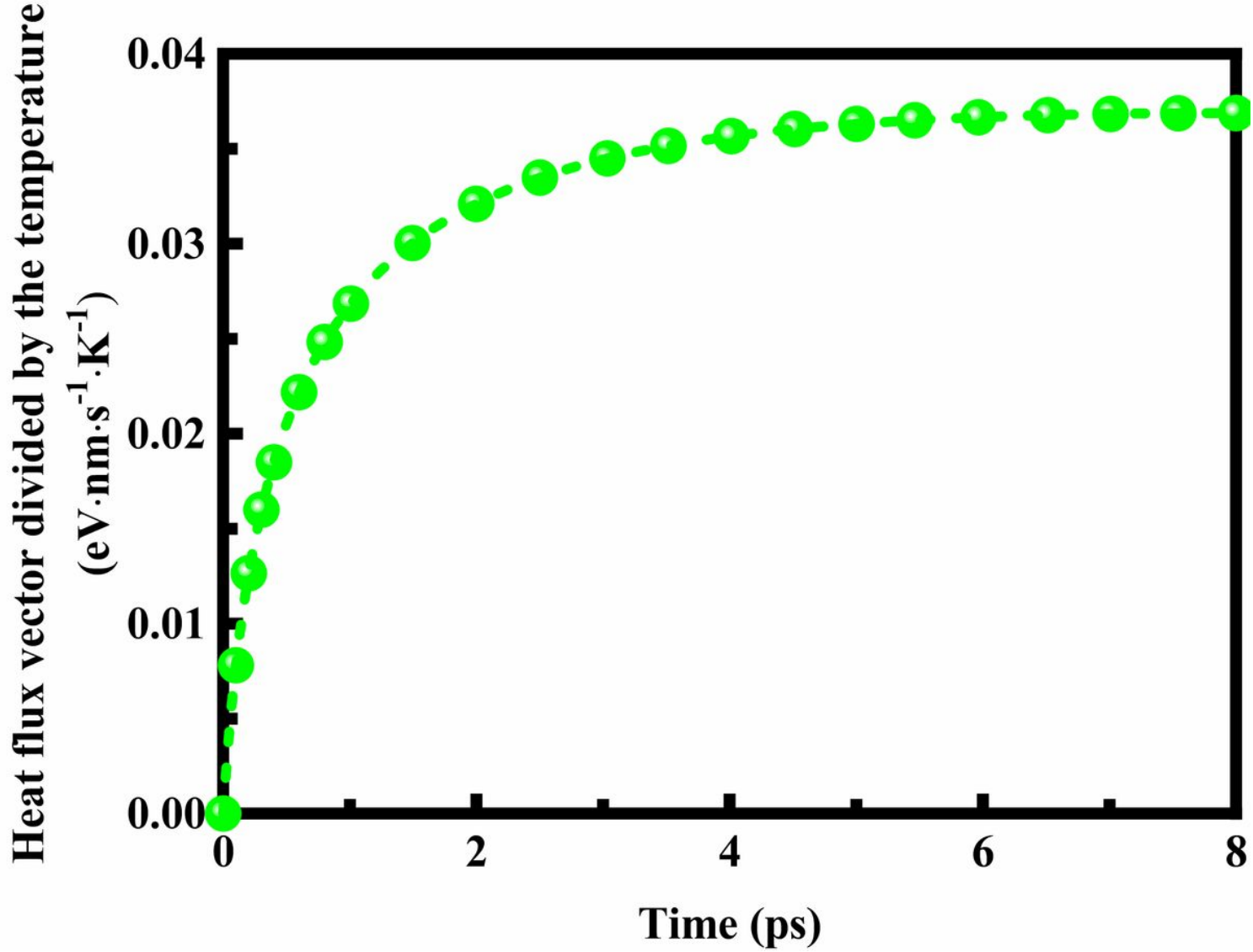

Figure 3

Heat flux vector divided by the temperature along an individual single-walled carbon nanotube as a function of time.

