Chapter 30
A Hierarchical Modeling Approach of Thermal Vias Using CNT-Based Composites

Jörg Hertwig, Holger Neubert and Jens Lienig

30.1 Introduction

The continuous down-scaling of electronic systems into the nano-scale era enforces a multitude of new design challenges. Thermal management is one of the most crucial issues that must be addressed when designing electronic systems with high-density nano-scale structures. Heat is an undesired byproduct which accrues in electrical devices and wires with negative impact on functionality and reliability. The increasing circuit-integration density and related down-scaling of circuit structures results in a higher power density per area or volume respectively. Thermal management becomes more important and thus heat dissipation has to be addressed during physical design of electronic circuits. It requires heat dissipating structures that transport thermal energy from a heat source, such as an electronic device, to a heat sink, such as a cooling fluid.

One bottleneck of heat dissipation in electronic circuits is the passage through the interconnect layers. Common substrates have a low thermal conductivity in the range of $0.2 \ldots 0.5\,\mathrm{W/(m \cdot K)}$ (organic substrate) or $1 \ldots 100\,\mathrm{W/(m \cdot K)}$ (ceramic substrate materials) respectively. Furthermore, the heat dissipation is affected by anisotropic heat conduction of the structure. Due to increased thermal conductivity of in-plane electrical conductors, the in-plane heat conduction is about tenfold better than the vertical conduction through the layer.

An established technology for heat conduction through substrates are *thermal vias*. Essentially, they act as a pipe to diffusively transport the heat from a higher temperature region, such as a cluster of devices within the circuit, through layers of low thermal conductivity (Fig. 30.1). Based on a significant greater thermal conductivity than the substrate or layer conductivity, these plated-through holes improve the vertical through-layer heat transport dramatically.

J. Hertwig · H. Neubert (✉) · J. Lienig
Institute of Electromechanical and Electronic Design, www.ifte.de,
Technische Universität Dresden, 01062 Dresden, Germany

G. Gerlach and K.-J. Wolter (eds.), *Bio and Nano Packaging Techniques for Electron Devices*, DOI: 10.1007/978-3-642-28522-6_30,

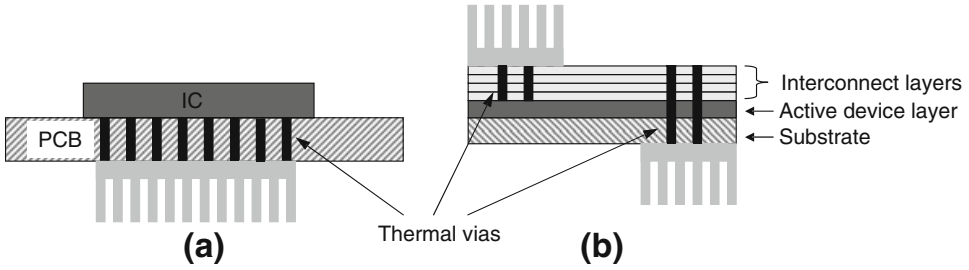

Fig. 30.1 Thermal vias integrated in **a** the substrate of a printed circuit board (PCB) and **b** in the interconnect layers of a bare integrated circuit

While the thermal conductivity of these vias has been sufficient for many applications so far, new nano-scale circuits with their higher heat density require better heat dissipation mechanisms. Furthermore, the continuous down-scaling of circuit structures is reducing the area provided for thermal vias, thus exacerbating this need.

Carbon nano tubes (CNTs) have recently been gaining attention due to their special characteristics. One of them is excellent heat conductivity which exceeds that of metallic materials (such as copper) by approximately an order of magnitude.

This chapter discusses the potential of improving thermal vias by using CNT-based composite materials. Specifically, a new hierarchical modeling approach is presented that allows an evaluation of the thermal behavior of various technological configurations. In this chapter, we refer to thermal vias using CNT-based composites as *CNT-based thermal vias*.

30.2 Thermal Management Using Nano Materials

In general, heat is emitted in active and passive components as well as in interconnect structures. The dissipation of heat by transferring it to a heat sink, such as a cooling device or a cooling fluid, is one of the most difficult tasks in electronic systems design. A *thermal path* describes the structural flow of heat. Based on a thermal model of an electronic device with different system levels, different thermal paths can be appointed. A thermal path is characterized by the total *thermal resistance* across the electronic device, from a source to a heat sink:

$$R_{th} = \frac{\Delta T}{P}, \tag{30.1}$$

which describes dissipation of the thermal power P due to the temperature difference ΔT. In solid state, as of interest here, heat dissipation is described by the heat diffusion equation:

$$c_p\, \rho\, \frac{\partial T}{\partial t} - \nabla \cdot k\, \nabla T = q. \tag{30.2}$$

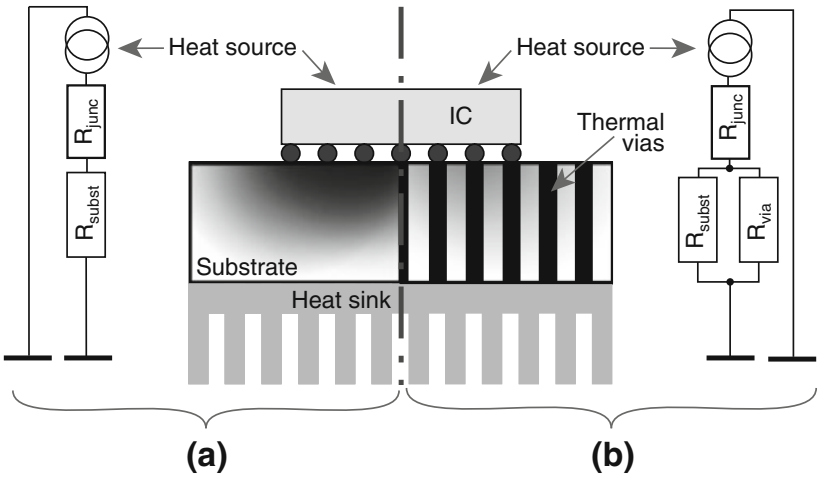

Fig. 30.2 Thermal paths and thermal-resistance network models for different system levels, **a** without and **b** with thermal vias. R_{subst}, R_{junc} and R_{via} are the thermal resistances of substrate, junction and vias, respectively

The constant k describes the specific thermal conductivity, c_p the specific heat, ρ the density of the solid, T the temperature field and q the heat-source density per volume. For the static thermal resistance of a planar solid, (30.1) can be specified using (30.2):

$$R_{th} = \frac{L}{k \cdot A} \tag{30.3}$$

with the length L and the constant cross section A of the thermal path across the solid.

30.2.1 Thermal Vias

An established technology to overcome the aforementioned bottleneck of heat transfer through substrates or interconnect layers are thermal vias. A via (Vertical Interconnect Access) is an interlayer connection. While vias are typically used to realize electrical connections between layers, thermal vias do not have an electrical function. Their sole purpose is to improve (vertical) interlayer heat transport, e.g. in integrated circuits and printed circuits boards (Fig. 30.2).

In general, copper is used for thermal vias in printed circuit boards because it is widely used in many process steps and is an inexpensive material with high thermal conductivity.

The application of thermal vias in real-world electronic circuits faces a multitude of problems. One of them is limited thermal conductivity due to both materials used and cross-section area limitations. Furthermore, thermal vias require large keep-out spaces, so their usage should be minimized. As a result, suitable placement

algorithms are required for placing thermal vias in areas where they are needed most [16]. Additionally, the efficiency of the thermal conductivity of vias themselves has to be improved in order to minimize the number of required thermal vias. These issues are expected to become more and more prominent with increased application of 3D integration technologies combined with further downscaling to nano-scale circuits. Hence, future applications require smaller thermal vias with a lower thermal resistance. According to (30.3), there exist three options to decrease the thermal resistance of single thermal vias:

1. downsizing the path length which is generally determined by the substrate or interconnect layer thickness,
2. enlargement of the available thermal conduction area, and
3. enhancement of the thermal conductivity along the thermal path.

