Cognitive Data Visualization of Chirality-Dependent Carbon Nanotubes Thermal and Electrical Properties

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Abstract. The paper presents different approaches to a cognitive visualization of multidimensional data of chirality-dependent carbon nanotubes thermal and electrical properties. It is remarkable that the proposed visual analytics approaches are able to demonstrate hidden relations between features of carbon nanotubes.

Keywords*:* Nanotubes, multidimensional data, data analysis, human visual perception

1 Introduction

In the natural world, color information plays an important role in human visual perception. In engineering application, color information is used for visualization of multidimensional data and representation of physical features of alternative design solutions.

Carbon nanotubes (CNT) are characterized by a sufficient large number of different parameters, such as thermal conductivity (*G*), the chirality indices (*m* and *n*), diameter (*D*), electrical properties (metallic or semiconducting), and etc (Marconnet, et al., 2013). In addition to the numerous data, the nanotubes are invisible for a human eye. Therefore, efficient information management is crucial for nanoengineering applications (de la Iglesia et al., 2013, Shakhnov et al., 2014). The paper presents the possible approaches to a cognitive visualization of multidimensional chirality-dependent carbon nanotubes thermal and electrical properties.

The visual analytics tool aimed to thermal properties investigation of carbon nanotubes has presented in (Shakhnov, et al., 2016) (Kazakov, et al., 2016).

In the paper, we present a new version of the tool visualizing thermal and electric properties simultaneously. Fig. 1 shows the screenshot of the main mode. We use different colors for the carbon nanotubes parameters. Red dots shows values of thermal conductivity of CNTs for the given chirality index *m*. Green color means that a carbon nanotube has metallic electrical properties, while blue color means semiconducting electrical properties. The green cross is used to show the parameters of the visualized carbon nanotube.

In addition, the pie chart shows the numerical proportion of carbon nanotubes with metallic and conducting electrical properties for the given chirality indices variations.

