Thermal parameters defined with graph theory approach in synthetized diamonds

Mitić, Vojislav; Randjelović, Branislav; Ribar, Srdjan; Čebela, Maria; Mohr, Markus; Vlahović, Branislav; Fecht, Hans

Source / Izvornik: **Thermal Science, 2022, 26, 2177 - 2186**

Journal article, Published version
Rad u časopisu, Objavljena verzija rada (izdavačev PDF)

https://doi.org/10.2298/TSCI210422284M

Permanent link / Trajna poveznica: https://urn.nsk.hr/urn:nbn:hr:217:408876

THERMAL PARAMETERS DEFINED WITH GRAPH THEORY APPROACH IN SYNTHETIZED DIAMONDS

by

Vojislav V. MITIĆ [a,b] ***Branislav M. RANDJELOVIĆ*** [a*], ***Srdjan N. RIBAR*** [c], ***Maria Ž. ČEBELA*** [d,e], ***Markus MOHR*** [f], ***Branislav D. VLAHOVIĆ*** [g], ***and Hans J. FECHT*** [h]

[a] Faculty of Electronic Engineering, University of Nis, Nis, Serbia
[b] Institute of Technical Sciences, SASA, University of Belgrade, Belgrade, Serbia
[c] Faculty of Mechanical Engineering, University of Belgrade, Belgrade, Serbia
[d] Vinča Institute of Nuclear Science, National Institute of the Republic of Serbia, University of Belgrade, Belgrade, Serbia
[e] Department of Physics, Faculty of Science, University of Zagreb, Zagreb, Croatia
[f] Institute of Functional Nanosystems, University of Ulm, Ulm, Germany
[g] North Carolina Central University (NCCU), Durham, North Carolina, USA
[h] Institute for Multifunctional Properties of Materialis, University Ulm, Ulm, Germany

Original scientific paper
https://doi.org/10.2298/TSCI210422284M

The Nanocrystaline diamonds are very important biomedical material with variety of applications. The experimental procedures and results have been done in the Institute of Functional Nanosystems at the University Ulm, Germany. There is an existing biocompatibility of the diamond layers, selectively improved by biomimetic 3-D patterns structuring. Based on that, we have been inspired to apply the graph theory approach in analysing and defining the physical parameters within the structure of materials structure samples. Instead the parameters values, characteristic at the samples surface, we penetrate the graphs deeply in the bulk structure. These values could be only, with some probability, distributed through the micro-structure what defines not enough precious parameters values between the micro-structure constituents, grains and pores. So, we originally applied the graph theory to get defined the physical parameters at the grains and pores levels. This novelty, in our paper, we applied for thermophysical parameters, like thermoconductiviy. By graph approach we open new frontiers in controlling and defining the processes at micro-structure relations. In this way, we can easily predict and design the structure with proposed parameters.

Key words: *nanocrystallinity, synthetized diamonds, biomaterials, biomimetics, graph theory, thermal parameters*

Introduction

Self similarity and biomimetic materials properties are getting very high importance, nowadays. One of the best examples is nanocrystalline diamond, with its unusual bioadaptive characteristics. The fabrication of these nanocrystalline diamonds with biomimetic surface layers is viable today, based on specific diamonds properties and possibilility to be synthesized by homogenous nanocrystalline diamond films. There are variety of applications, from biomedi-

* Corresponding author, e-mail: banedg2483@gmail.com

cal, up to high professional fields. In that sense, the properties characterization and parameters defining is very important. One of the most important research goals in this paper is based on idea that we can predict and in advance to prognose the physical properties in process of micro-structure creation. From this point of view, we develop the graph theory application with one important novelty to understand and calculate the property values, instead only at the samples surface, in the micro-structure grains and pores levels. We understand the differences between the structure and morphology in synthesized and nanocrystalin diamonds, but here in this paper we just, on the thermophysical field characteristics, develop the first phase new frontiers.

New frontiers in applications of graph theory

Graph theory is already implemented on modelling the processes, in order to calculate physical characteristics of materials [1-4], and modelling some parameters of electrophysyical nature [5]. Graphs are simple and easy for use. They are visual and there are a large number of possibilities for applications, especially if we use graph matrices. Application of graphs in research of intergranular impedances is introduced in [6]. The concept of graph theory application and artificial neural networks is a part of our extended research in the field of electronic ceramic materials, sintering science and micro-structure analysis and related phenomena especially based on fractal nature analysis and involved corrections [7-13].