Decreasing the substrate or layer thickness is limited because of mechanical stability considerations and the required number of layers. Due to already limited wiring space, the enlargement of thermal-via sites is difficult to realize. The most promising option is the enhancement of thermal conductivity along the thermal path by using thermal vias with thermally high-conductive materials. As described in the next section, composites in which carbon nano tubes are mixed are a promising option for such materials with high thermal conductivity.

30.2.2 CNT-Based Composite Materials

A *composite* is a material compound containing two or more constituent materials with different physical and chemical characteristics. Composites are usually engineered to achieve particular characteristics. In this chapter, composites containing *carbon nano tubes* are investigated.

CNTs are cylindrical, nanoscopic structures of carbon, comparable to a rolled-up monomolecular graphite layer sheet, forming a tube. Theoretically, their thermal conductivity can reach $6000\,\mathrm{W/(m \cdot K)}$, while measured values range from 2000 to $3000\,\mathrm{W/(m \cdot K)}$ [20]. These values, which are approximately ten times higher compared to metals, characterize CNTs as the best available heat conductors. Furthermore, due to the absence of electromigration, using CNTs as electrical vias has also become an interesting application [43].

Different types of CNTs are characterized by their *roll angle* or *chirality*. In general, the chirality is denoted as a pair of indices (n, m) (Fig. 30.3a). Depending on the chirality, CNTs can be distinguished in three classes: (i) armchair (n, n), (ii) zig-zag $(n, 0)$, and (iii) chiral (n, m), as illustrated in Fig. 30.3b. Furthermore, nanotubes are categorized into single-walled (SWNTs) and multi-walled nano tubes (MWNTs).

In previous investigations of CNT-based composites for thermal applications, CNTs are (mostly disorderly) mixed into a composite in order to enhance its thermal conductivity. The most commonly used structural-matrix material for CNT-based

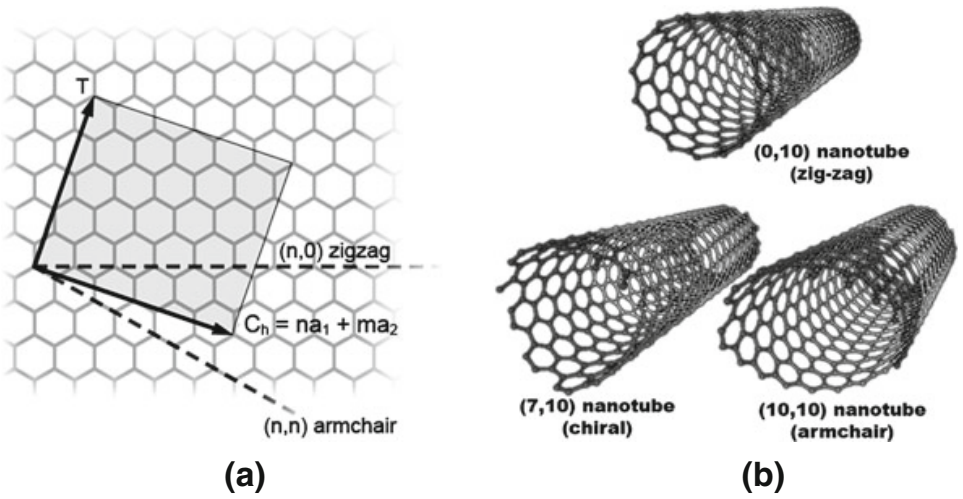

Fig. 30.3 Naming scheme for CNTs represented by **a** the unit vectors of a graphite monolayer and **b** different chiralities of CNTs [54]

composites is epoxy. Typically, CNTs occupy a volume fraction equivalent to 1 . . . 10 mass-% of the composite. This increases thermal conductivity of the CNT-based composite by a factor of up to 3.6, compared to unfilled matrix material [17, 21, 69]. Other polymers and metals (e.g., copper and aluminum) have also been investigated for their applicability as matrix material for thermal interfaces, leading to similar results [9, 51].

Disordered mixing of CNTs in matrices results in only poor improvement of thermal conductivity. This is understandable since the heat conduction in a CNT primarily occurs in axial direction. In order to exploit the full potential of their thermal conductivity, CNTs must be aligned. The following options of CNT alignment are known:

- fluidic alignment using straight channels to arrange multiple CNTs [23],
- alignment along an electric field by dielectrophoresis [14, 21, 31, 32, 35, 52],
- directional growth of CNTs on a catalyzer [2, 4, 38, 57],
- spin assembly process [22], and
- manual placing of single CNTs on a functionalized surface [3, 49].

While these approaches allow the alignment of a small number of CNTs, their application within composites is still a challenge. Furthermore, CNT alignment results in an anisotropic thermal behavior.

Exploiting the full thermal potential of embedded CNTs requires detailed studies on the mechanical bonding to the material adjacent to the composite. Several options to realize bonding to a material with low thermal boundary resistance are:

- soldering the contact with metallic solder [7],
- contacting with functionalized groups [6, 61],
- galvanic bonding of the CNTs [21], or
- mechanical connection of the CNTs [14, 39].

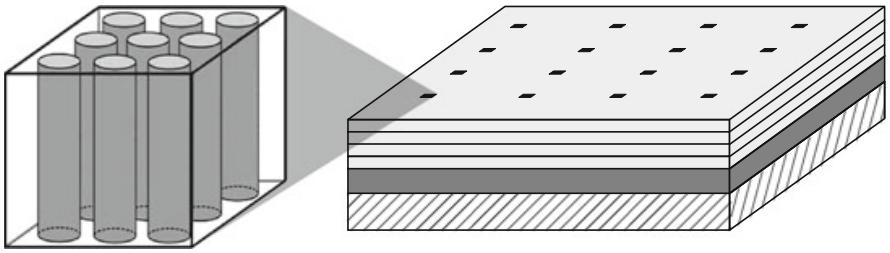

Fig. 30.4 Thermal via arrays in an integrated circuit

While contacting CNTs at the surface of the composite lowers the thermal boundary resistance, direct CNT-to-CNT contacts within the composite disrupt the phonon transport along the CNTs and increase the thermal resistivity of the composite [13]. Since CNTs tend to agglomerate, smart CNT alignment has to avoid direct CNT-to-CNT contacts in composites. This is still a major challenge in up-to-date composite applications [55].

30.3 Thermal Modeling

Due to the complex behavior of CNTs in composites, the effectiveness of practical approaches can only be determined in numerous experimental investigations. This also applies to future CNT-based thermal via applications. Hence, a modeling approach is required in order to predict the thermal system behavior. Its goal is to reduce the uncertainty of practical solutions with regard to their applicability as effective heat-dissipation solutions.

It is obvious that the level of modeling has to be adapted in order to account for relevant characteristics, which are varying from nanoscopic up to macroscopic range. Models for thermal behavior of via arrays must be valid in both the nanometer and the millimeter range. Therefore, hierarchical models are required to properly adjust and limit the degrees of freedom.

30.3.1 Hierarchical Models of CNT-Based Thermal Via Arrays

Due to the pressing thermal-dissipation problem of ICs and PCBs, the placement of via arrays rather than single vias has been gaining importance during the last years. Here, specific areas within the circuit are designated as potential via sites (Fig. 30.4). The density of thermal vias within these sites can be determined accordingly to thermal requirements. Another advantage of this approach is the large granularity for the thermal analysis, significantly reducing computational efforts.

