

Visual analytics in investigation of chirality-dependent thermal properties of carbon nanotubes

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Abstract. In the paper, we present our approach to visual analytics application to investigation of thermal properties of carbon nanotubes. A thermal properties carbon nanotube framework is developed to investigate remarkable features of carbon nanotubes. Visual analytics is useful for comparison of their thermal properties and the corresponding analysis. The preliminary results are reported.

1. Introduction

Currently, many different mathematical models of nano-objects are used for calculation of their properties [1-5]. Using a mathematical model, a designer obtains a big numerical data file, that has to be analyzed. However, it is difficult to choose the best design solution from the two objects that are invisible. In our approach, data and designed objects are visualized [6]. A designer can analyze the obtained numerical and visual information simultaneously.

In the paper, we present an application of our approach to visual analytics support for research of carbon nanotube variation and its influence on thermal conduction phenomena. The outstanding thermal conductivity of carbon nanotubes attracts designers [1, 2, 7]. Carbon nanotubes FETs are promising candidates for the post silicon era. However, the fabrication of carbon nanotubes with the predefined performance is a big challenge [8]. Carbon nanotube specific variations, including nanotube diameter and chirality variations, influence the thermal conductivity of carbon nanotube [9]. A designer has to compare thermal properties of carbon nanotubes with different chiral indices. However, carbon nanotubes are invisible for a human eye. Therefore, special efforts are required to compare alternative design solutions.

We illustrate our approach for investigation of thermal properties of single-walled carbon nanotubes. In the paper, we proposed a novel approach based on visual analytics. The approach supports a nanotube devices design process and simplifies a design solution choice.

In the paper, we focus on design solution with the predefined diameter. First, we find all possible chiral indices for the given diameter and then visualize all possible design solutions with their thermal properties. The corresponding statistical data is reported as well.

The rest of the paper is structured as follows. The next section reviews the related works in the field of carbon nanotubes thermal conductivity. Section 3 presents our approach for visual analytics support in research of chirality-dependent thermal properties of carbon nanotubes. We use single-walled CNTs as our test case. Finally, conclusions are derived in Section 4.



2. Mathematical model of thermal conductivity of carbon nanotubes

The carbon film (graphene) and nanotubes are allotropes of carbon with unique transport properties [3, 4]. Nanotubes come in a variety of lengths L and diameters D . The distance between the adjacent carbon atoms in carbon nanotubes is equal to $d_0 = 0.142$ nm. Therefore, the atomic structure of a single-walled CNT is well described by a pair of indices (chiral indices), n and m . The diameter is calculated as follows:

$$D = \frac{\sqrt{m^2 + n^2 + m * n}}{\pi} \frac{\sqrt{3} * d_0}{\pi} \quad (1)$$

The CNT thermal conductivity is dependent on the temperature, the nanotube length L and the average phonon mean free path l_0 [1, 2]. If $l_0 > L$ the ballistic conduction mechanism is dominant. A quantum of thermal conductance is given as follow:

$$G_{th} = \frac{\pi^2 k_B^2 T}{3h} = 9,46 \times 10^{-13} \frac{W}{K^2} T \quad (2)$$

where k_B is the Boltzmann constant;

T is the temperature;

h is the Planck constant.

The thermal conductivity of nanotubes per unit length is calculated as follows:

$$G = G_{th} N_p \quad (3)$$

where N_p is the number of phonon channels in a nanotube.

The number of phonon channels N_p is equal to the triple number of atoms in the unit cell $2N$, where N is calculated as follows:

$$N = \frac{2(n^2 + m^2 + nm)}{d_R} \quad (4)$$

where d_R is equal to the greatest common divisor of the numbers $(2n + m)$ and $(n + 2m)$.

According to [3, 4] a single-walled carbon nanotube with the chiral indices (5, 5) and the diameter $D = 0,678$ nm contains 60 phonon channels and its thermal conductivity is given as follows:

$$G = 60 G_{th} \quad (5)$$

A single-walled carbon nanotube with the chiral indices (10, 10) and the diameter $D = 1,356$ nm contains 120 phonon channels and its thermal conductivity is given as follows:

$$G = 120 G_{th} \quad (6)$$

Table I summaries the data for the thermal conductivity of two nanotubes.

It should be noted, that experimental data for the thermal properties of nanotubes has been published in [4]. In particular, the experimental value of thermal conductivity of the nanotube (10, 10) is equal to

$$G = 128 G_{th} \quad (7)$$

Through inspecting other experimental data points [4], we can validate that the measured values lie very close to the curves proposed by (3).

3. Thermal properties carbon nanotube framework

We developed a framework for analysis and visualization of nanotubes transport properties [10]. Our framework has been implemented using C# programming language and Microsoft Visual Studio 2015. We use the libraries of Tao Framework, including the OpenGL library [11].

Our framework provides a comparison of thermal properties of two different nanotubes and supports nanotubes variation analysis. More details about the first feature can be found in [12].

In the paper, our focus is on nanotube variation visualization and its analysis.

