

WITHDRAWN: Effects of structure, purity, and alignment factors on the heat conduction properties of nanostructured materials comprising single-walled carbon nanotubes

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Abstract

The increasing popularity of single-walled carbon nanotubes has created a demand for greater scientific understanding of the characteristics of thermal transport in nanostructured materials. However, the effects of structure, purity, and alignment factors on the specific heat capacity and thermal conductivity of single-walled carbon nanotubes are still poorly understood. The effects of structure, purity, and alignment factors on the heat conduction properties of single-walled carbon nanotubes were investigated by using the nonequilibrium molecular dynamics method. The specific heat capacity and thermal conductivity of carbon nanotube-based materials were determined to understand the characteristics of thermal transport in the nanostructured materials. The effect of single-walled carbon nanotube loading on the heat conduction properties of carbon nanotube-based polymer composites was investigated. The results indicated that single-walled carbon nanotubes are very efficient at conducting heat. The structure, purity, and alignment factors play a fundamentally important role in determining the heat conduction properties of single-walled carbon nanotubes. The difference in specific heat capacity between graphene and single-walled carbon nanotubes is larger at lower temperatures but becomes very small at higher temperatures. The purity strongly affects the heat conduction properties of single-walled carbon nanotubes, whereas the effect of alignment on the thermal conductivity is considerable. The lattice thermal conductivity of carbon nanotube-based materials first increases and then decreases with temperature. Single-walled carbon nanotube reinforced epoxy composites are able to achieve significant improvements in thermal properties at much lower loadings. A significant improvement in heat conduction properties can be achieved when single-walled carbon nanotubes serve as thermal reinforcements for epoxy composite systems with further promise of multifunctionality.

1. Introduction

Carbon nanotubes, also called buckytubes, are nanoscale hollow tubes composed of carbon atoms. The cylindrical carbon molecules feature high aspect ratios, length-to-diameter values, typically above 10^3 , with diameters from about one nanometer up to tens of nanometers and lengths up to millimeters [1, 2]. This unique one-dimensional structure and concomitant properties endow carbon nanotubes with special natures, rendering them with unlimited potential in nanotechnology-associated applications [3, 4]. Carbon nanotubes are members of the fullerene family. Although the first fullerene molecules were discovered in 1985 [5], it was not until Sumio Iijima reported his findings in 1991 about needlelike carbon tubes in *Nature* that carbon nanotubes came to public awareness [6]. Since then, carbon nanotubes with various structures have been discovered. According to the number of graphic shells, they are mainly categorized as single-walled and multi-walled carbon nanotubes. The carbon nanotubes reported by Sumio Iijima were multi-walled carbon nanotubes synthesized by arc discharge methods [6]. Two years later, two sets of researchers working independently, Sumio Iijima and Toshinari Ichihashi [7], along with Donald Stimson Bethune and his colleagues at International Business Machines Corporation [8], synthesized single-walled carbon nanotubes, using transition-metal catalyzed arc discharge.

A single-walled carbon nanotube can be described as a long tube formed by wrapping a single graphene sheet into a cylinder with diameter of about one nanometer, the ends of which are capped by fullerene cages. The fullerene structures, with alternating structures of five hexagons adjacent to one pentagon, form the surface with desired curvature to enclose the volume. The sidewalls of carbon nanotubes are made of graphene sheets consisting of neighboring hexagonal cells. Other polygon structures, such as pentagons and heptagons, constitute defects of sidewalls. The cylindrical sidewalls can be produced from different rolling directions to make single-walled carbon nanotubes with distinct structures and properties [9, 10]. Due to cylindrical symmetry, there are only a handful of methods that are effective in making seamless cylinders, and they are characterized by the chiral vectors with integer indices (n, m) . To establish the chiral vector, two atoms in the graphene sheet are selected, with one serving as the origin of the vector pointing toward the other atom. The graphene sheet is then rolled in a way that allows the two atoms to coincide. Under these circumstances, the chiral vectors form a plane perpendicular to the longitude direction of nanotubes and the lengths of the chiral vectors are equal to the circumference. Three different types of single-walled carbon nanotubes are distinctly characterized, named "zigzag", "armchair", and "chiral". These structural variations result in differences in electrical conductivity and mechanical strength [9, 10]. Multi-walled carbon nanotubes are concentrically aligned single-walled carbon nanotube assemblies with different diameters. The distance between adjacent shells is about 0.34 nanometer [11, 12]. Multi-walled carbon nanotubes differ from single-walled carbon nanotubes not only in their dimensions, but also in their corresponding properties.

Various techniques have been developed to produce carbon nanotubes in sizable quantity, high yield, and purity, while maintaining a reasonable cost [13, 14]. Well-developed techniques include arc discharge, laser ablation, and chemical vapor deposition, and most processes involve costly vacuum conditions [15, 16]. Arc discharge was initially used for the synthesis of fullerenes [17]. In a typical experimental setup, a chamber filled with low-pressure, 50 to 700 mbar, inert gas, helium or argon, is where the reaction takes place. Two carbon rods are placed end-to-end as the electrodes, separated by a few millimeters, and a direct current of 50 to 100 A, driven by a potential difference of 20 V, generates a high discharge temperature to sublime the negative electrode, leaving soot where carbon nanotubes are found [18]. This method is the most common way to synthesize carbon nanotubes and perhaps the easiest way. The quality of carbon nanotubes depends on the uniformity of plasma arc, catalysts, and the selection of filling gases. A mixture of carbon nanotubes is usually produced. Consequently, purification processes are needed to remove the fullerenes, amorphous carbon, and catalysts. Laser ablation was first employed to produce carbon nanotubes in 1995 [19]. A pulsed or continuous laser is used to vaporize a graphite, or graphite metal mixture, target in a 1,200°C oven filled with inert gas at a pressure of 500 torr. Carbon vapors cool down rapidly during expansion, and carbon atoms quickly condense to form tubular structures with the help of catalyst particles. Multi-walled carbon nanotubes can be synthesized when pure graphite is vaporized, and single-walled carbon nanotubes are grown from graphite-transition metal mixtures. The method is primarily used to synthesize single-walled carbon nanotubes with high selectivity and in a diameter-controllable way by tailoring reaction temperatures. The resulting products are usually in the form of bundles. Laser ablation is the most-costly technique due to the involvement of expensive

lasers and high-power input [20]. Chemical vapor deposition is the most promising way to produce carbon nanotubes on an industrial scale [21]. This process utilizes high energy, 600–900°C, to atomize gaseous carbon sources, such as methane, carbon monoxide, and acetylene. The resulting reactive carbon atoms diffuse toward a catalyst-coated substrate and condense to form carbon nanotubes [22]. Well-aligned carbon nanotubes can be synthesized with precisely controlled morphology, provided that proper reaction conditions are maintained, including preparation of substrates and selection of catalysts.