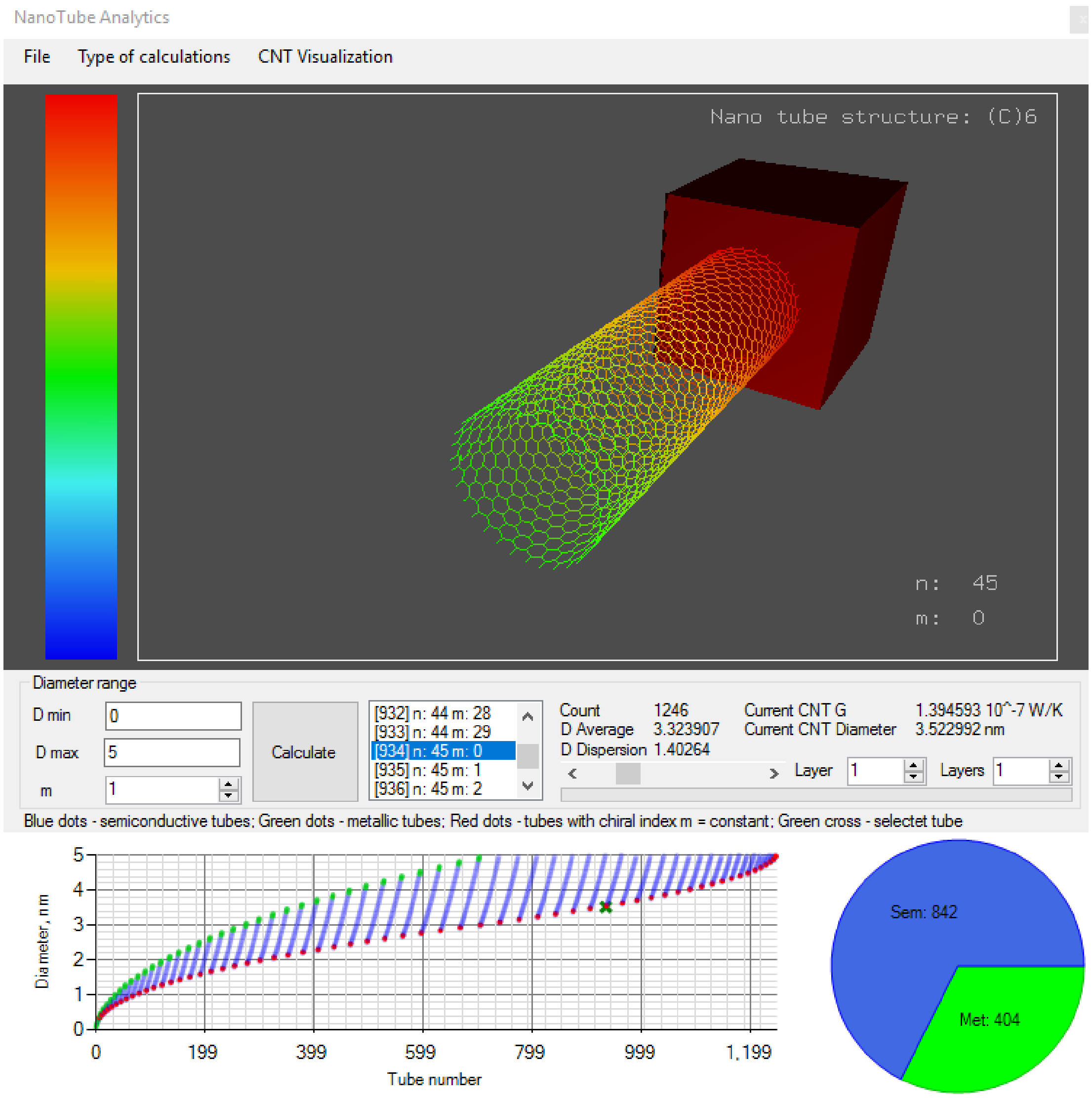


Fig. 1. The main mode

2 The use of color transparency in chirality-dependent carbon nanotube properties visualization

In order to enhance information management for our application, we use color transparency. Two-dimensional graphs (Fig. 1) can be analyzed easily, but the information capacity is low. In order to overcome the deficiency we vary the degree of transparency of each point according to the value of a variable. The degree of transparency we propose to calculate as follows:

$$R = \frac{(k - min_1)*(max_2 - min_2)}{max_1 - min_1} + min_2 \qquad (1)$$

where max_1 and min_1 are equal to the maximal and minimal values of input data;

max_2 and min_2 are equal to the values of maximal and minimal values of output data;

k is a given constant;

R is the degree of transparency.

Fig. 2 shows an example of the visualization based on this evaluation. Each line shows a different density value distribution.

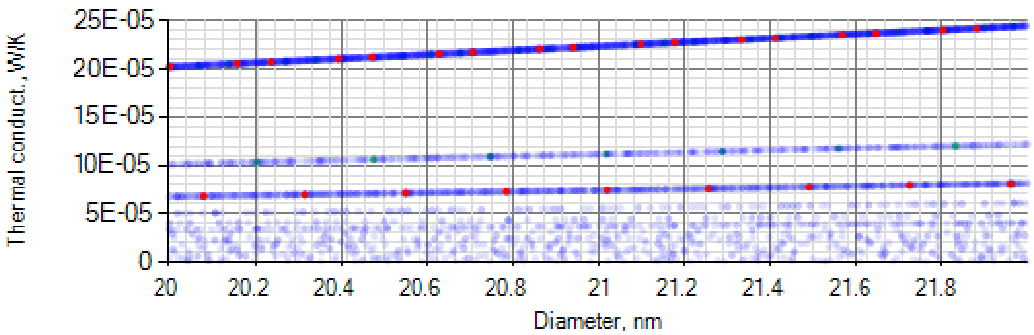


Fig. 2. An example of visualization of carbon nanotubes thermal properties for the given diameter variations

3 3D representation of chirality-dependent carbon nanotubes properties

In order to improve information representation, we use a 3D representation as well. Fig. 3 shows an example of 3D visualization of chirality-dependent carbon nanotubes thermal and electrical properties for the given chirality indices variations.

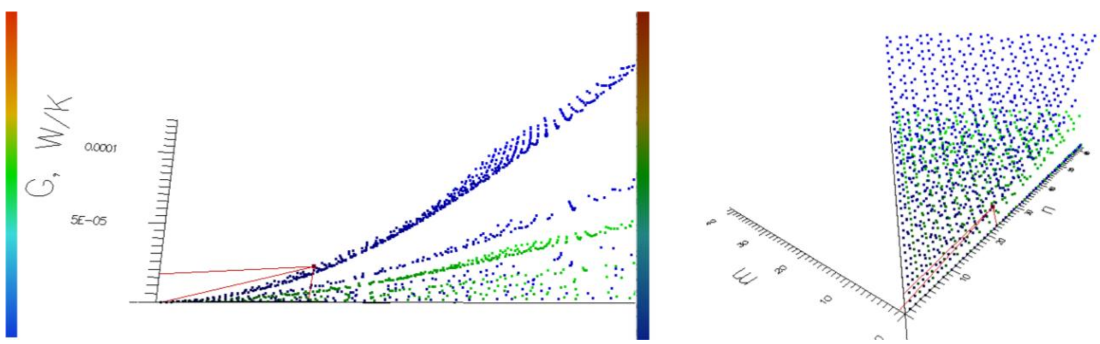


Fig. 3. 3D visualization of carbon nanotubes thermal and electrical properties for the given chirality indices variations

It is obvious that the discrete nanotube structure results in discrete layered structure. Each layer includes a specific distribution of thermal conductivity values. Values in the top layer represent hexagons.