Table 1. The thermal conductivity of nanotubes.

	Indices		Temperature, K		
	<i>n</i>	<i>m</i>	233	273	333
The thermal conductivity of the nanotube, <i>G</i> , W/K	5	5	$1,32 \cdot 10^{-8}$	$1,54 \cdot 10^{-8}$	$1,89 \cdot 10^{-8}$
The thermal conductivity of the nanotube, <i>G</i> , W/K	10	10	$2,64 \cdot 10^{-8}$	$3,09 \cdot 10^{-8}$	$3,78 \cdot 10^{-8}$

3. 1. Nanotubes variation analysis

Nanotubes parameters vary in diameter and chirality indices. In our framework, we provide three different types of diameters variation settings:

1. Min / Max (Figure 1).
2. Deviation, %.
3. Deviation, nm.

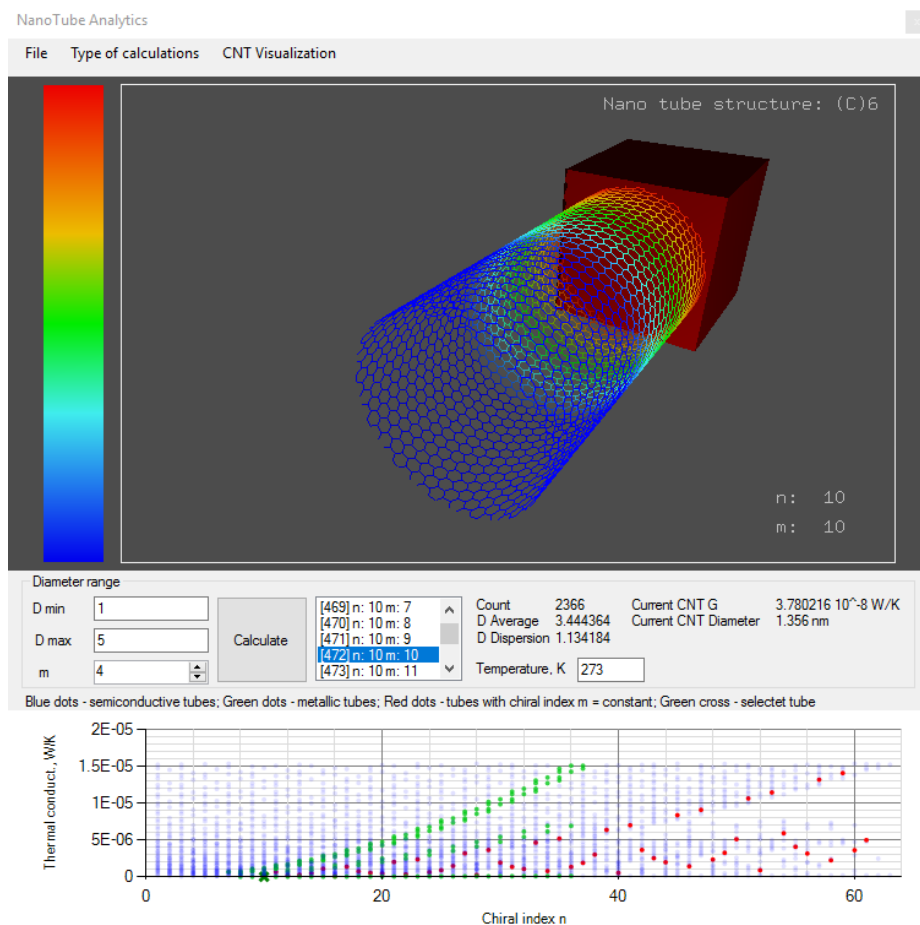


Figure 1. The variation tube analysis mode. Diameters vary from 1 nm to 5 nm, *m* = 10. \times depicts experimental measures [4] for the nanotube (10, 10).

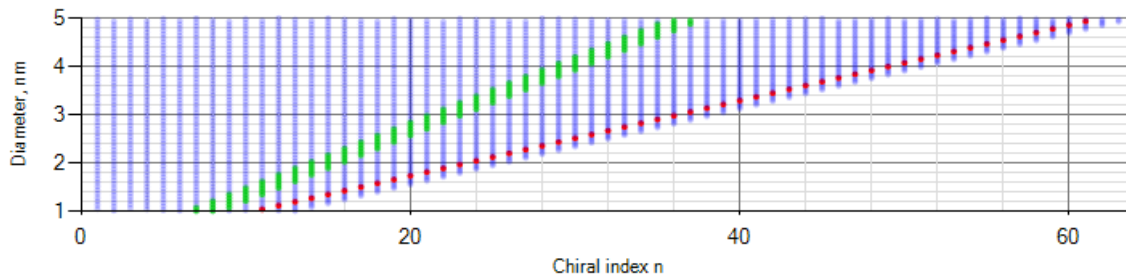


Figure 2. Diameters variation for different chiral indices n .

For all settings, our framework calculates an average nanotube diameter and a nanotube diameter dispersion.