In order to obtain the characteristics of an array containing several thermal vias, a bottom-up modeling approach is required. It comprises the calculation of thermal

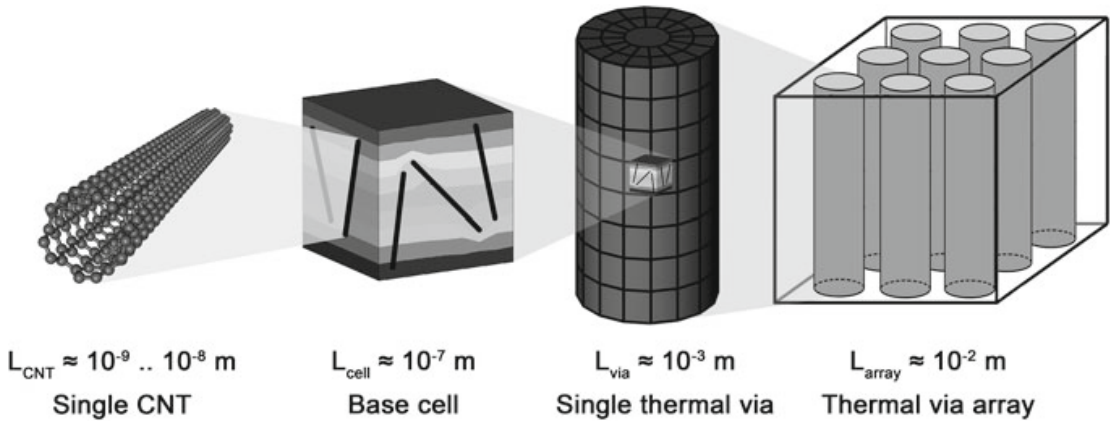

Fig. 30.5 Hierarchical model structure of a CNT-based thermal-via array

characteristics of single CNTs and the application of their characteristics in a base cell model of the composite, containing a specific number of CNTs. Next, a model of a thermal via or a thermal-via array respectively is created while accounting for the thermal properties of the base cell. The dimensions of the base cell must be chosen such that modeling the cell minimizes the overall degrees of freedom. Furthermore, local inhomogeneous allocations of CNTs must be considered. Figure 30.5 illustrates a hierarchical model structure that spans from a single CNT to a thermal via array consisting of numerous thermal vias.

The basic problem of modeling interdependencies between CNTs and materials has to be addressed on the level of both a single CNT and the base cell. Modeling higher system levels should use base cell properties. However, to enable CNT-based models, the following considerations must also be taken into account:

- anisotropic heat conduction,
- thermal conductivity depending on physical conditions, e.g. temperature, geometry, alignment, and
- locally inhomogeneous distribution of CNTs.

30.3.2 Thermal Model of Single CNTs

Due to the large aspect ratio, the geometry of CNTs can be considered one-dimensional. Diameters are nearly as large as the mean free path of phonons. Therefore, their thermal behavior is very anisotropic, as illustrated in Table 30.1. Heat dissipation perpendicular to the CNT axis can be neglected.

Considering only stationary processes, the thermal resistance of a CNT transporting heat along its axis may be expressed by a parameter Λ and the length L_{CNT} of the CNT according to (30.4).

$$R_{th-CNT} = \frac{L_{CNT}}{\Lambda} \tag{30.4}$$

Table 30.1 Thermal conductivity of different occurrences of CNTs [60]

Occurrence	Thermal conductivity in $W/(m \cdot K)$
Parallel alignment of single SWNT (10, 10)	2980
Aligned bundled nanotubes	950
Perpendicular alignment of a single CNT	5.6

Hence, in spatial models (e.g., with spatial discretization), CNTs can be represented by a *line element* with a thermal conductivity Λ. This approach is based on (30.2), which solely represents energy conservation using thermal conductivity to describe stationary heat transfer in solids. The parameter Λ, which represents the thermal resistance of a CNT, is not constant since it dependents on different CNT properties. Strictly speaking, Fourier's law is invalid at nanoscale dimensions. If phenomenological aspects only have to be modeled and the physics of heat dissipation is not of primary interest, as it is here, such an approach may be adequate.

The influence of relevant CNT properties must be determined in order to predict the thermal resistance of a CNT. Here, experimental results or molecular dynamics simulation (MD) can be used. One benefit provided by MD is that the properties of CNTs can be calculated based on their structural qualities and consideration of interface effects.

Unfortunately, the experimental as well as the MD approach, are complex. Due to a large number of structural parameters and the practical issues preparing appropriate samples, experimental results are hard to obtain. In contrast, MD is computationally expensive and thus inapplicable to complex problems with a large number of CNTs.

Several characteristics influence the thermal conductivity of CNTs and must be considered while using parameter Λ within a CNT line-element model. They are described next in detail. It should be noted that diameter and length of CNTs and the temperature have a major impact on thermal conductivity. Other structural properties, such as chirality and isotope impurities, are less relevant.

Chirality. Relating to CNTs, the *chirality* describes at which angle the carbon layers are rolled up (Sect. 30.2.2). Most studies have reported an impact of the chirality on the specific thermal conductivity; determined values consider scattering. While some studies report higher conductivity of armchair-CNTs compared to CNTs in the zigzag-configuration [65], others report a lower conductivity [37, 70]. Chiral CNTs have a lower thermal conductivity than the mentioned armchair-CNTs [70]. The impact of the chirality on the thermal conductivity is illustrated in Table 30.2 according to [65] and [70]. It appears that the influence of this effect is in general low compared to the influence of length or temperature [1, 37, 65]. At low temperatures (close to 0 K), the chirality has no impact on the thermal conductivity [59].

Diameter. CNTs are characterized by different diameters, depending on their chirality. Disparities of thermal conductivity values provided in Table 30.2 are also based on different radii of the CNTs. The impact of the diameter on thermal properties

Table 30.2 Thermal conductivity values for different chiralities

Chirality	(9, 0) zigzag	(10, 0) zigzag	(5, 5) armchair	(20, 0) zigzag	(11, 11) armchair	(10, 10) armchair	(10, 13) chiral
$\Lambda(\mathrm{W}/(\mathrm{m}\cdot\mathrm{K}))$	880	770	960	7800	3600	2200	1200
Source	[65]	[65]	[65]	[70]	[70]	[70]	[70]

strongly depends on the length of CNTs. For short CNTs, heat transport is ballistic and the influence of the diameter is negligible. The longer the CNT, the lower the coherence of phonons and the heat transfer becomes more and more diffusive. Hence, the impact of the diameter on the thermal properties increases. For very long CNTs, the thermal conductivity reaches its maximum at small diameters (non-linear phonon collision decreases with smaller growing diameter) [45, 53, 65]. At low temperatures (close to 0 K), the diameter (similar to the chirality) has no impact on the thermal conductivity [59].

Length. The thermal conductivity of a CNT directly depends on its length. This effect is well investigated and appears to be consistent for different studies [1, 28, 40, 44–46, 65]. These studies provide a similar heat conductivity of approximately 350 $\mathrm{W}/(\mathrm{m}\cdot\mathrm{K})$ for a (5.5) SWNT with a length of 100 nm. In principle, longer CNTs have a higher thermal conductivity.

Isotope impurities. An *isotope* is a nuclide with a constant number of protons, but the number of neutrons varies for different isotopes. For example, common carbon is composed of 98.9% ^{12}C atoms and of 1.1% ^{13}C atoms. Such impurities may influence many physical properties, such as thermal, elastic or oscillation states. They can also reduce thermal conductivity to 60% (Fig. 30.6). CNTs which consist of either ^{12}C atoms or ^{13}C atoms provide the highest thermal conductivity [29].