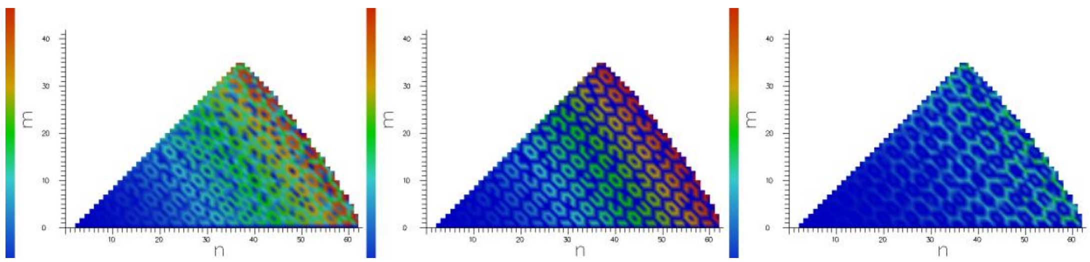
It is remarkable that semiconducting carbon nanotubes are located in one layer. Then two metallic carbon nanotubes layers are observed. The combination is observed for all chirality indices variations.

4 Cognitive representation of chirality-dependent thermal properties of carbon nanotubes

Unfortunately, Fig. 3 does not clearly present structure of each layer and correlation between the layers. In order to overcome this deficiency, an additional mode has been introduced. Fig. 4 illustrates our approach.

The chirality indices variations (Fig. 4) correspond to the variations of carbon nanotubes diameters from 0 nm to 5 nm. Fig. 4, a shows all thermal conductivity layers for the given chirality indices variations, while the only top layer is selected in Fig. 4, b. Fig. 4, c presents the remaining layers.

We use OpenGL graphics library tools to show gradients between discrete points of the given values. This color gradient variation is useful for analysis of chirality-dependent thermal properties features (Patrikalakis, 1991).



a b c

Fig. 4. Charts thermal conductivity of CNTs

Blue color is used to show areas with the minimal thermal conductivity, while red color shows areas with maximal thermal conductivity for the given chirality indices variations.

We also combine 3D visualization and the cognitive representation of chirality-dependent thermal properties of carbon nanotubes. Fig. 5 illustrates this option in our software. It is should be noted that Fig. 5 shows the only top layer of thermal conductivity in the cognitive visualization.

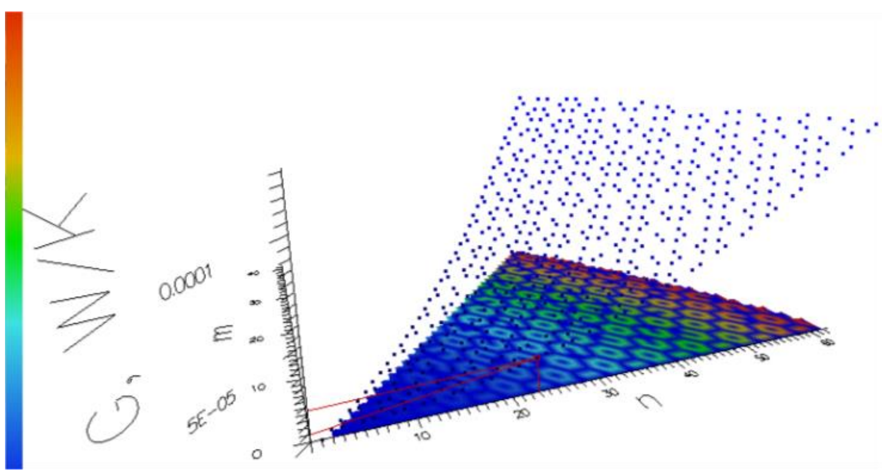


Fig. 5. Combined way of presenting data on the thermal conductivity of CNTs

5 Conclusion

In the paper, we discussed several approaches to cognitive visualization of chirality-dependent carbon nanotubes properties. It is obvious that visualization of electrical and thermal properties allows us to find hidden features of carbon nanotubes. The use of visual channel features simplifies analysis of multidimensional data of chirality-dependent transport properties of carbon nanotubes. The approach can be easily expanded for design of carbon nanotubes based on evolutionary adaptation (Red'ko, 2007).

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