Modelling heat transfer of carbon nanotubes

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Abstract

Modelling heat transfer of carbon nanotubes is important for the thermal management of nanotube-based composites and nanoelectronic devices. By using a finite element method for three-dimensional anisotropic heat transfer, we have simulated the heat conduction and temperature variations of a single nanotube, a nanotube array and a part of a nanotube-based composite surface with heat generation. The thermal conductivity used is obtained from the upscaled value from the molecular simulations or experiments. Simulations show that nanotube arrays have unique cooling characteristics due to their anisotropic thermal conductivity.

1. Introduction

Carbon nanotubes (CNTs) have attracted worldwide attention in both research and industry since the discovery by Iijima in 1991 [17]. Extensive studies of this novel nanocomposite material suggests that it has many potential applications such as in nanomachines, nanoelectronic and nanomedicine due to its super-high stiffness, strength and resilience, and its exceptional electrical and thermal properties [6, 11–13, 18, 19, 25, 39]. It has become one of the hottest research topics in the important field of nanotechnology. There have been extensive studies on the properties of CNTs [1,2,15,27,34,38,40]. In addition, there have been important developments in the multi-scale computer simulation techniques to imbue the continuum-based models with more realistic details at quantum and atomistic scales [7]. There are many technical challenges such as the experimental studies of the mechanical, thermal and electronic properties of CNTs (e.g. [9,32,34]). Even though there have been extensive theoretical modelling studies in terms of atomistic, molecular dynamics (MD), quantum mechanics and continuum approach, many computational issues remain unsolved or unsatisfied. Among these important issues are the modelling of the nano-rheological behaviour and heat transfer of CNTs, the fluid flow inside a nanotube or interconnected nanotube networks.

The modelling of nanothermal processes such as heat transfer and thermal stress of CNTs has interesting challenges. The complexity of the nanotubes makes the analytical approach intractable, while the experimental measurement is very expensive and time-consuming. This
makes the computational modelling a better, quick and yet efficient alternative for studies and analysis of the structure of CNTs and nanocomposites [8, 22, 23, 26, 28, 30, 36]. Finite element analysis (FEA) has been quite successful in the modelling of macroscale phenomena such as heat transfer, engineering mechanics and fluid flow. However, special care should be taken before it can be applied to model the nanoscale structure. In recent years, there have been several interesting studies using the continuum mechanical method to study the microscale structure and mechanical properties (e.g. [1, 8, 22, 23, 26, 31]). However, there has been little progress in the modelling of heat transfer and thermal management of CNTs or nanotube-based composites.

This paper aims at the development of the FEA of the nanoscale heat transfer of CNTs. We first formulate the finite element method for three-dimensional heat transfer analysis of nanotubes. Then, we study the heat conduction and temperature variations of single-walled nanotubes, nanotube array and nanotube-based composites to simulate the thermal behaviour of such materials such as nano-electronic devices and nanoswitch, followed by a discussion and implication of the simulation results.

2. Finite element formulation

In the modelling of CNTs, molecular modelling is a discrete approach and the conventional finite element method is a continuum-based approach. FEA on nanoscales is different from both these approaches. In fact, it is the combination of these two approaches and the bridging of their gaps. The finite element method uses the most elaborate finite element method while its input materials properties are estimated from molecular-based modelling.

2.1. Scaling gaps

CNTs and nanocomposites have a length scale range from molecular to macroscopic scales. There are two conventional computational methods working on different scales. Molecular-based computational modelling tries to predict the mechanical and thermal properties using quantum mechanics and discrete \textit{ab initio} calculations [2, 4, 24, 28, 33], while macroscopic solid mechanics treats the media as a continuum using homogenized bulk material properties [1, 12, 41]. However, the intermediate nanoscale is just between these two extreme scales. A proper methodology is needed to bridge these two scales in the hierarchy.

Such important intermediate scaling of material properties have only started to emerge recently. Odegard \textit{et al} [26] proposed an instructive and interesting approach. Another promising method is the molecular mechanical modelling approach [22, 37]. These methods often use the molecular level phonon theories to derive the thermal conductivity [4].