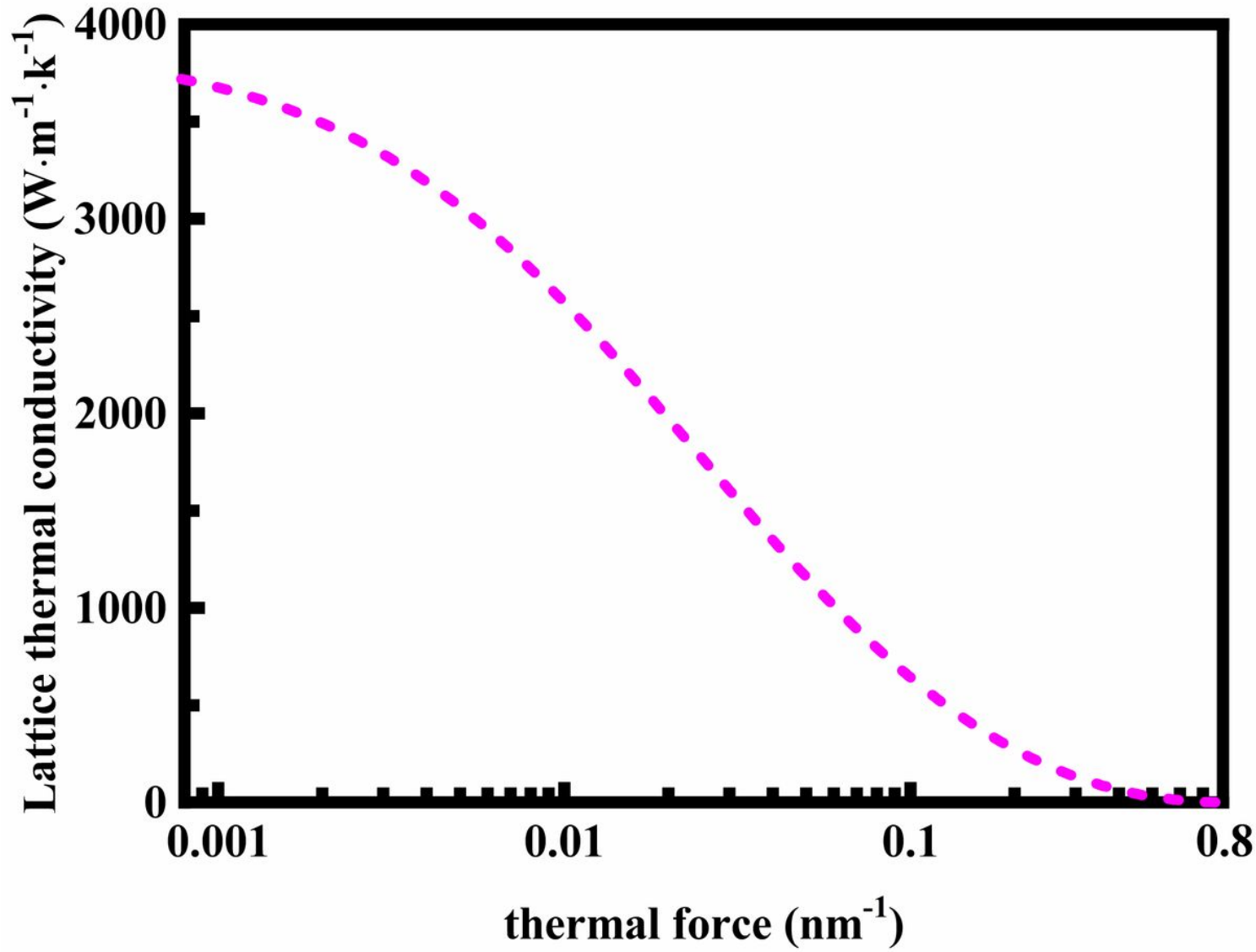

Figure 4

Lattice thermal conductivity of single-walled carbon nanotubes as a function of thermal force at a temperature of 80 K.