Novel chemical, electrical, and mechanical properties absent in other materials have been discovered in carbon nanotubes [23, 24]. Pristine carbon nanotubes are inert to most chemicals and need to be grafted with surface functional groups to increase their chemical reactivity and add new properties [25, 26]. For single-walled carbon nanotubes, electrical conductivity is dependent on the chiral vector and independent of the length as determined by quantum mechanics [27]. Considering a chiral vector with indices (n, m) , carbon nanotubes can be metallic and semiconducting in some cases [28]. Along the longitudinal directions, carbon nanotubes show superior mechanical strength, with the highest known tensile strength and elastic modulus among known materials [29]. As for thermal properties, carbon nanotubes outperform diamond as the best thermal conductor [30]. Applications of carbon nanotubes are aimed to make use of their unique properties to solve problems at the nanoscale [31, 32]. Their high surface area, together with the unique ability to carry any chemical compounds after surface modification, offers carbon nanotubes the potential to be used as nanoscale catalyst supports with high catalytic reactivity and chemical sensors [33]. They are known to be the best field emitters due to their sharp tips, which can concentrate electric field easily, enabling them to emit electrons at low voltages [34]. This property has special applications in field emission flat-panel displays and cold-cathode electron guns used in microscopes [35, 36]. In nanoelectronics, single-walled carbon nanotubes have been used to fabricate transistors that can function at room temperature and are potential candidates for devices operating at terahertz frequencies [37, 38]. Engineering materials using carbon nanotubes as additives have exhibited capability to make plastic composite materials with enhanced electrical conductivity and mechanical strength [39, 40]. While carbon nanotubes exhibit extremely high thermal conductivity, the interplay of structure and alignment factors and heat conduction properties is poorly understood.

This study relates to the heat conduction properties of single-walled carbon nanotubes. The effects of structure, purity, and alignment factors on the heat conduction properties of single-walled carbon nanotubes were investigated by using the nonequilibrium molecular dynamics method. The specific heat capacity and thermal conductivity of single-walled carbon nanotube-based materials were determined to understand the characteristics of thermal transport in the nanostructured materials. The effect of single-walled carbon nanotube loading on the heat conduction properties of carbon nanotube-based polymer composites was investigated. 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 specific heat capacity and thermal conductivity on single-walled carbon nanotubes, with an attempt to improve the heat conduction properties for single-walled carbon nanotube-based materials.

2. Numerical Methods

The lattice thermal conductivity of carbon nanotube-based materials is expressed as

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

1

,

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. In the physical sciences, relaxation usually means the return of a perturbed system into equilibrium. Each relaxation process can be categorized by a relaxation time. In condensed matter physics, relaxation is usually studied as a linear response to a small external perturbation.

The mean free path of phonons is given by

$$\Lambda = v \tau_c$$

2

,

wherein Λ is the mean free path of phonons.

The lattice thermal conductivity can be written as follows:

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

3

.

Equilibrium molecular dynamics simulations are performed and the Green-Kubo method is used. The lattice thermal conductivity of carbon nanotubes can be written as follows:

$$k_{\alpha\beta} = \frac{1}{V} \frac{1}{k_B T^2} \int_0^\infty \langle J_\alpha(t) \cdot J_\beta(t) \rangle dt$$

4

,

wherein $k_{\alpha\beta}$ is the (α, β) component of the thermal conductivity tensor, V is the volume, k_B is the Boltzmann constant, and J_α and J_β are the components of the heat current in the α and β directions, respectively. The Boltzmann constant is the proportionality factor that relates the average relative kinetic

energy of particles in a gas with the thermodynamic temperature of the gas. The Boltzmann constant has dimensions of energy divided by temperature.

The lattice thermal conductivity is determined by applying either a fixed temperature gradient or heat flux to the system. The lattice thermal conductivity is related to the thermal gradient by

$$J_{\alpha} = - \sum_{\beta} k_{\alpha\beta} \frac{\partial T}{\partial x_{\beta}}$$

5

wherein $\frac{\partial T}{\partial x_{\beta}}$ is the temperature gradient along the β direction. A temperature gradient is a physical quantity that describes in which direction and at what rate the temperature changes the most rapidly around a particular location. The temperature gradient is a dimensional quantity expressed in units of degrees per unit length.

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

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

6

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.

The phonon density of states per branch per mode is expressed as

$$g_{ph,br}(\omega) = \frac{3\omega^2}{\omega_D^3}$$

7

wherein ω_D is the Debye cutoff frequency.

The Debye temperature is defined as

$$\theta_D = \frac{\hbar\omega_D}{k_B}$$

8

wherein θ_D is the Debye temperature and \hbar is the reduced Planck's constant. The reduced Planck's constant is of fundamental importance in quantum mechanics.

3. Results And Discussion

3.1. Specific heat

The results obtained for the specific heat capacity of an individual single-walled carbon nanotube at low temperatures are presented in Fig. 1, in which the temperature varies from 0 to 8 K. The specific heat capacity varies with temperature, with a substantially linear temperature dependence. Heat capacity is the ratio of heat absorbed by a material to the temperature change. It is usually expressed as calories per degree in terms of the actual amount of material being considered, most commonly a mole. Specific heat is the quantity of heat required to raise the temperature of one gram of a substance by one Celsius degree. In thermodynamics, the specific heat capacity of a substance is the heat capacity of a sample of the substance divided by the mass of the sample, also sometimes referred to as mass heat capacity. Informally, it is the amount of heat that must be added to one unit of mass of the substance in order to cause an increase of one unit in temperature. The SI unit of specific heat capacity is joule per kelvin per kilogram. At a temperature of 8 K, there is an increase in the slope of the temperature dependence. At sufficiently low temperatures, the specific heat capacity tends to be very small for single-walled carbon nanotubes.

The effects of structure factors on the heat conduction properties of nanostructured materials are investigated, including an individual single-walled carbon nanotube, graphene, graphite, and a single-walled carbon nanotube rope. The results obtained for the specific heat capacity of the nanostructured materials at different temperatures are presented in Fig. 2, in which the temperature varies from 8 to 300 K. The specific heat capacity of graphene is significantly higher than that of the other nanostructured materials. The difference in specific heat capacity between the nanostructured materials is larger at lower temperatures but becomes very small at higher temperatures. Graphene is a two-dimensional form of crystalline carbon, either a single layer of carbon atoms forming a hexagonal lattice or several coupled layers of this honeycomb structure. Graphene is a parent form of all graphitic structures of carbon: graphite, which is a three-dimensional crystal consisting of relatively weakly coupled graphene layers; carbon nanotubes, which may be represented as scrolls of graphene; and buckyballs, spherical molecules made from graphene with some hexagonal rings replaced by pentagonal rings. Graphite, also called plumbago or black lead, is a mineral consisting of carbon. Graphite has a layered structure that consists of rings of six carbon atoms arranged in widely spaced horizontal sheets. Graphite thus crystallizes in the

hexagonal system, in contrast to the same element crystallizing in the octahedral or tetrahedral system as diamond. Such dimorphous pairs usually are rather similar in their physical properties, but not so in this case. The specific heat capacity of single-walled carbon nanotubes is higher than that of graphite and single-walled carbon nanotube ropes. The specific heat capacity of graphite is slightly higher than that of single-walled carbon nanotube ropes. At sufficiently high temperatures, the heat capacity per atom tends to be the same for all elements. For metals of higher atomic weight, this approximation is already a good one at room temperature, giving rise to the law of Dulong and Petit [41, 42]. The law of Dulong and Petit is initially used as an empirical rule, along with other empirical rules, in determining approximate atomic weights of the elements. For other materials, heat capacity and its temperature variation depend on differences in energy levels for atoms. At sufficiently high temperatures, the specific heat capacity tends to be the same for all the nanostructured materials.