In order to *granulate* and distribute-disperse the grains, by associating graph vertices at the top of the grain and at the bottom of the grain there are researches and results focused on 1-D, 2-D, and 3-D graphs [2, 3, 5]. This novel approach offers variety of further possibilities, especially if we locate vertices in some imaginary points, at positions in the middle of a grain, or in the space between grains. In this paper v represents any electrothermical or magnetic property for our interest, in this paper particulary thermal conductivity.

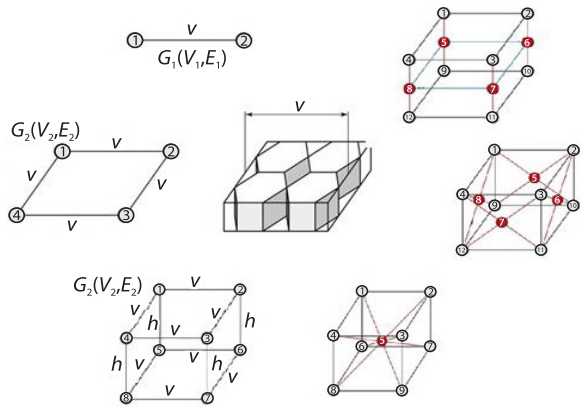

Figure 1. Different (1-D, 2-D, and 3-D) graph representations of 2 × 2 × 1 sample (diamond particle, considered as grain sample, shown in the middle)

In previous works there were applications of 1-D graph with two vertices, 2-D graphs with four vertices, and 3-D graphs with eight vertices. There were, also, applications using other geometrical shapes or displacement of vertices, inside graph, especially in 3-D case, in order to mapp simple 2 × 2 × 1 sample, on those various shapes. Some of them are shown in fig. 1.

Very important results, based on 3-D graph theory application, within the measurements and calculation the values of some thermophysical parameters on microstructural level,

are chosen to be scope of this research. This direction came over our previous results by implementation graph theory, see [2, 3], which are considering capacity as the parameter. So, this is some kind of top of the pyramidal hierarchy structure, with the essence of graph theory applied in electronic, ceramics, materials area.

Using this method, developed in acccordance to results [3-5], we disposed completely new approach for getting much more precise value calculations of conductivity, which are concretely connected with experimental sources. Based on graph theory we can dispose one unique reviewed feature, which explains what have we done and what can we do in next steps [14, 15].

Experimental methods for measurment of thermal conductivity

In order to obtain the cross-plane thermal conductivity of nanocrystalline diamond films, we employed the 3ω-method [16]. To this end, a thin metal line, placed on the surface of the diamond layer is used as heater and thermometer. A current $I_{1\omega}$ with angular frequency ω is applied to the heater. The linear dependence of the resistance on temperature leads to a voltage component $U_{3\omega}$ with angular frequency 3ω that can be measured by means of a lock-in amplifier. Knowing the linear temperature coefficient of the resistance:

$$\alpha = \frac{1}{R_0}\frac{\mathrm{d}R}{\mathrm{d}T}$$

where the voltage $U_{3\omega}$ and current $I_{1\omega}$ can be used to calculate the temperature oscillation of the metal line:

$$\Delta T = \frac{2U_{3\omega}}{\alpha R_0 I_{1\omega}}$$

When the thin metal heater is placed directly on a semi-infinite substrate, the amplitude of the temperature oscillation can be calculated:

$$\Delta T_{\mathrm{subs}} = -\left(\frac{P}{l\pi\lambda}\right)\left[\ln(\omega) - \ln\left(\frac{ib^2}{D}\right) + \mathrm{const}\right]$$

When a thin film exists between the heater stripe and the semi-infinite substrate, an additional, frequency independent temperature drop is added across the film with thickness t and thermal conductivity λ_{film}. This offset can be expressed:

$$\Delta T_{\mathrm{film}} = \frac{Pt}{2lb\lambda_{\mathrm{film}}}$$

Hence, the temperature oscillation measured by the metal line is $\Delta T = \Delta T_{\mathrm{subs}} + \Delta T_{\mathrm{film}}$. The thermal resistance that is added by the thin film consists however of the thermal resistance of the film and the additional interface resistance between the heater and the film, as well as the interface resistance between the film and the substrate. Since the interface resistance between gold and diamond is known, the interface resistance between the diamond layers and the silicon substrate can be obtained by the measurement of several films with different thicknesses [17].

In our experiment, we obtained some experimental results, for thermal conductivity, that are shown in tab. 1.

Table 1. Thermal conductivity in dependence of grain size

Grain size [nm]	6.00	7.40	9.30	9.80	12.30	12.90	13.60	14.60
Thermal conductivity [$W^{-1}mK^{-1}$]	0.56	1.29	5.92	9.28	22.35	13.66	27.70	38.21

We will use those results in following theoretical experiment.