Temperature. The temperature is not a structural property of a CNT, but has major impact on their thermal conductivity. The conductivity increases with rising temperature until a peak is reached (at approx. 500 K). With further rising temperature, conductivity decreases again (Fig. 30.7). The peak depends on the diameter of the CNT. As with chirality, reported simulation results vary for different studies [26].

30.3.3 Thermal Model of CNT-Based Composites

The correlation between the design of CNT-based composites, the structural properties of the composite (such as volume fraction, CNT alignment and local inhomogeneities of the CNT concentration), and the resulting thermal behavior and other properties has not been completely understood yet.

Today, CNTs are only available as as conglomerate of different CNT types, with varying chiralities, diameters and lengths. Therefore, their properties have to be

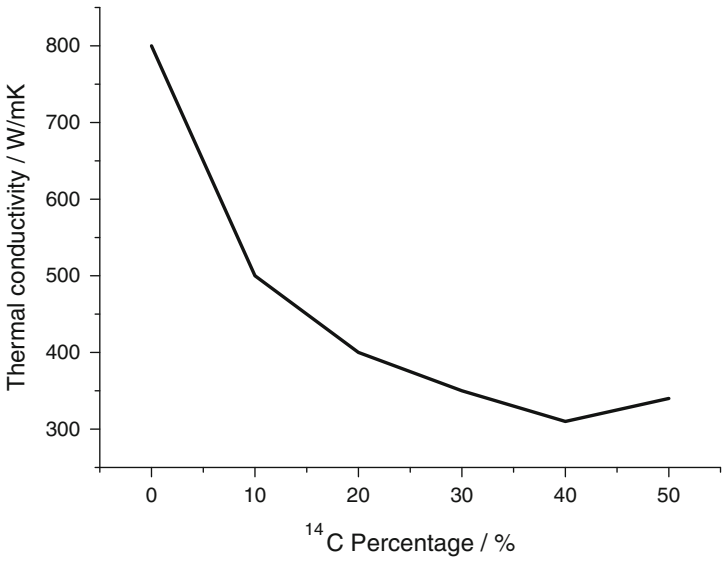

Fig. 30.6 Impact of isotope impurities of ^{14}C on thermal conductivity [65]

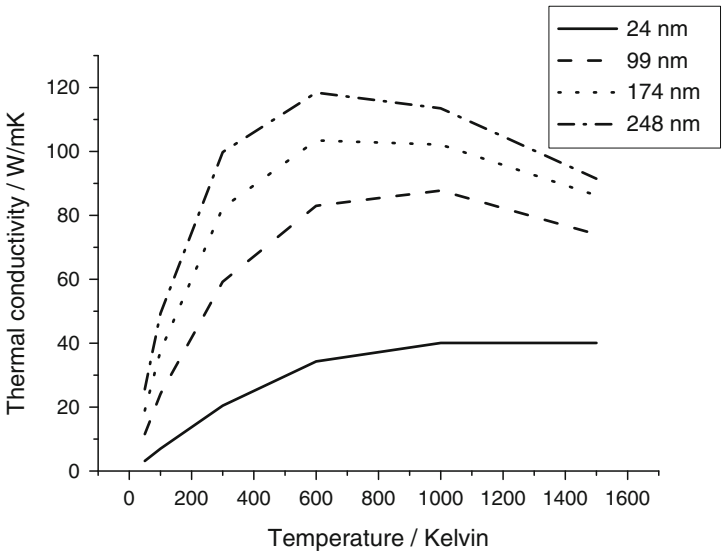

Fig. 30.7 Impact of temperature on thermal conductivity for different CNT lengths [56]

described in terms of distribution functions, increasing modeling complexity. The thermal properties cannot be calculated by using molecular dynamics simulations since this method is computationally intensive and hence inapplicable for tasks with a large number of CNTs. Thus, other simulation methods must be used to determine the thermal properties of the CNT-based composites.

In the literature, various modeling approaches for CNT-based composites have been reported. In most cases, the *effective medium approach (EMA)* is applied. Studies differ in simplifications while modeling CNTs embedded in matrix materials, the dimensionality of the problems to be solved, and the problem-solving methods. Several simple CNT models are used, such as *prolate spheroidal inclusions* [5], *tubes* [48, 60], *prismatic beams* [41, 50] or *rigid lines* [36]. Two-dimensional [36] or three-dimensional [41, 48, 60] base-cell units are created. In order to solve the equation system used to model the composite, different methods are applied, such

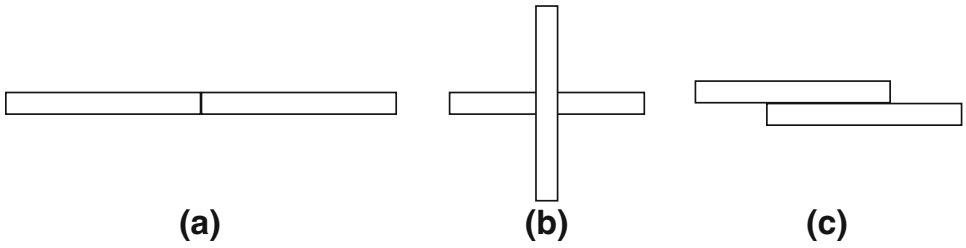

Fig. 30.8 Contact arrangements of single CNTs. **a** CNTs contacted on front surfaces. Shell surface of two CNTs are contacted either in **b** one point or **c** at a limited surface for parallel CNTs

as the *boundary element method (BEM)* [25], *boundary integral equations* [36], *finite element method (FEM)* [48, 60], *element-free Galerkin method* [47], *dissipative particle dynamics (DPD)* [27], or the equations are solved analytically [33, 34, 58]. Stochastic distribution of the embedded CNTs in a random unit cell is reported in [41]. The authors of [63] give a comprehensive review on multi-scale modeling and simulation of polymer composites.

All these studies consider only particular parameters of CNTs and/or CNTs in composites. Furthermore, only structures in the scale of the CNTs are taken into account, which renders these models inapplicable for much larger thermal vias.

A reasonable modeling approach should use a EMA based on structured base cells or should control volume to derive phenomenological thermal properties of the composite material. In such a base-cell model, the following effects have to be accounted for:

- heat transport in embedded CNTs,
- impact of mutual interactions of CNT-to-CNT contacts on heat transport within the composite,
- heat transport in plain matrix material, and
- interfacial heat transport between CNT and matrix material.

The heat transfer within CNTs embedded in matrix material can be modeled by a line element or other adequate approaches, as described in Sect. 30.3.2. The heat transport in the plain matrix material is described by the heat diffusion (30.2).

Mutual interactions at contacts between single CNTs might occur for multiple CNTs within a composite or if a CNT bundle is used. Different cases of contact arrangements can be distinguished (Fig. 30.8). A study has shown that case (a) rarely occurs [11]. It should also be noted that this contact arrangement (two front surfaces in contact) results in negligible impact on the heat conduction. However, a contact of CNT shells, as illustrated in cases (b) and (c), can reduce the thermal conductivity of both CNTs due to lattice vibrations [60]. This effect must be accounted for in the base-cell model for embedded CNTs by describing a specific correlation between the thermal line-element parameter Λ and the proximity to neighboring CNTs.