The effects of purity factors on the heat conduction properties of nanostructured materials are investigated. The results obtained for the specific heat capacity of single-walled carbon nanotubes with different degrees of purity at different temperatures are presented in Fig. 3, in which the temperature varies from 8 to 300 K. The purity strongly affects the heat conduction properties of single-walled carbon nanotubes. The specific heat capacity differs by one or more order of magnitude, especially at higher temperatures. Thermal conduction is the transfer of energy arising from temperature differences between adjacent parts of a body. Thermal conductivity is attributed to the exchange of energy between adjacent molecules and electrons in the conducting medium. The rate of heat flow in a rod of material is proportional to the cross-sectional area of the rod and to the temperature difference between the ends and inversely proportional to the length. The specific heat capacity of all the nanostructured materials tends to become zero at sufficiently low temperatures. Therefore, the difference in specific heat capacity between the nanostructured materials becomes very small at sufficiently low temperatures. Heat is energy that is transferred from one body to another as the result of a difference in temperature. If two bodies at different temperatures are brought together, energy is transferred from the hotter body to the colder. The effect of this transfer of energy usually, but not always, is an increase in the temperature of the colder body and a decrease in the temperature of the hotter body. A substance may absorb heat without an increase in temperature by changing from one physical state to another, as from a solid to a liquid, from a solid to a vapor, from a liquid to a vapor, or from one solid form to another. Heat is a form of energy and temperature a measure of the amount of that energy present in a body. However, single-walled carbon nanotubes have no melting point at atmospheric pressure [43, 44]. Melting point is the temperature at which the solid and liquid forms of a pure substance can exist in equilibrium. In such a context, the specific heat capacity of single-walled carbon nanotubes tends to become zero at sufficiently low temperatures, regardless of the degree of purity.

The effects of structure factors on the heat conduction properties of nanostructured materials are investigated at low temperatures, including an individual single-walled carbon nanotube, graphene, graphite, and a single-walled carbon nanotube rope. The results obtained for the specific heat capacity of the nanostructured materials at low temperatures are presented in Fig. 4, in which the temperature varies from 0 to 8 K. At low temperatures, the specific heat capacity of graphene is significantly higher than that

of the other nanostructured materials. The difference in specific heat capacity between the nanostructured materials is large in all the cases studied here. At sufficiently low temperatures, the specific heat capacity tends to be the same for all the nanostructured materials. In general, the amount of energy required to raise a unit mass of a substance through a specified temperature interval is called the heat capacity, or the specific heat, of that substance. The quantity of energy necessary to raise the temperature of a body one degree varies depending upon the restraints imposed [45, 46]. If heat is added to a gas confined at constant volume, the amount of heat needed to cause a one-degree temperature rise is less than if the heat is added to the same gas free to expand and so do work. In the first case, all the energy goes into raising the temperature of the gas, but in the second case, the energy not only contributes to the temperature increase of the gas but also provides the energy necessary for the work done by the gas on the piston. Consequently, the specific heat of a substance depends on these conditions. The most commonly determined specific heats are the specific heat at constant volume and the specific heat at constant pressure. However, the nanostructured materials relate to a solid form. Solids exhibit certain characteristics that distinguish them from liquids and gases. The energy required to melt a solid to a liquid is called the heat of fusion, and the heat of sublimation is the energy necessary to change a solid directly to a vapor, these changes also taking place under conditions of constant temperature and pressure. However, all the nanostructured materials have no melting point at atmospheric pressure. To distinguish between the energy associated with the phase change and the energy required for a temperature change, the concept of sensible heat was introduced. In a mixture of water vapor and air, the sensible heat is the energy necessary to produce a particular temperature change excluding any energy required for a phase change. It is impossible to determine the sensible heat the nanostructured materials, since these solids have no melting point at atmospheric pressure.

3.2. Thermal conductivity

The effects of temperature factors on the heat conduction properties of nanostructured materials are investigated. The results obtained for the thermal conductivity of single-walled carbon nanotubes at different temperatures are presented in Fig. 5, in which the temperature varies from 8 to 300 K. The temperature strongly affects the heat conduction properties of single-walled carbon nanotubes. The thermal conductivity of a material is a measure of its ability to conduct heat. Heat transfer occurs at a lower rate in materials of low thermal conductivity than in materials of high thermal conductivity. For instance, metals typically have high thermal conductivity and are very efficient at conducting heat, while the opposite is true for insulating materials. Correspondingly, materials of high thermal conductivity are widely used in heat sink applications, and materials of low thermal conductivity are used as thermal insulation. The reciprocal of thermal conductivity is called thermal resistivity. Thermal conduction is defined as the transport of energy due to random molecular motion across a temperature gradient. It is distinguished from energy transport by convection and molecular work in that it does not involve macroscopic flows or work-performing internal stresses. 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 has been associated directly with the effective relaxation length for processes without directional correlation. The extraordinary thermal properties of single-walled carbon nanotubes have attracted widespread interest [47, 48]. The carbon nanotubes exhibit a very low coefficient of thermal expansion, high strength, high elastic modulus, and uniquely high thermal conductivity along their longitudinal axis, but exhibit only average properties orthogonal to longitudinal axis, similar to those of graphite. However, the thermal conductivity of single-walled carbon nanotubes first increases and then decreases with temperature. The thermal conductivity of single-walled carbon nanotubes at room temperature is significantly higher than that of a highly conductive metal, for example, copper. The thermal conductivity differs by about one order of magnitude. The thermal conductivity of single-walled carbon nanotubes spans about one order of magnitude.

The effect of alignment on the thermal conductivity of single-walled carbon nanotubes at different temperatures is illustrated in Fig. 6, in which the temperature varies from 8 to 300 K. The temperature strongly affects the heat conduction properties of single-walled carbon nanotubes, regardless of the degree of alignment. The thermal conductivity differs by less than about 2000 K. The effect of temperature on thermal conductivity is identical for single-walled carbon nanotubes and highly aligned single-walled carbon nanotubes. Because heat is energy in transition, some discussion of the mechanisms involved is pertinent. There are three modes of heat transfer, which can be described as the transfer of heat by conduction in solids or fluids at rest, the transfer of heat by convection in liquids or gases in a state of motion, combining conduction with fluid flow, and the transfer of heat by radiation, which takes place with no material carrier. However, all the nanostructured materials relate to a solid form. Therefore, the mode of heat transfer within single-walled carbon nanotubes can be described as the transfer of heat by conduction in solids at rest. A particularly important concept is thermodynamic equilibrium, in which there is no tendency for the state of a system to change spontaneously. The concept of temperature is fundamental to any discussion of thermodynamics. In this case, the temperature varies from 8 to 300 K. As temperatures approach absolute zero, the thermal conductivity of single-walled carbon nanotubes decreases sharply, regardless of the degree of alignment. Single-walled carbon nanotubes have a peak thermal conductivity at lower temperatures. Heat conductivity in single-walled carbon nanotubes is mainly due to lattice vibrations. Except for high-quality crystals at low temperatures, the mean free path of phonons is not reduced significantly at higher temperatures. As the temperature increases from 8 to 300 K, the difference in thermal conductivity between single-walled carbon nanotubes and highly aligned single-walled carbon nanotubes increases from about 100 K to about 200 K. However, single-walled carbon nanotubes can exhibit different thermal conductivities along different crystal axes. When anisotropy is present, the direction of heat flow may differ from the direction of the thermal gradient. In this case, However, the tensorial description becomes necessary in single-walled carbon nanotubes which are anisotropic.