2.2. Thermal conductivity

The thermal conductivity ($K$) for CNTs varies greatly and is highly anisotropic as the conductivity is much higher along the axis of the nanotube than in other directions. Although it is extremely difficult to obtain experimental measurements, there has been some important progress in the experimental studies of the thermal properties of CNTs [16, 32, 35]. Small \textit{et al} [35] discussed in detail the mesoscopic experimental measurements of phonon thermal transport and thermoelectronic phenomena in individual CNTs. They measured the temperature distributions in electrically heated individual multiwalled CNTs with a scanning thermal microscope and a microfabricated suspended device to obtain the thermal conductivity.
The bulk thermal conductivity is estimated to be in the range of 150–6000 W mK\(^{-1}\), and it varies with the temperature and size of the nanotubes [4,24,35]. However, there is a significant gap between experiment-derived values and theoretical predictions. Choi et al [5] used 2000 W mK\(^{-1}\) for thermal conductivity, and Kim et al [21] obtained a value of 3000 W mK\(^{-1}\) for the room temperature thermal conductivity of individual multiwalled nanotubes. Biercuk et al [3] demonstrated that samples loaded with 1 wt% unpurified single-walled CNTs showed a 70% increase in thermal conductivity at 40 K and 125% at room temperature. Small et al obtained that the ‘bulk’ thermal conductivity at room temperature is over 3000 W mK\(^{-1}\), while the earlier results suggested a lower value of 36 W mK\(^{-1}\) for the densely-packed single-walled CNT mat, and with the estimated bulk longitude thermal conductivity of a nanorope in the range of 1600–6000 W mK\(^{-1}\) [16,35]. In addition, there is also a large difference between single tube and bulk measurements and there is stronger temperature dependence in individual nanotubes than in the bulk measurements as clearly pointed out by Small et al [35]. Che et al theoretically predicted that the thermal conductivity along the tube axis approaches 2980 W mK\(^{-1}\) for (10,10) single-walled nanotubes for a tube length up to 40 nm with a thickness of 1 Å. They also predicted a value of 950 W mK\(^{-1}\) for nanotube bundles along the tube axis and a much lower thermal conductivity of 5.6 W mK\(^{-1}\) in the direction perpendicular to the tube, and this value is comparable to the graphite out-of-plane thermal conductivity of 5.5 W mK\(^{-1}\) [4]. Similarly, the mechanical properties are also unusually unique with a very high Young’s modulus 1000–3700 GPa and Poisson’s ratio of 0.18–0.3 [9,15,20,34,36,38]. In fact, the thermal conductivity of nanotubes is highly anisotropic with the value along the tube axis usually two orders of magnitude higher than the perpendicular to the tube. Thus, the aligned nanotubes, nanoropes and bundles are also highly anisotropic.

The highly anisotropic properties in thermal conductivity and the large difference between single-tube and bulk measurements suggest that more extensive studies are needed. From the point of view of FEA, the formulation will be especially taken care of so that the method will be able to analyse the anisotropic characteristics in heat transfer of nanotubes. For the continuum-based finite element method there have been many ways to ensure this capability. However, for the FEA on the nanoscale, some modifications and a special choice of element types should be investigated. In the rest of the section, we will formulate the essential implementation of the FEA for the modelling heat transfer of CNTs.

2.3. Continuum-based finite element formulation

Once the parameters of thermal properties are estimated or upscaled from the molecular simulations or \textit{ab initio} simulations, an equivalent continuum-based finite element formulation can be used. The main procedure is the same as the conventional finite element procedure, and many finite element algorithms and element types can be similarly constructed. However, the continuum-based finite element method only works from the scale of one micron to very large scales [41]. For smaller scales, the continuum-based representative volume does not work on the atomistic scale. There are two ways to overcome this difficulty. One way is to use the discrete molecular–mechanical simulations based on quantum mechanics, and this may lead to very large numbers of computations [8,22,29]. The other is to use the discrete-based modelling to upscale the continuum-equivalent material properties such as thermal conductivity. Then, the normal procedure of FEA can be used.

For the FEA of nanoscale heat transfer of CNTs, two natural models for element types are: the truss model and the hexagon model. The truss model is very popular in solid mechanics for the analysis of engineering structures. Odegard et al [26] use a truss model to simulate the mechanical behaviour of the nano-structured systems in terms of the displacement of the atoms
and the total molecular potential energy. The hexagon model will be studied in more detail in this paper. The beam and truss models are based on the one-dimensional line model, and thus it is unlikely to give accurate results for three-dimensional structures, especially since the geometry is more complex. The anisotropic feature of the heat conduction of CNTs requires the full three-dimensional formulation of the heat transfer equation, and proper initial and boundary conditions will be implemented.

In the rest of this paper, we will formulate a full three-dimensional finite element method and use the hexagon element with six nodes being the atoms of the basic carbon structure. We will then simulate the heat transfer of CNTs and compare different methods for the same configuration so as to find a better and suitable method for the finite element method.

The governing equation of three-dimensional heat conduction can be written as

\[ \rho c_p \frac{\partial T}{\partial t} = \nabla \cdot \left( K \nabla T \right) + Q(t, T), \tag{1} \]

where \( K_x, K_y, K_z \) are the principal thermal conductivities and \( \rho \) and \( c_p \) are density and specific heat capacity, respectively. \( Q \) is the rate of heat generation, and \( f(t, T) \) is the source term which is a known function of time \( t \) and temperature \( T \).