Interfacial effects influence the heat dissipation from one medium to another. By means of molecular dynamic simulation, mainly single CNTs are examined, which are in contact with neighboring tubes or water [19, 29, 44]. Using a one-parameter

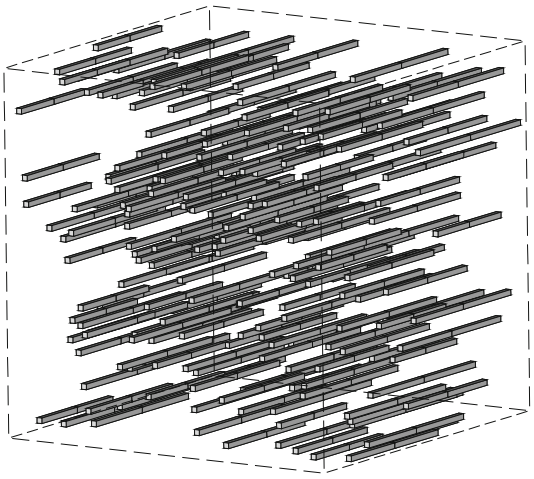

Fig. 30.9 Composite with aligned CNTs

line-element model, interfacial effects cannot be modeled except for CNT boundaries. This restriction seems to be adequate regarding the anisotropic thermal behavior of CNTs. Results of empirical investigations on CNT-based composites can be used to validate the model results. The following parameters have been investigated:

CNT orientation. The orientation of CNTs in a substrate describes their alignment with regard to the heat flow (Fig. 30.9). Due to the predominantly axial heat conduction of CNTs, an alignment parallel to the heat flow provides highest thermal conductivity. This observation and a considerable dependency on the orientation of the CNT has been confirmed. Specifically, a alignment perpendicular to the heat flow reduces thermal conductivity by a factor of 3.5 compared to parallel alignment and by a factor of 2 compared to unaligned CNTs [12, 15]. The influence of a small twist angle (0 . . . 10 degrees) between straightened CNTs is negligible [47]. The influence of anisotropism is more dominant for single-walled CNTs (SWNT) composites than for multi-walled (MWNTs) composites [12].

Volume fraction. The influence of the volume fraction of CNTs in the composite has been examined in different studies [12, 36, 47]. A linear or an exponential increase of thermal conductivity with increasing fraction of CNTs has been reported (Table 30.3). The thermal conductivity of SWNT-based composites increases by 100% [12] compared to MWNTs of equal CNT volume fraction. Interestingly, the examined volume fractions range from 0 to 20%. In composites with larger volume fractions, more CNTs contact each other. Obviously, the thermal resistance for a direct CNT-to-CNT contact is larger than for a CNT contacting the surrounding medium. Thus, for volume fractions greater than 20%, thermal conductivity is decreased by approximately a factor of 4 [12].

Length. For single CNTs, their length influences the thermal conductivity in composites. In [36], the authors show that the thermal conductivity of a CNT-based composite could be improved by approx. 55% using 100 CNTs with length of 80 µm or by using 10,000 CNTs with length of 8 µm. This indicates the importance of long CNTs in future applications (Fig. 30.10).

Table 30.3 Correlation of CNT volume fraction and thermal conductivity

Study	Singh 2007 [47]	Duong 2005 [12]	Nishimura 2004 [36]
Volume fraction	4…16%	1…8%	0…0.7%
Max. enhancement of thermal conductivity	30%	30%	200% (simulation) 120% (measured)

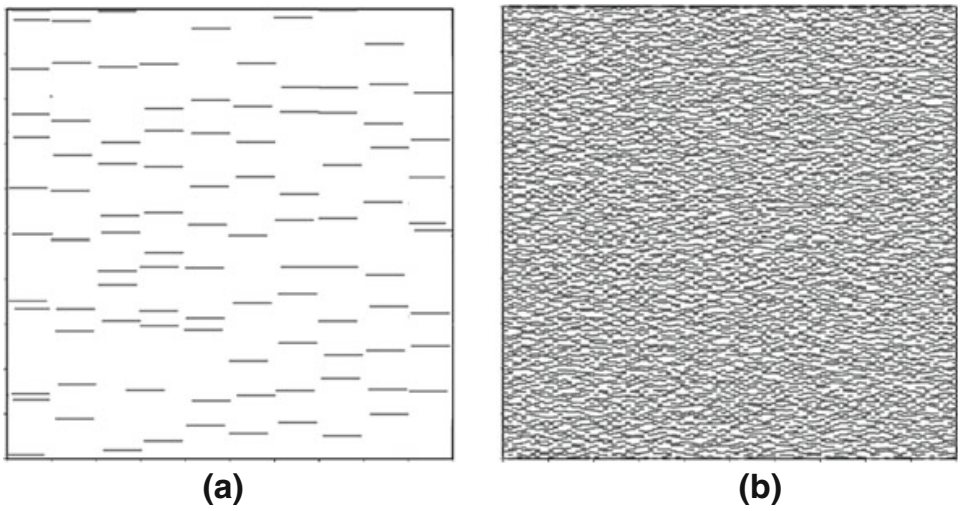

Fig. 30.10 Impact of the CNT lengths on the thermal conductivity of CNT-based composites. Both mixtures provide approximately the same thermal conductivity despite different CNT densities; the composite in **a** contains 100 CNTs with a length of 80 µm, the composite in **b** 10,000 CNTs with a length of 8 µm [36]

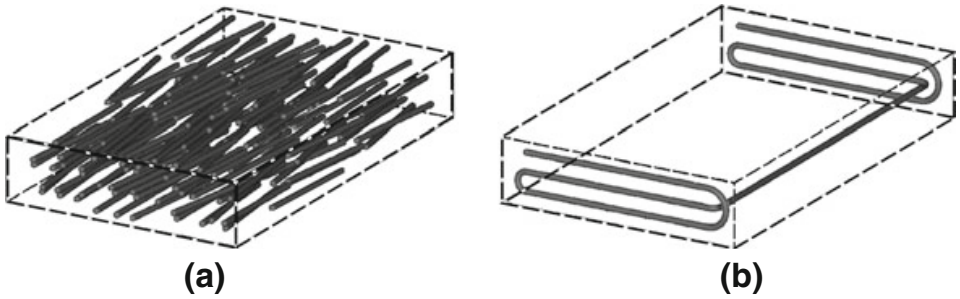

Fig. 30.11 Impact of the CNT shape on thermal conductivity of a composite. **a** A composite with a higher volume fraction of CNTs but lower thermal conductivity compared to **b** a single CNT with a "C" shape [67]

Shape. Not only the length but also the shape of CNTs influences the thermal conductivity of CNT-filled composites. The composite illustrated in Fig. 30.11a has a CNT volume fraction of 8.4% and a thermal conductivity of 3.75 $W/(m \cdot K)$. In case of Fig. 30.11b, the composite has a CNT volume fraction of only 0.88%. However, due to the CNT shape, the thermal conductivity of 11.76 $W/(m \cdot K)$ is three times larger [66]. Furthermore, for certain CNT lengths, a "C" shape has been found to be the best heat conductor [67].

Besides structural parameters of the composite, the temperature also has a major influence, as already mentioned in Sect. 30.3.2. Specifically, temperature dependencies had been reported for aligned and randomly arranged CNTs [15], and for CNT-filled interface materials [68]. Hence, temperature dependencies must be considered for both the CNT model and the matrix material.

It is obvious that the influences of the CNT's orientation and length are stochastic parameters. Hence, the model of a base cell must allow a distribution of these parameters. Furthermore, the influence of the volume fraction can differ locally.

30.3.4 Thermal Model of CNT-based Thermal Vias and Via Arrays

The properties of the base cell have been discussed in detail in the previous Sect. 30.3.3. Following the effective medium approach, the calculated anisotropic, specific thermal conductivity of a CNT-based composite has to be applied in the thermal-via model or the via-array model. Normally, these parameters are location-dependent, i.e., multiple composite models with different parameters have to be solved for a thermal-via model or a via-array model.