Theoretical experiment

Theoreticaly, we will split the diamond surface into a small particles. On each of them we will implement similar approach like with grains in [18-20]. Lets consider one infinitely small part of diamond surface, of *dimension* 2 × 2 × 1, shown in the middle of fig. 1. We will locate graph vertices in upper surface of diamond, then vertices on lower surface of diamond. Additionally, we can locate some vertices in the middle of the diamond sample, shown on fig. 2(a). This will be basis for construction of appropriate 3-D graph, for simulation and calculation of thermoconductiv property on this sample, between vertices of our graph. This graph is shown on fig. 2(b).

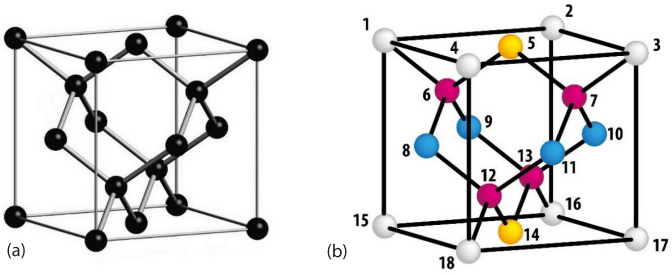

Figure 2. Diamond internal structure and appropriate 3-D graph model

We will use this graph model and we will calculate elements of weight matrix fro that graph. This matrix will represent thermoconductive properties between vertices in graph *i.e.* between parts of sample. We can assume that thermoconductivity will be noted with v, and we can assign values on those graph edges, so we can represent this graph with weight matrix W.

Graph $G = (V, E)$, has a set of vertices $V = \{1, 2, 3,... 18\}$ and a set of edges:

$$E = \{\{1,2\}, \{1,4\},\{1,6\},\{1,15\},\{2,3\},\{2,16\},\{3,4\},\{3,7\},\{3,17\},\{4,18\},\{5,6\},\{5,7\},$$
$$\{6,8\},\{6,9\}, \{7,10\},\{7,11\},\{8,12\}, \{9,13\}, \{10,13\}, \{11,12\},\{12,14\}, \{12,18\},\{13,14\},$$
$$\{13,16\},\{15,16\},\{15,18\},\{16,17\},\{17,18\}$$

Horizontal edges of this graph will have weight v, direct *vertical* edge also v, and *skew* edges, through the structure, with weight $v/4$. It is divided with 4, because in this model every algebraic path through this graph, starting from upper surface down to lower surface, consist from 4 edges, *i.e.* length of algebraic path is 4.

Results and discussion

First particular case of measured thermalconductivity, from tab. 1, will map to graph with a set of 18 vertices and 28 edges, and corresponding weight matrices. Size of grain is 6.00 nm and thermal conductivity 0.56 W/mK, fig. 3.

$$W = \begin{bmatrix}
0 & 0.56 & 0 & 0.56 & 0 & 0.14 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.56 & 0 & 0 & 0 \\
0.56 & 0 & 0.56 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.56 & 0 & 0 \\
0 & 0.56 & 0 & 0.56 & 0 & 0 & 0.14 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.56 & 0 \\
0.56 & 0 & 0.56 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.56 \\
0 & 0 & 0 & 0 & 0 & 0.14 & 0.14 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0.14 & 0 & 0 & 0 & 0.14 & 0 & 0 & 0.14 & 0.14 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0.14 & 0 & 0.14 & 0 & 0 & 0 & 0 & 0.14 & 0.14 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0.14 & 0 & 0 & 0 & 0 & 0 & 0.14 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0.14 & 0 & 0 & 0 & 0 & 0 & 0 & 0.14 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0.14 & 0 & 0 & 0 & 0 & 0 & 0.14 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0.14 & 0 & 0 & 0 & 0 & 0.14 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.14 & 0 & 0 & 0.14 & 0 & 0 & 0.14 & 0 & 0 & 0 & 0.14 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.14 & 0.14 & 0 & 0 & 0 & 0.14 & 0 & 0.14 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.14 & 0.14 & 0 & 0 & 0 & 0 & 0 \\
0.56 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.56 & 0 & 0.56 \\
0 & 0.56 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.14 & 0 & 0.56 & 0 & 0.56 & 0 \\
0 & 0 & 0.56 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.56 & 0 & 0.56 \\
0 & 0 & 0 & 0.56 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.14 & 0 & 0 & 0.56 & 0 & 0.56 & 0
\end{bmatrix}$$