The effects of temperature factors on the heat conduction properties of nanostructured materials are investigated. The results obtained for the thermal conductivity divided by temperature of single-walled carbon nanotubes at different temperatures are presented in Fig. 7, in which the temperature varies from 8 to 300 K. The temperature strongly affects the heat conduction properties of single-walled carbon

nanotubes. The thermal conductivity divided by temperature of single-walled carbon nanotubes decreases with increasing temperature. The unusual thermal properties of single-walled carbon nanotubes are governed by their unusual and simple atomic structure. A single-walled carbon nanotube consists of an atomic layer of carbon atoms rolled into the form of a nanotube. The axis of the nanotube can form along many different directions in the carbon layer, yielding single-walled carbon nanotubes with different chirality and diameters. Heat conduction by single-walled carbon nanotubes is dominated by the coupled vibrations of carbon atoms and therefore can be analyzed as phonon transport. Phonon transport dominates over heat conduction by electrons even in those carbon nanotubes chirality that exhibit metallic properties. The phonon dispersion relationship consists of four acoustic modes and many optical modes. The twist acoustic mode arises from torsion of the nanotube about its axis, which can be described as a twisting motion. The phonon conductivity can be computed from the phonon dispersion relationship, the heat capacity of each phonon mode, and their scattering rates or mean free paths. The Debye temperature is significantly higher than room temperature and likely similar to graphene, graphite, and diamond. Consequently, even at room temperature the heat capacity and thermal conductivity are impacted by quantum effects. Single-walled carbon nanotubes and other low-dimensional carbon-based nanomaterials including graphene can have very high thermal conductivities, despite very small cross-sectional dimensions. This is in contrast to many crystalline nanowires with small cross-sectional dimensions in which the thermal conductivity is strongly reduced by the increased rate of phonon-boundary scattering. The long-range crystallinity, long mean free path of phonons, and large speed of sound of single-walled carbon nanotubes lead to the large thermal conductivity. The phonon mean free path in carbon nanotubes depends on phonon-phonon, phonon-boundary, and phonon-defect scattering processes. However, single-walled carbon nanotubes do not have very high thermal conductivity divided by temperature, especially at higher temperatures.

The effect of single-walled carbon nanotube loading on the heat conduction properties of carbon nanotube-based polymer composites is investigated. The results obtained for the thermal conductivity enhancement of single-walled carbon nanotube-based epoxy composites are presented in Fig. 8, in which the carbon nanotube loading varies from 0 to 0.08. In materials science, a polymer matrix composite is a composite material composed of a variety of short or continuous fibers bound together by a matrix of organic polymers. Polymer matrix composites are designed to transfer loads between fibers of a matrix. Epoxy systems currently dominate the advanced composite industry. Single-walled carbon nanotube reinforced epoxy composites are able to achieve significant improvements in thermal properties at much lower loadings. However, in order to take advantage of the exceptional thermal properties of single-walled carbon nanotubes, the load transfer between the single-walled carbon nanotubes and the polymer matrix must be very large. Fundamental processing challenges must be overcome in order to fully enable the reinforcement by single-walled carbon nanotubes. In general, long and high aspect ratio single-walled carbon nanotubes lead to greater enhancement of thermal properties, but are more difficult to process. The interface between the single-walled carbon nanotubes and the polymer matrix is of exceptional importance. Therefore, the dispersion property has become more important when single-walled carbon nanotubes are blended with polymers. Additional processing difficulties for single-walled carbon

nanotube reinforced epoxy polymer composites come from the significant increase of viscosity when the single-walled carbon nanotubes are added directly into the epoxy. Sidewall functionalization of single-walled carbon nanotubes, like end-cap functionalization, offer opportunity, if the right functional moiety is attached, to covalently integrate into epoxy polymer matrices, but they offer far more opportunities for such integration by virtue of having more functional groups with which to interact. The functionalization can be used to get better dispersion, to get specific interactions between the materials in the composite system, and to promote alignment. A significant improvement in heat conduction properties can be achieved when single-walled carbon nanotubes serve as thermal reinforcements for epoxy composite systems with further promise of multifunctionality.

4. Conclusions

The effects of structure, purity, and alignment factors on the heat conduction properties of single-walled carbon nanotubes were investigated by using the nonequilibrium molecular dynamics method. The specific heat capacity and thermal conductivity of carbon nanotube-based materials were determined to understand the characteristics of thermal transport in the nanostructured materials.

The results indicated that the thermal properties of single-walled carbon nanotubes are directly related to their unique structure. 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 difference in specific heat capacity between graphene and single-walled carbon nanotubes is larger at lower temperatures but becomes very small at higher temperatures. At low temperatures, the specific heat capacity of graphene is significantly higher than that of single-walled carbon nanotubes. The purity strongly affects the heat conduction properties of single-walled carbon nanotubes. The effect of alignment on the thermal conductivity is considerable. The lattice thermal conductivity of carbon nanotube-based materials first increases and then decreases with temperature. Single-walled carbon nanotube reinforced epoxy composites are able to achieve significant improvements in thermal properties at much lower loadings. However, in order to take advantage of the exceptional thermal properties of single-walled carbon nanotubes, the load transfer between the single-walled carbon nanotubes and the polymer matrix must be very large. A significant improvement in heat conduction properties can be achieved when single-walled carbon nanotubes serve as thermal reinforcements for epoxy composite systems with further promise of multifunctionality.

Declarations

Declaration of competing interest

The authors declare that there is no conflict of interest.