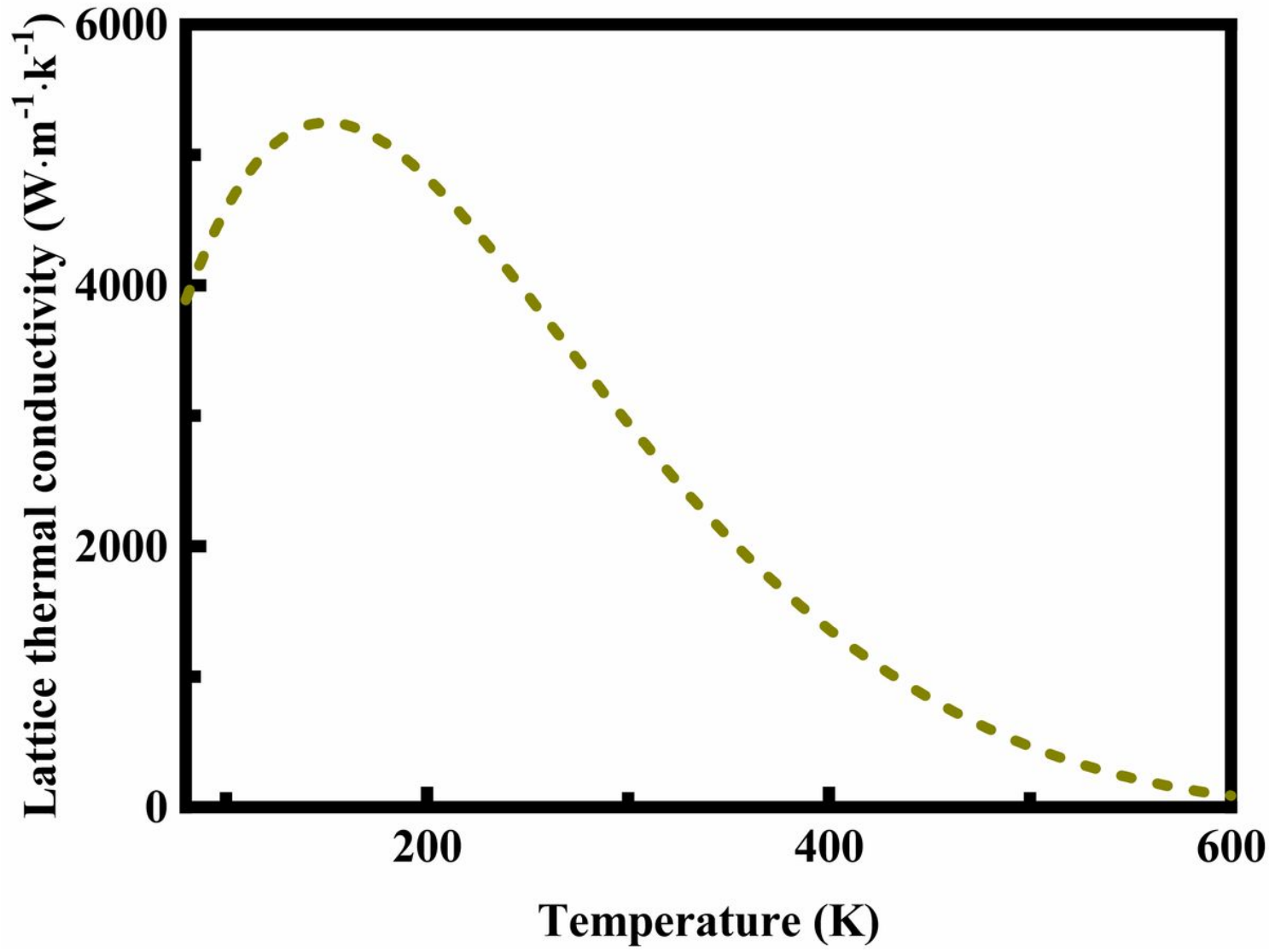

Figure 5

Lattice thermal conductivity of single-walled carbon nanotubes as a function of temperature. The temperature varies from 80 to 600 K.