For an ambient temperature \( T_\infty \) and the typical temperature \( T_\ast \) of the system, any temperature can be written as \( T = T_\infty + \Theta \Delta T \). The temperature variation is very small \( \Delta T = T_\ast - T_\infty \ll T_\infty \), and typically \( \Delta T \) is the order of 1 K. Equivalently, we can define a dimensionless temperature

\[ \Theta = \frac{T - T_\infty}{T_\ast - T_\infty} \tag{2} \]

For the ambient room temperature \( T_\infty = 300 \text{ K} \) and the typical temperature \( T_\ast = T_\infty + 1 = 301 \text{ K} \) of interest, we have \( \Theta = 1 \) when \( T = 301 \text{ K} \), and \( \Theta = 0 \) when \( T = 300 \text{ K} \). In fact, we can choose any temperature \( T_\ast \) of interest so that the dimensionless temperature difference is \( O(1) \).

By choosing the typical length \( L \), thermal conductivity \( K_0 = 2500 \text{ W m}^{-1} \text{ K}^{-1} \) and time scale \( \tau \sim L^2 \rho c_p / K_0 \), the governing equation in the dimensionless form becomes

\[ \frac{\partial \Theta}{\partial \tau} = \nabla \cdot \left( \kappa \nabla \Theta \right) + \lambda f(t, \Theta), \tag{3} \]

where \( \lambda = QL^2 / K_0(T_\ast - T_\infty) \) and \( \kappa = K_{ij} / K_0 \) is a \( 3 \times 3 \) matrix depending on the anisotropic thermal conductivity. If there is no heat generation, then \( Q = 0 \) or \( \lambda = 0 \). For a uniform time-independent heat source, \( f(t, \Theta) = 1 \).

Substituting \( \Theta = \sum_{j=1}^{N} u_j(t)N_j(x, y) \) into the above equation and after some elaborate calculations, the finite element formulation usually leads to a generic form

\[ M \dot{u} + Ku = F \tag{4} \]

and

\[ u = [u_1 v_1 u_2 v_2 \ldots u_n v_n] \tag{5} \]

where \( M = \int_{\Omega} N_i N_j \text{ d}\Omega \), \( K \) are the coefficient matrix and the stiffness matrix, respectively. \( F_i = \int_{\Omega} \lambda N_i f \text{ d}\Omega + \int_{\Gamma} q \text{ d}\Gamma \) is the contribution of the heat source and boundary conditions.

### 3. Simulations and results

Using the finite element method formulated in the above section, we can simulate some typical characteristics concerning the heat transfer of CNTs. We first study the heat conduction of a
single nanotube, and then investigate the heat conduction of an array of parallel nanotubes and the temperature variations of a nanodevice with heat generation.

CNTs are of three major types: armchair tubes (e.g. \((n, n)\)), chiral tubes (e.g. \((8, 2)\)) and zigzag tubes such as \((n, 0)\) [11,36]. We shall focus on one type of the nanotube such as zigzag. For other types such as chiral or armchair, the methodology used is the same. Once the detailed configuration of the nanotubes is known, the finite element nodes and elements are essentially the same. In all the following simulations, we assume all the carbon bonds are equal in length, 1.42 Å with equal angles 120°. The bulk thermal conductivity \(K_0 = 2500 \text{ W mK}^{-1}\) and the ratio of transverse to longitude thermal conductivity \(\gamma = 0.01\). Thus, the thermal conductivity matrix \(\kappa = \text{diag}(1, 1, \gamma)\). The radius \(R\) of the CNT is 1–1.5 nm (normalized in the dimensional form as 1), while the length is 20 nm (normalized as 1), and the thickness of the single-walled CNT is taken to be 0.34 nm [30, 36].

In the finite element simulations, we use two major element types: hexagonal element and beam element. The 6-noded hexagon element has the same structure as the basic carbon structure (see figure 1). We shall present the results using these two element types and a comparison will be made whenever relevant.

3.1. Heat conduction of a nanotube

Nanoelectromechanical devices such as nanoswitches may have many potential applications in nanomedicine and nanoelectronics [10,35]. The thermal behaviour of a nanodevice and its heat management is of great interest and has practical applications. For a single nanotube with a radius of 1 nm and a length of 20 nm, by fixing the temperature \(\Theta = 1\) or \(T_0 = 301\) K at one end and a radiation boundary at the other with the ambient temperature \(T_\infty = 300\) K, then heat conduction of the nanotube is computed. The left figure in figure 2 shows the dimensionless temperature distribution at time \(t = 10\). For the same CNT, if we fix the temperature at one contact line as \(\Theta = 1\), then transverse heat conduction leads to the temperature distribution shown on the right in the figure 2. We can see that temperature decreases more quickly along the tube axis than that in the transverse direction, and this is because of the anisotropic thermal conductivity of the nanotube.