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Figures

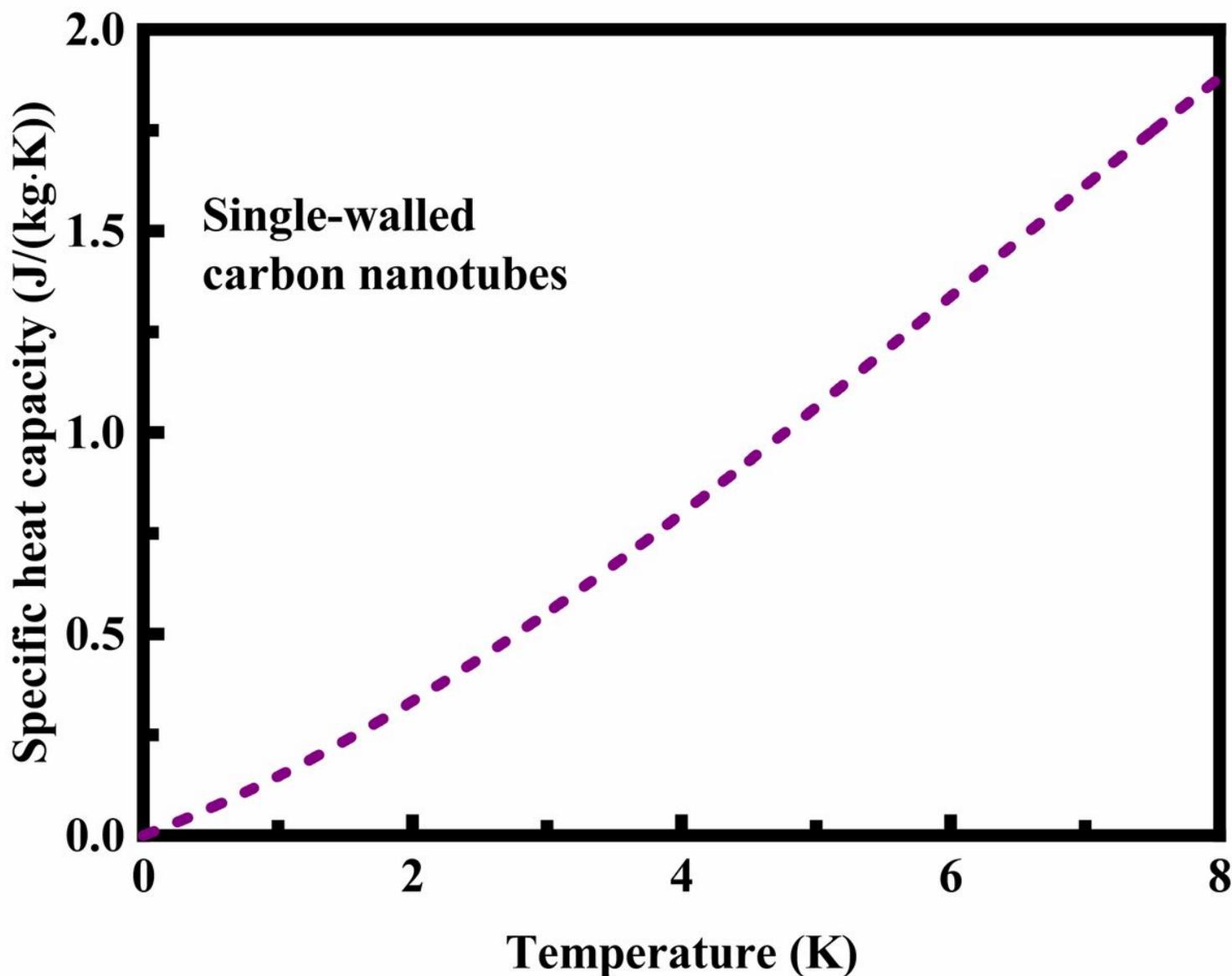


Figure 1

Specific heat capacity of an individual single-walled carbon nanotube at low temperatures. The temperature varies from 0 to 8 K.

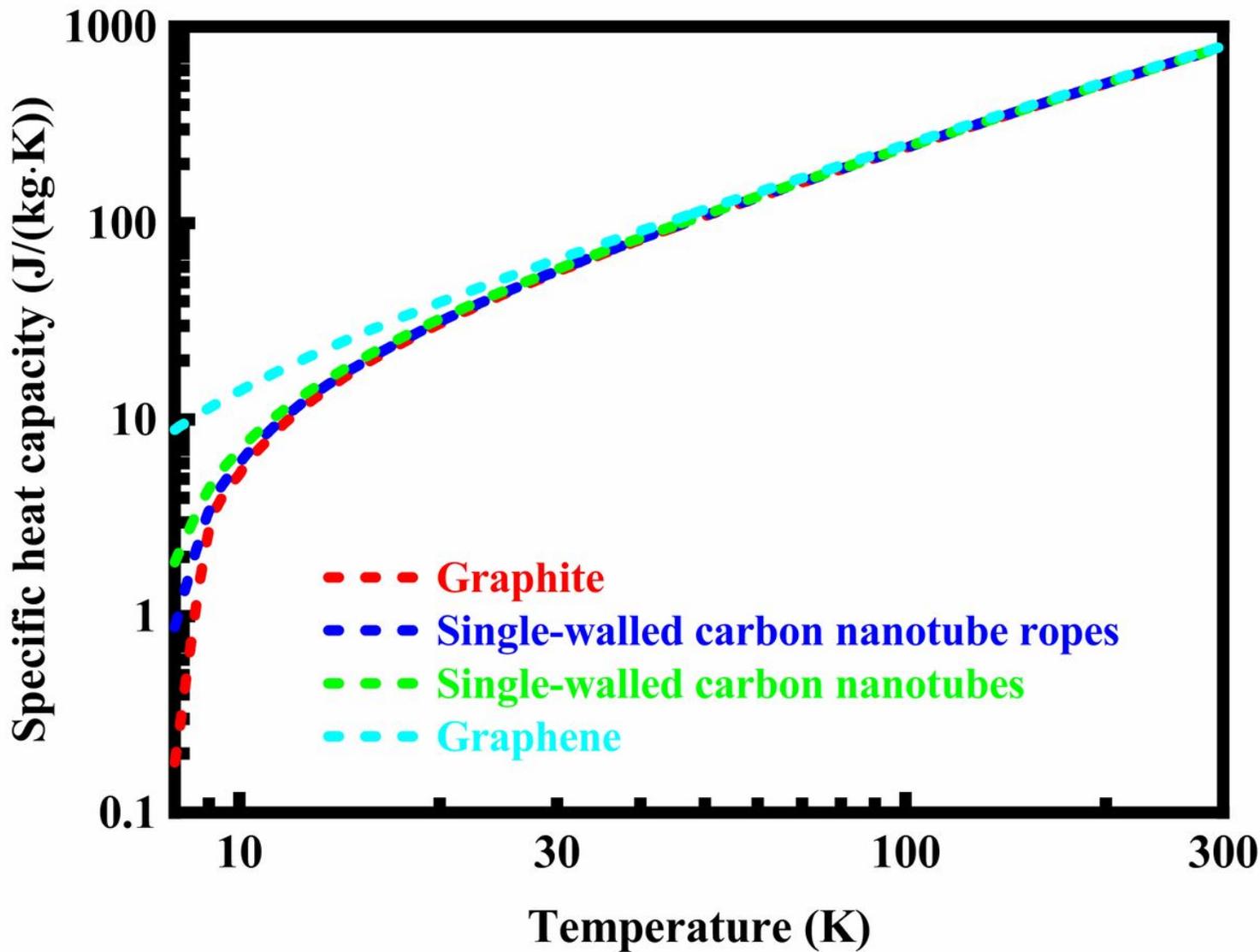


Figure 2

Specific heat capacity of an individual single-walled carbon nanotube, graphene, graphite, and a single-walled carbon nanotube rope. The temperature varies from 8 to 300 K.