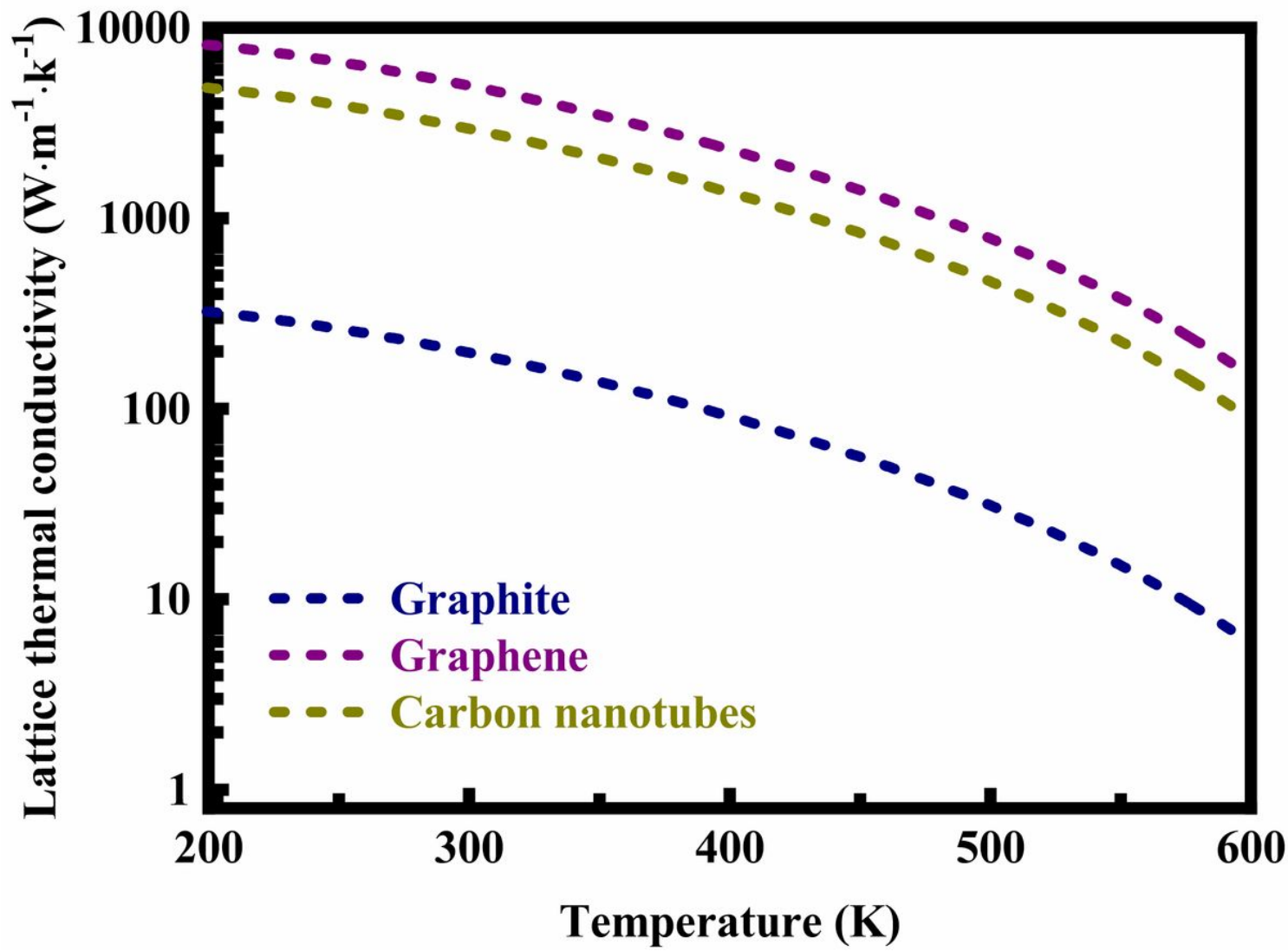

Figure 6

Lattice thermal conductivity of single-walled carbon nanotubes, graphite, and graphene as a function of temperature. The temperature varies from 200 to 600 K.