A thermal model of a thermal via or via array, respectively, is based on the heat diffusion equation (30.2). Thus, regular arrangements of vias often can be calculated analytically. However, complex via arrangements and design-optimization problems usually require numerical methods. The most widely used numerical techniques for heat-diffusion problems (e.g., thermal analysis of electronic components and assemblies) are categorized into *finite difference method*, *finite element method*, and *boundary element method* using Green functions [64]. Basically, these methods differ in formulating the equation set describing the problem, the domain discretization, and the applicable solvers. A comprehensive overview on these techniques is given in [30].

For example, a thermal via model can be generated by conventional 3D-Finite Element Analysis (FEA). Here, as illustrated in Fig. 30.12, thermal-via-array designs can be analyzed and optimized.

30.4 Application Potential

A modeling approach has been presented that can be used to calculate the thermal behavior of (i) CNT-based composites and (ii) elements based on such composites. Since this approach involves mutual interactions between CNTs, the impact of the CNT volume fraction on the thermal behavior can also be calculated. It is important to note that this approach overcomes the limits of established models that usually neglect these interactions. Hence, the presented modeling approach allows to account for most relevant properties of CNTs.

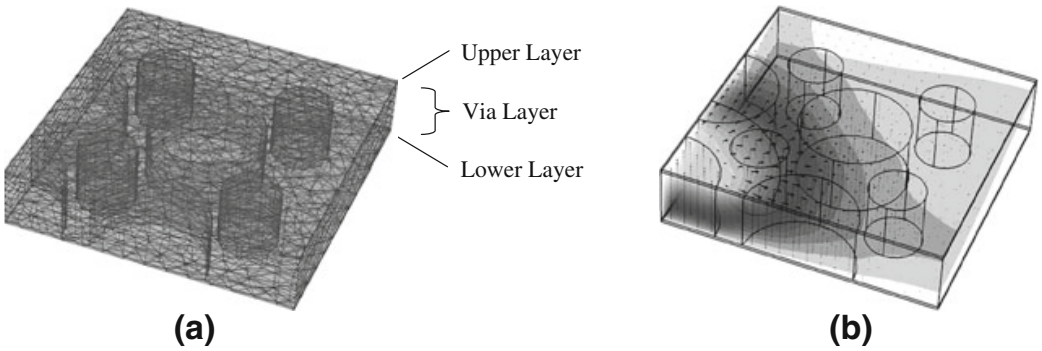

Fig. 30.12 Finite element analysis model of a thermal-via array. **a** A discretized model and **b** numerical results are used to describe the isothermal surfaces

Design optimization is one of the main applications of the proposed models. For optimization purposes, all sub-models of the several hierarchy levels have to be formulated parametrically. Suitable global optimization techniques, such as [18], are applicable.

Using the developed hierarchical modeling method, promising technological approaches and optimized arrangements of thermal vias can be developed that, among others, account for

- shape and dimensions at arbitrary, hierarchical level of the model,
- CNT orientation, and
- volume fraction.

Moreover, reasonable ranges of thermal resistance for different technological approaches can be estimated. This allows a comprehensive comparison with conventional thermal-via design [8, 10, 16, 24, 62]. Furthermore, the presented modeling approach helps to evaluate the application potential of CNT-based composites more precisely. Justified suggestions for technological researchers and designers can be derived.

Probabilistic simulation techniques allow to estimate the distributions of the thermal behavior of thermal vias, caused by stochastic deviations of dimension, shape and material properties, or local inhomogeneities (see Chap. 6). Combined with optimization methods, these techniques allow a robust design optimization of thermal-via arrays. This is an important issue since manufacturing tolerances must be considered throughout the whole design process.

Thermally-driven design of integrated circuits and electronic assemblies requires the temperature distribution to be computed within certain design steps, e.g., during floorplanning and placement. For this purpose, adequately fast computing models are required. Normally, network models are used. However, spatial models like finite-element models have been applied additionally during the last years. If elements like CNT-based thermal vias are used, all used models have to refer to sub-models describing the thermal behavior of these elements. The developed models can be used for this purpose as well.

Thermal design is a key issue for emerging 3D designs (see Chap. 5). Here, the power density is significantly higher and the thermal paths are longer than in 2D designs [42]. As mentioned before, the usage of conventional thermal vias based on copper becomes more and more insufficient. The high thermal conductivity of CNTs used in composites can significantly increase the efficiency of thermal vias with regard to their thermal conductivity. Hence, thermal vias and thermal-via arrays using CNT-based composites are a promising approach for the thermal management of 3D electronic systems.

30.5 Outlook

More and more electronic circuits contain thermal vias in order to improve vertical thermal conductivity. However, continuous down-scaling of circuit structures and the related increased heat density require new approaches for thermal management. Since the efficiency of thermal vias directly depends on the used via material, the application of any highly heat-conducting material can significantly improve the thermal conductivity of these vias. CNT-based composites could replace conventional via materials like copper due to their unique thermal conductivity. However, simulations and practical applications of thermal vias using CNT-based composites have rarely been carried out yet.

The presented hierarchical modeling approach of thermal vias is based on CNT-composites. Using the heat diffusion equation, the approach models the thermal behavior of CNTs phenomenologically by line elements. By using the effective medium approach in a base cell, CNTs can be integrated into a macroscopic model despite their nanometer scale. Such an optimized model of thermal-via arrays using CNT-based composites significantly simplifies thermal simulations of these nano-scale structures.

The modeling results allow an efficient comparison of various technological solutions prior to practical experiments. For example, the impact of CNT orientation, volume fraction and other composite characteristics on the thermal conductivity can be simulated in order to obtain the most promising settings for these experiments. Once the technology has been established, the models can also be used to optimize the thermal management of the electronic system.

References

1. Alaghemandi, M.: The thermal conductivity and thermal rectification of carbon nanotubes studied using reverse non-equilibrium molecular dynamics simulations. Nanotechnology. **20**, 1–8 (2009). doi:10.1088/0957-4484/20/11/115704
2. Ando, Y., Zhao, X., Sugai, T., Kumar, M.: Growing carbon nanotubes. Mater. Today **7**(10), 22–29 (2004)