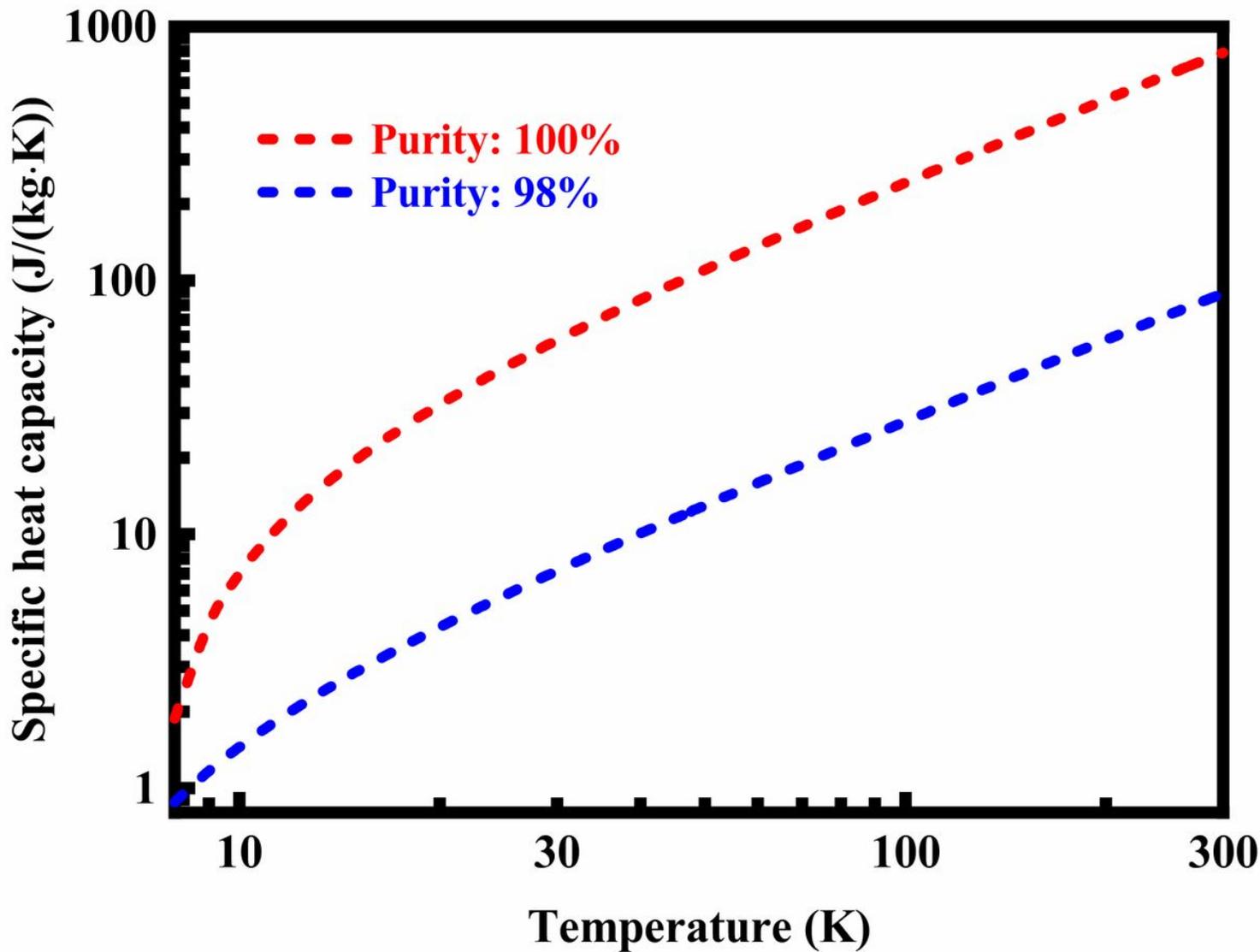


Figure 3

Specific heat capacity of single-walled carbon nanotubes with different degrees of purity at different temperatures. The temperature varies from 8 to 300 K.

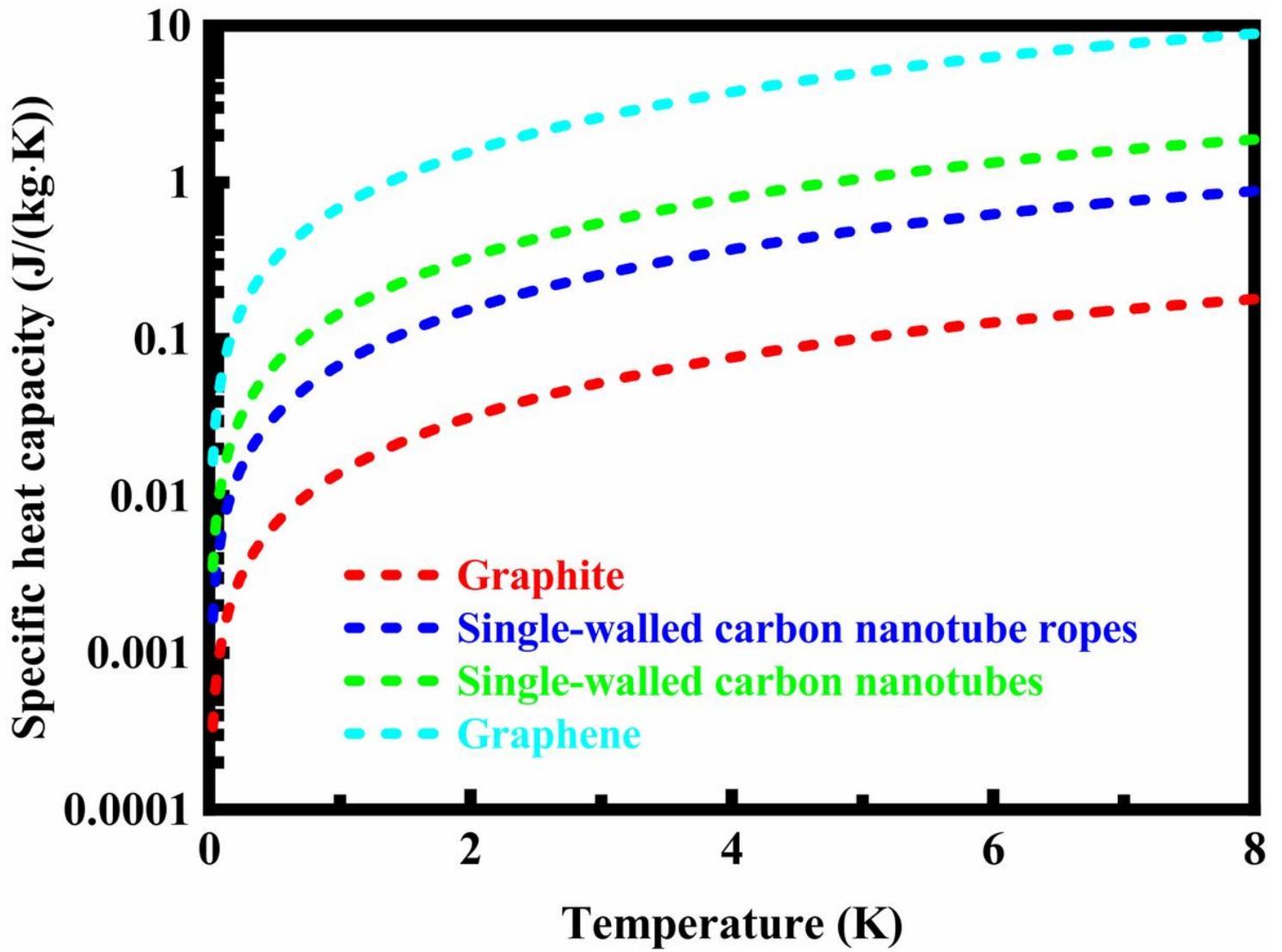


Figure 4

Specific heat capacity of an individual single-walled carbon nanotube, graphene, graphite, and a single-walled carbon nanotube rope at low temperatures. The temperature varies from 0 to 8 K.