Our framework generates the following output information:

1. Nanotubes diameters variation.
2. The sorted nanotubes diameters.
3. Dispersion of nanotubes diameters.
4. A curve $D(n, m)$.
5. Chiral indices variations.
6. A curve $G(D)$.
7. A curve $G(n, m)$
8. A dispersion of nanotube thermal conductivity.

For a given tube, our framework shows the corresponding thermal conductivity, the diameter and the dot in the curve.

Figure 1 illustrates the variation nanotubes analysis mode of our framework. The curve shows a change of thermal conductivity for different chirality indices. Each blue dot corresponds to semiconductor dots. Green dots show metallic nanotubes. Transparency of each point allows us to estimate the density of the distribution of values in different areas. Figure 1 shows the case $m = 10$.

Figure 2 summaries a diameter variation for variation of the chiral index n , while Figure 3 shows all possible chirality indices n and m for the diameter variations from 1 nm to 5 nm.

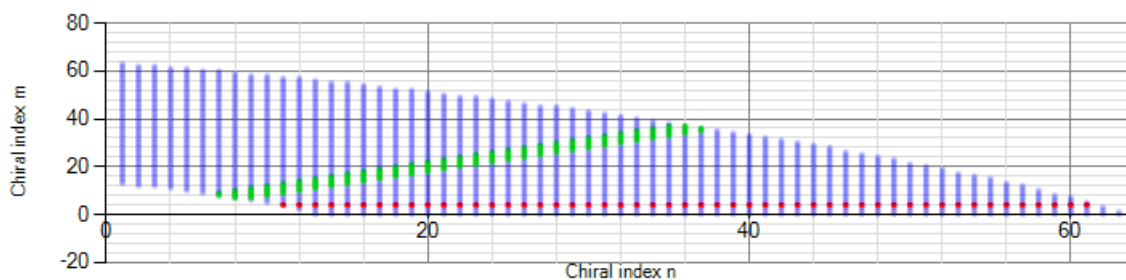


Figure 3. Chirality indices variations for the diameter variations from the 1 nm to 5 nm.

Figure 4 shows thermal conductivity variation for diameter variations. It is obvious that tubes divided into clusters. Tubes with equal m are observed in different clusters. It is remarkable that metallic and semiconductor nanotubes are observed in each cluster.

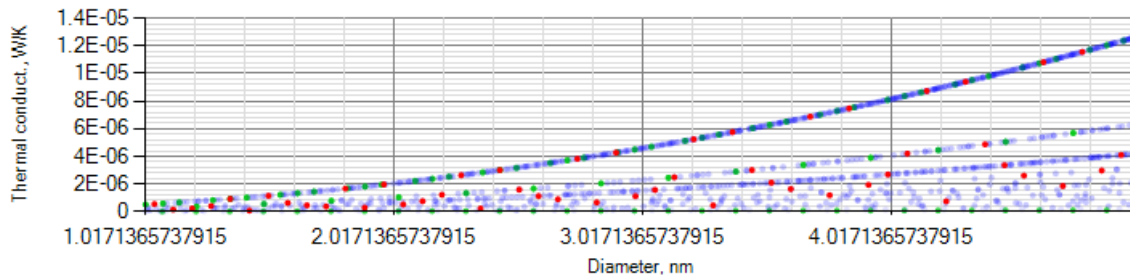


Figure 4. Thermal conductivity variations

Figure 5 represents a dispersion of thermal conductivity for nanotube diameter variation from 4 nm to 5 nm. It is remarkable, that some values of thermal conductivity are missing.

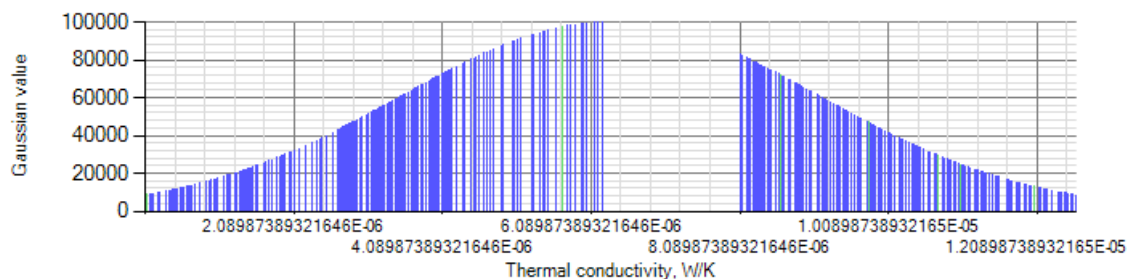


Figure 5. Thermal conductivity dispersion.

4. Conclusion

In the paper, we have presented our approach to visual analytics support for investigation of carbon nanotube variations. We have illustrated our approach using the single walled carbon nanotubes thermal conductivity as our test case. Our tool visualizes variation of nanotubes parameters and performance. It is obvious that visual analytics is useful for investigation of thermal properties of carbon nanotubes.

It should be mentioned, that our approach uses only the visual information channel. However, the approach simplifies a nanotube design flow.

Acknowledgments

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