3. Avouris, P., Chen, Z., Perebeinos, V.: Carbon-based electronics. Nat. Nanotechnol. **2**, 605–615 (2007). doi:10.1038/nnano.2007.300
4. Awano, Y.: Carbon nanotube technologies for LSI via interconnects. IEICE Trans. Electron. **E89**-C(11), 1499–1503 (2006). doi:10.1093/ietele/e89-c.11.1499
5. Bagchi, A., Nomura, S.: On the effective thermal conductivity of carbon nanotube reinforced polymer composites. Compos. Sci. Technol. **66**, 1703–1712 (2006). doi:10.1016/j.compscitech.2005.11.003
6. Bijua, V., Itoha, T., Makitab, Y., Ishikawa, M.: Close-conjugation of quantum dots and gold nanoparticles to sidewall functionalized single-walled carbon nanotube templates. J. Photochem. Photobiol., A **183**, 315–321 (2006). doi:10.1016/j.jphotochem.2006.06.032
7. Borca-Tasciuc, D.A., Pietruszka, L., Borca-Tasciuc T., Vajtai, R., Ajayan, P.: Thermal transport measurements in multi-wall carbon nanotube strands using the 3ω method. In: IEEE Twenty First Annual Semiconductor Thermal Measurement and Management Symposium, pp. 247–252 (2005). doi:10.1109/STHERM.2005.1412187
8. Bower, C.A., Malta, D., Temple, D., Robinson, J.E., Coffman, P.R., Skokan, M.R., Welch, T.B.: High density, vertical interconnects for 3-D integration of silicon integrated circuits. In: 56th Proceedings of Electronic Components and Technology Conference, pp. 399–403 (2006). doi:10.1109/ECTC.2006.1645677
9. Chai, Y., Zhang, K., Zhang, M., Chan, P.C.H., Yuen, M.M.F.: Carbon nanotube/copper composites for via filling and thermal management. In: Proceedings of 57th Electronic Components and Technology Conference (ECTC '07), pp. 1224–1229 (2007). doi:10.1109/ECTC.2007.373950
10. Chiriac, V.A., Lee, T.Y.T.: Thermal assessment of RF integrated LTCC front end module (FEM). In: Proceedings of Eighth Intersociety Conference on Thermal and Thermomechanical Phenomena in Electronic Systems (ITHERM), pp. 520–527 (2002). doi:10.1109/ITHERM.2002.1012500
11. Cola, B.A., Xu, J., Fisher, T.S.: Contact mechanics and thermal conductance of carbon nanotube array interfaces. Int. J. Heat Mass Transfer **52**, 3490–3503 (2009)
12. Duong, H.M., Papavassiliou, D.V.: Random walks in nanotube composites: Improved algorithms and the role of thermal boundary resistance. Appl. Phys. Lett. **87**, 013101-1–013101-3 (2005). doi:10.1063/1.1940737
13. Duong, H.M., Yamamoto, N., Papavassiliou, D.V., ShigeoMaruyama, Wardle, B.L.: Inter-carbon nanotube contact in thermal transport of controlled-morphology polymer nanocomposites. Nanotechnology. **20**, 1–23 (2009). doi:10.1088/0957-4484/20/15/155702
14. Evoy, S., Riegelman, M.A., Naguib, N., Ye, H., Jaroenapibal, P., Luzzi, D.E., Gogotsi, Y.: Dielectrophoretic assembly of carbon nanofiber nanoelectromechanical devices. IEEE Trans. Nanotechnol. **4**(5), 570–575 (2005). doi:10.1109/TNANO.2005.851404
15. Gonnet, P.: Thermal conductivity of magnetically aligned carbon nanotube buckypapers and nanocomposites. Current Applied Physics **6**, 119–122 (2006). doi:10.1016/j.cap.2005.01.053
16. Goplen, B., Sapatnekar, S.S.: Placement of thermal vias in 3-D ICs using various thermal objectives. IEEE Trans. Comput. Aid. Des. **25**(4), 692–709 (2006). doi:10.1109/TCAD.2006.870069
17. Heimann, M., Lemm, J., Wolter, K.J.: Characterization of carbon nanotubes/epoxy composites for electronics applications. In: Proceedings of 30th International Spring Seminar on Electronics Technology, pp. 1–6 (2007). doi:10.1109/ISSE.2007.4432811
18. Horst, R., Pardalos, P.M., Thoai, N.V.: Introduction to Global Optimization, 2nd edn. Springer, New York (2009)
19. Igarashi, Y., Shibuta, Y., Maruyama, S.: Heat transfer problems related with carbon nanotubes by molecular dynamics-based simulations. In: 1st International Forum on Heat Transfer (2004)
20. Kim, P., Shi, L., Majumdar, A., McEuen, P.L.: Thermal transport measurements of individual multiwalled nanotubes. Phys. Rev. Lett. **87**, 1–4 (2001). doi:10.1103/PhysRevLett.87.215502
21. Koker, T.: Konzeption und Realisierung einer neuen Prozesskette zur Integration von Kohlenstoff-Nanoröhren über Handhabung in technischen Anwendungen, Universitätsverlag Karlsruhe (2006)

22. LeMieux, M.C., Roberts, M., Barman, S., Jin, Y.W., Kim, J.M., Bao, Z.: Self-sorted, aligned nanotube networks for thin-film transistors. Science **321**(5885), 101–104 (2008). doi:10.1126/science.1156588
23. Li, J., Zhang, Q., Yan, Y., Li, S., Chen, L.: Fabrication of carbon nanotube field-effect transistors by fluidic alignment technique. IEEE Trans. Nanotechnol. **6**(4), 481–484 (2007). doi:10.1109/TNANO.2007.897868
24. Li, Z., Hong, X., Zhou, Q., Zeng, S., Bian, J., Yu, W., Yang, H.H., Pitchumani, V., Cheng, C.K.: Efficient thermal via planning approach and its application in 3-D floorplanning. IEEE Trans. Comput. Aid. Des. **26**(4), 645–658 (2007). doi:10.1109/TCAD.2006.885831
25. Liu, Y.J., Chen, X.L.: Continuum models of carbon nanotube-based composites using the boundary element method. Electron. J. Boundary Elem. **1**, 316–335 (2003)
26. Lukes, J.R., Zhong, H.: Thermal conductivity of individual single-wall carbon nanotubes. J. Heat Transf. **129**, 705–716 (2007)
27. Maiti, A.: Multiscale modeling with carbon nanotubes. Microelectron. J. **39**, 208–221 (2008). doi:10.1016/j.mejo.2006.06.003
28. Maruyama, S.: A molecular dynamics simulation of heat conduction in finite length SWNTs. Physica B **323**, 193–195 (2002)
29. Maruyama, S., Igarashi, Y., Taniguchi, Y., Shiomi, J.: Anisotropic heat transfer of single-walled carbon nanotubes. J. Therm. Sci. Technol. **1**, 138–148 (2006). doi:10.1299/jtst.1.138
30. Minkowycz, W.J., Sparrow, E.M., Murthy, J.Y. (eds.): Handbook of Numerical Heat Transfer. Wiley, New York (2006)
31. Mirza, S.M., Grebel, H.: Thermoelectric properties of aligned carbon nanotubes. Appl. Phys. Lett. **92**, 203116 (2008). doi:10.1063/1.2931084
32. Monica, A.H., Papadakis, S.J., Osiander, R., Paranjape, M.: Wafer-level assembly of carbon nanotube networks using dielectrophoresis. Nanotechnology. **19**, 085303 (2008). doi:10.1088/0957-4484/19/8/085303
33. Nan, C.W., Liu, G., Lin, Y., Li, M.: Interface effect on thermal conductivity of carbon nanotube composites. Appl. Phys. Lett. **85**, 3549–3551 (2004). doi:10.1063/1.1808874
34. Nan, C.W., Shi, Z., Lin, Y.: A simple model for thermal conductivity of carbon nanotube-based composites. Chem. Phys. Lett. **375**, 666–669 (2003). doi:10.1016/S0009-2614(03)009564
35. Narayanan, A., Dan, Y., Deshpande, V., Lello, N.D., Evoy, S., Raman, S.: Dielectrophoretic integration of nanodevices with CMOS VLSI circuitry. IEEE Trans. Nanotechnol. **5**(2), 101–109 (2006). doi:10.1109/TNANO.2006.869679
36. Nishimura, N., Liu, Y.J.: Thermal analysis of carbon-nanotube composites using a rigid-line inclusion model by the boundary integral equation method. Comput. Mech. **35**, 1–10 (2004). doi:10.1007/s00466-004-0580-2
37. Osman, M.A., Srivastava, D.: Molecular dynamics simulation of heat pulse propagation in single-wall carbon nanotubes. Phys. Rev. B: Condens. Matter **72**, 125413-1–125413-7 (2005). doi:10.1103/PhysRevB.76.155424
38. Rao, C.N.R., Müller, A., Cheetham, A.K. (eds.): The Chemistry of Nanomaterials. Wiley-VCH, Weinheim (2005). doi:10.1002/352760247X
39. Romero, J.J.: Carbon nanotubes take the heat off chips. IEEE Spectr. **12**, 12–14 (2007)
40. Rui-Qin, P., Zi-Jian, X., Zhi-Yuan, Z.: Length dependence of thermal conductivity of single-walled carbon nanotubes. Chin. Phys. Lett. **24**, 1321–1323 (2006)
41. Sanada, K., Tada, Y., Shindo, Y.: Thermal conductivity of polymer composites with close-packed structure of nano and micro fillers. Composites Part A **40**, 724–730 (2009). doi:10.1016/j.compositesa.2009.02.024
42. Sapatnekar, S.S.: Computer-Aided Design for 3D Circuits at the University of Minnesota. In: Garrou, P., Bower, C., and Ramm, P. (eds.): Handbook of 3D Integration: Technology and Applications of 3D Integrated Circuits, pp. 583–597. Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim (2008)
43. Scheffer, L.K.: CAD implications of new interconnect technologies. In: Proceedings of the 44th annual conference on Design automation (DAC), pp. 576–581. New York, USA (2007). doi:10.1145/1278480.1278626