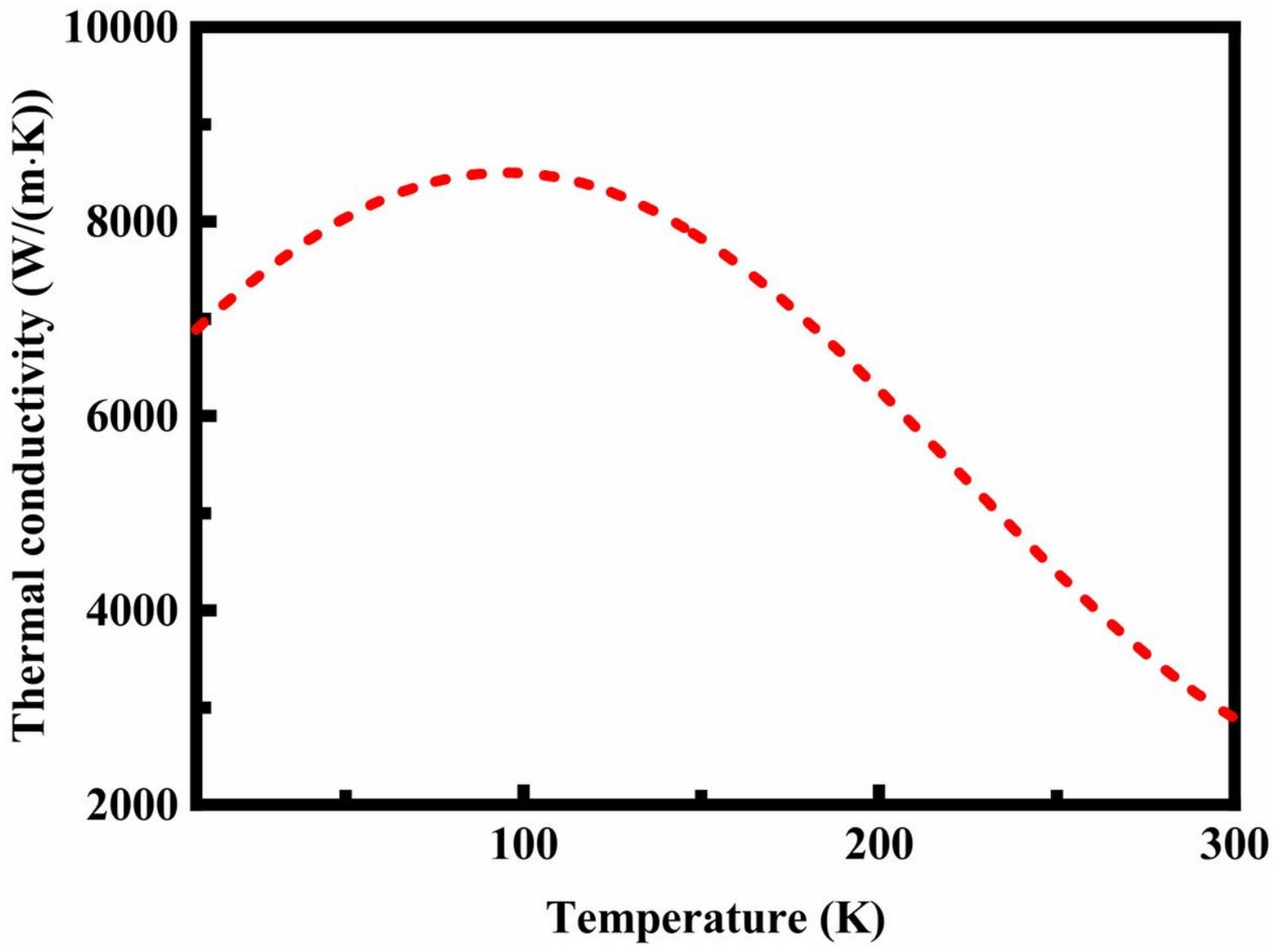


Figure 5

Thermal conductivity of single-walled carbon nanotubes at different temperatures. The temperature varies from 8 to 300 K.

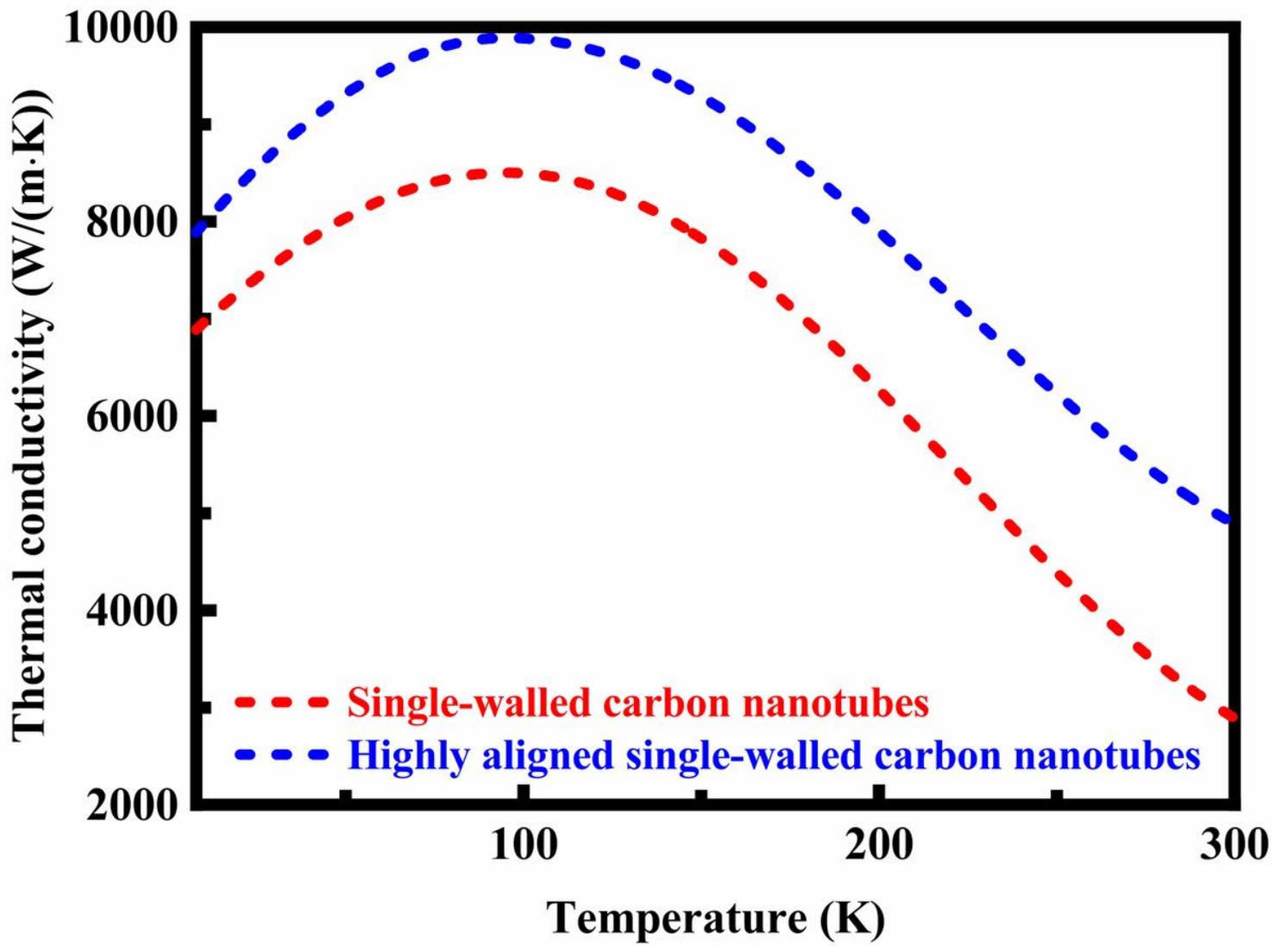


Figure 6

Effect of alignment on the thermal conductivity of single-walled carbon nanotubes at different temperatures. The temperature varies from 8 to 300 K.