For the practical purpose of modelling CNTs, the hexagonal elements and the truss element give essentially the same results. Thus, the choice of element types is for the convenience of computation and programming. However, when the structure is not thin, the full three-dimensional finite element method will be used, and the hexagonal element generally works better.
3.2. Nanotube array

The simulation of an array of parallel CNTs is of more practical interest due to the experimental development of CNT fabrication and the amorphous carbon deposition [14]. This makes it more relevant to the nanoscale device. The heat transfer process on this scale is also important. For an array of parallelled nanotubes with a radius of 1 nm and a spacing of 2.6 nm, the base stays at a fixed temperature. The heat conduction of a nanotube array is shown figure 3 where the fixed base temperature \( \Theta = 1 \) or \( T_0 = 301 \text{ K} \), and the ambient room temperature \( T_\infty = 300 \text{ K} \) are used. The normalized temperature distribution is shown in colour calculated using the hexagon elements. The temperature decreases more quickly along the direction of the axis of the nanotubes while the transverse temperature variation along the amorphous base is relatively small. This suggests that an array of CNTs can serve as a good cooling device or that the nanotube array-based nanodevice may have very good heat dissipation properties.

3.3. Nanotube-based composite surface with heat generation

Nanotube-based composites are very promising due to their very unique mechanical, thermal and nanoelectronic properties. In practice, most nanoelectronic devices will meet the problem of heat management due to the energy dissipation, heat generation and thermal transport. For a representative volume of such composites, the continuum-based simulation can focus on a regular array of nanotubes parallel to each other. For the CNT array discussed earlier, we embedded them onto a composite surface and added the heat generation in the system. Figure 4 shows the two cross-sections of three-dimensional finite element results for a representative volume with three CNTs embedded onto a composite surface. The composite matrix is assumed to be isotropic and its thermal conductivity is taken as 500 W mK\(^{-1}\). The initial temperature is \( T_0 = 300.5 \text{ K} \) with a uniform heat generation rate \( \lambda = 0.2 \). The ambient temperature is \( T_\infty = 300 \text{ K} \).
Figure 3. Temperature distribution of a nanotube array at $t = 10$. The temperature decreases more quickly along the direction of the axis of the nanotubes.

The simulation of this configuration is different from that in figure 3 in that the present simulation uses the continuum-based tetrahedrons and thus the temperature distribution of the nanotubes is smoothly averaged, while the distribution in figure 3 is based on hexagonal elements with the nodes being the same as the atoms. Due to the large number of atoms involved in the composites, the hexagonal elements are no longer practical and very time-consuming. The best choice for composites is the tetrahedron elements. We can see from figure 4 that the temperature variations are much bigger along the nanotubes than in the transverse direction. This is because the thermal conductivity is much higher along the tube axis than in the other directions. This interesting characteristic of heat transfer may imply that the properly aligned nanotubes can have a better cooling mechanism and thus better heat management properties. This may also imply that these composites can be a better choice for nanoelectronic circuits and other nanomechanical devices. From the above simulations, we see that CNTs have anisotropic heat conduction properties. The thermal conductivity is quite high compared with the usual materials.

4. Conclusions

We have formulated a finite element method to simulate the nanoscale heat transfer of a CNT and nanotube array. This method is based on the three-dimensional continuum-mechanical approach by using material parameters upscaled from the molecular simulations. The conventional finite element method usually works from the micron-scale up to a very large scale. As it reduces to atomic scales, the continuum approach needs special modifications. These include the upsampling and continuum-equivalent homogenization of material properties such as thermal conductivity. For a CNT with a radius of 1–1.5 nm, thermal conductivity of
Figure 4. Temperature variation relative to the initial temperature $T_0 = 300.5 \, \text{K}$ at $t = 10$. Heat is generated at a constant rate $\dot{\lambda} = 0.2$ and the temperature variations are bigger along the nanotubes than in the transverse direction.

2500 W mK$^{-1}$ and a ratio of 0.01 (perpendicular thermal conductivity to axial conductivity), the heat conduction and temperature variations with heat generation have been investigated under possible conditions such as a nanomechanical device. From the natural structure of the CNTs, we have used two major element types: the hexagonal elements and beam elements in the simulations. The comparison of the hexagonal elements and beam elements shows that for thin structures they give essentially the same results.

In our simulations, we assume the nanotubes are regular cylindrical shapes with a uniform thickness. In real nanotubes, caps are an important part of a CNT, thus the effect of the cap may not be negligible. In principle, we can use the the present method to simulate its effect. In addition, the multi-walled nanotubes and nanotube-based composites need more extensive studies concerning their thermal behaviour and how their nanothermal behaviours differ from the single-walled nanotubes. These will become the computational modelling issues for further research.

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