44. Shiomi, J., Maruyama, S.: Heat conduction of single-walled carbon nanotube in various environments. In: 2nd International Symposium on Micro- and Nano-technology (2006)
45. Shiomi, J., Maruyama, S.: Diameter and length effect on diffusive-ballistic phonon transport in a carbon nanotube. In: ASME-JSME Thermal Engineering Summer Heat Transfer Conference (2007)
46. Shiomi, J., Maruyama, S.: Diffusive-ballistic heat conduction of carbon nanotubes and nanographene ribbons. Int. J. Therm. Sci. **29**, 1–12 (2008). doi:10.1007/s10765-008-0516-8
47. Singh, I.V., Tanaka, M., Endo, M.: Effect of interface on the thermal conductivity of carbon nanotube composites. Int. J. Therm. Sci. **46**, 842–847 (2007). doi:10.1016/j.ijthermalsci.2006.11.003
48. Song, Y.S.: Evaluation of effective thermal conductivity for carbon nanotube/polymer composites using control volume finite element method. Carbon **44** 710–717, 2006. doi:10.1016/j.carbon.2005.09.034
49. Stevens, R., Nguyen, C., Meyyappan, M.: Nanomanipulation and fabrication by ion beam molding. IEEE T. Nanotechnol. **5**(3), 255–257 (2006). doi:10.1109/TNANO.2006.874056
50. Tserpes, K.I., Papanikos, P.: Continuum modeling of carbon nanotube-based super-structures. Compos. Struct. **91**, 131–137 (2009)
51. Ueno, T., Yoshioka, T., Ogawa, J., Ozoe, N., Sato, K., Yoshino, K.: Highly thermal conductive metal/carbon composites by pulsed electric current sintering. Synth. Met. 159, 2170–2172 (2009). doi:10.1016/j.synthmet.2009.10.006
52. Vijayaraghavan, A., Blatt, S., Weissenberger, D., Oron-Carl, M., Hennrich, F., Gerthsen, D., Hahn, H., Krupke, R.: Ultra-large-scale directed assembly of single-walled carbon nanotube devices. Nano Lett. **7**(6), 1556–1560 (2007). doi:10.1021/nl0703727
53. Wang, J., Wang, J.S.: Carbon nanotube thermal transport: Ballistic to diffusive. Appl. Phys. Lett. **88**, 111909-1–111909-3 (2006). doi:10.1063/1.2185727
54. Wikipedia: http://en.wikipedia.org/wiki/file:cntnames.png (01.10.2005)
55. Wirts-Rutters, M., Heimann, M., Kolbe, J., Wolter, K.J.: Carbon nanotube (CNT) filled adhesives for microelectronic packaging. In: Proceedings of the 2nd Electronics Systemintegration Technology Conference (ESTC), pp. 1057–1062 (2008). doi:10.1109/ESTC.2008.4684498
56. Wu, M.C.H., Hsu, J.Y.: Thermal conductivity of carbon nanotubes with quantum correction via heat capacity. Nanotechnology. **20**, 1–6 (2009). doi:10.1088/0957-4484/20/14/145401
57. Xu, T., Wang, Z., Chen, J.M.X., Tan, C.M.: Aligned carbon nanotubes for through-wafer interconnects. Appl. Phys. Lett. **91**(042108), 1–3 (2007). doi:10.1063/1.2759989
58. Xue, Q.Z.: Model for thermal conductivity of carbon nanotube-based composites. Physica B **368**, 302–307 (2005). doi:10.1016/j.progpolymsci.2007.09.002
59. Yamamoto, T., Watanabe, S., Watanabe, K.: Low-temperature thermal conductance of carbon nanotubes. Thin Solid Films **464**, 350–353 (2004)
60. Yang, X.S.: Modelling heat transfer of carbon nanotubes. Modelling Simul. Mater. Sci. Eng. **13**, 893–902 (2005). doi:10.1088/0965-0393/13/6/008
61. Ye, H., Gu, Z., Yu, T., Gracias, D.H.: Integrating nanowires with substrates using directed assembly and nanoscale soldering. IEEE T. Nanotechnol. **5**(1), 62–66 (2006). doi:10.1109/TNANO.2005.861399
62. Yu, H., Ho, J., He, L.: Simultaneous power and thermal integrity driven via stapling in 3D ICs. In: Proceedings of the IEEE/ACM international conference on Computer-aided design, pp. 802–808. ACM Press, New York, USA (2006). doi:10.1145/1233501.1233666
63. Zeng, Q.H., Yu, A.B., Lu, G.Q.: Multiscale modeling and simulation of polymer nanocomposites. Prog. Polym. Sci. **33**, 191–269 (2008). doi:10.1016/j.progpolymsci.2007.09.002
64. Zhan, Y., Goplen, B., Sapatnekar, S.S.: Electrothermal analysis and optimization techniques for nanoscale integrated circuits. In: Proceedings of the 2006 Asia and South Pacific Design Automation Conference ASP-DAC 2006, pp. 219–222. Yokohama, Japan (2006)
65. Zhang, G., Li, B.: Thermal conductivity of nanotubes revisited: Effects of chirality, isotope impurity, tube length, and temperature. J. Chem. Phys. **123**, 114714-1–114714-4 (2005). doi:10.1103/PhysRevB.78.085431

66. Zhang, J., Tanaka, M.: Systematic study of thermal properties of CNT composites by the fast multipole hybrid boundary node method. Eng. Anal. Boundary Elem. **31**, 388–401 (2007). doi:10.1016/j.enganabound.2006.07.011
67. Zhang, J., Tanaka, M.: Fast HdBNM for large-scale thermal analysis of CNT-reinforced composites. Comput. Mech. **41**, 777–787 (2008). doi:10.1007/s00466-007-0161-2
68. Zhang, K., Fan, H., Yuen, M.M.F.: Molecular dynamics study on thermal performance of CNT-array-thermal interface material. In: Proceedings of the International Conference on Electronic Materials and Packaging (EMAP), pp. 1–4 (2006). doi:10.1109/EMAP.2006.4430586
69. Zhang, K., Xiao, G.W., Wong, C.K.Y., Gu, H.W., Yuen, M.M.F., Chan, P.C.H., Xu, B.: Study on thermal interface material with carbon nanotubes and carbon black in high-brightness LED packaging with flip-chip. In: Proceedings of the 55th Electronic Components and Technology Conference, pp. 60–65 (2005). doi:10.1109/ECTC.2005.1441246
70. Zhang, W., Zhu, Z., Wang, F., Wang, T., Sun, L., Wang, Z.: Chirality dependence of the thermal conductivity of carbon nanotubes. Nanotechnology. **15**, 936–939 (2004). doi:10.1088/0957-4484/15/8/010