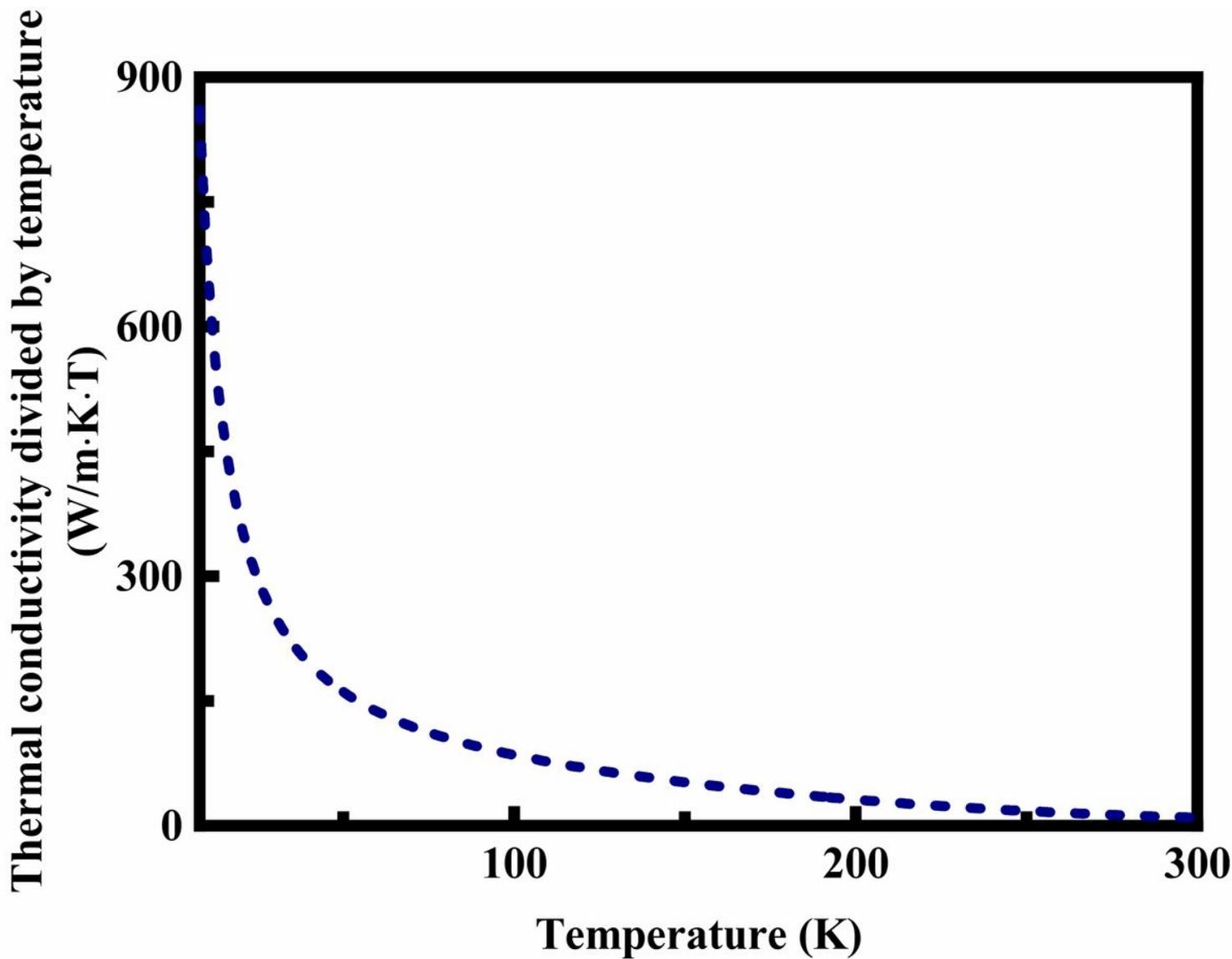


Figure 7

Thermal conductivity divided by temperature of single-walled carbon nanotubes at different temperatures. The temperature varies from 8 to 300 K.

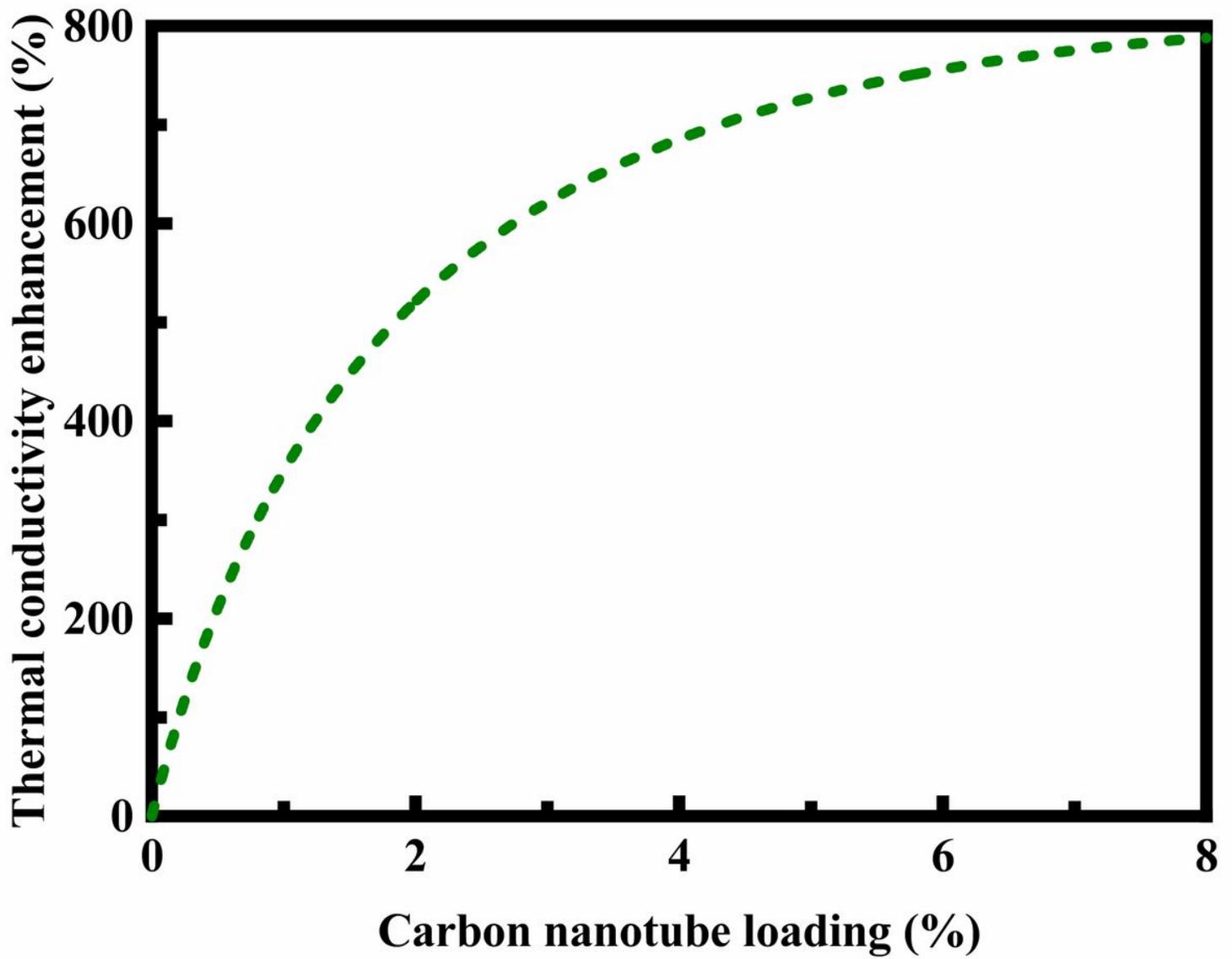


Figure 8

Thermal conductivity enhancement of single-walled carbon nanotube-based epoxy composites. The carbon nanotube loading varies from 0 to 0.08.