Same type of graph, for grain size 7.40 nm and thermal conductivity 1.29 W/mK, has matrix fig. 4:

$$W = \begin{bmatrix}
0 & 1.29 & 0 & 1.29 & 0 & 0.325 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.29 & 0 & 0 & 0 \\
1.29 & 0 & 1.29 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.29 & 0 & 0 \\
0 & 1.29 & 0 & 1.29 & 0 & 0 & 0.325 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.29 & 0 \\
1.29 & 0 & 1.29 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.29 \\
0 & 0 & 0 & 0 & 0 & 0.325 & 0.325 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0.325 & 0 & 0 & 0 & 0.325 & 0 & 0 & 0.325 & 0.325 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0.325 & 0 & 0.325 & 0 & 0 & 0 & 0 & 0.325 & 0.325 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0.325 & 0 & 0 & 0 & 0 & 0 & 0.325 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0.325 & 0 & 0 & 0 & 0 & 0 & 0 & 0.325 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0.325 & 0 & 0 & 0 & 0 & 0 & 0.325 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0.325 & 0 & 0 & 0 & 0 & 0.325 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.325 & 0 & 0 & 0.325 & 0 & 0 & 0.325 & 0 & 0 & 0 & 0.325 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.325 & 0.325 & 0 & 0 & 0 & 0.325 & 0 & 0.325 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.325 & 0.325 & 0 & 0 & 0 & 0 & 0 \\
1.29 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.29 & 0 & 1.29 \\
0 & 1.29 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.325 & 0 & 1.29 & 0 & 1.29 & 0 \\
0 & 0 & 1.29 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.29 & 0 & 1.29 \\
0 & 0 & 0 & 1.29 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.325 & 0 & 0 & 1.29 & 0 & 1.29 & 0
\end{bmatrix}$$

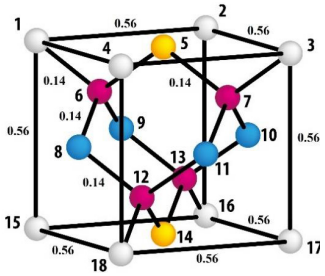

Figure 3. Graph for size of grain 6.00 nm and thermal conductivity 0.56 W/mK

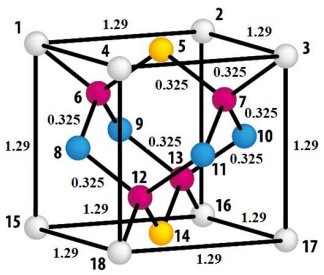

Figure 4. Graph for size of grain 7.40 nm and thermal conductivity 1.29 W/mK

Same type of graph, for grain size 9.30 nm and thermal conductivity 5.92 W/mK, has matrix fig. 5:

$$W = \begin{bmatrix}
0 & 5.92 & 0 & 5.92 & 0 & 1.48 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 5.92 & 0 & 0 & 0 \\
5.92 & 0 & 5.92 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 5.92 & 0 & 0 \\
0 & 5.92 & 0 & 5.92 & 0 & 0 & 1.48 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 5.92 & 0 \\
5.92 & 0 & 5.92 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 5.92 \\
0 & 0 & 0 & 0 & 0 & 1.48 & 1.48 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1.48 & 0 & 0 & 0 & 1.48 & 0 & 0 & 1.48 & 1.48 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1.48 & 0 & 1.48 & 0 & 0 & 0 & 0 & 1.48 & 1.48 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1.48 & 0 & 0 & 0 & 0 & 0 & 1.48 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1.48 & 0 & 0 & 0 & 0 & 0 & 0 & 1.48 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1.48 & 0 & 0 & 0 & 0 & 0 & 1.48 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1.48 & 0 & 0 & 0 & 0 & 1.48 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.48 & 0 & 0 & 1.48 & 0 & 0 & 1.48 & 0 & 0 & 0 & 1.48 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.48 & 1.48 & 0 & 0 & 0 & 1.48 & 0 & 1.48 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.48 & 1.48 & 0 & 0 & 0 & 0 & 0 \\
5.92 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 5.92 & 0 & 5.92 \\
0 & 5.92 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.48 & 0 & 5.92 & 0 & 5.92 & 0 \\
0 & 0 & 5.92 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 5.92 & 0 & 5.92 \\
0 & 0 & 0 & 5.92 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.48 & 0 & 0 & 5.92 & 0 & 5.92 & 0
\end{bmatrix}$$

Same type of graph, for grain size 9.80 nm and thermal conductivity 9.28 W/mK, has matrix fig. 6:

$$W = \begin{bmatrix}
0 & 9.28 & 0 & 9.28 & 0 & 2.32 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 9.28 & 0 & 0 & 0 \\
9.28 & 0 & 9.28 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 9.28 & 0 & 0 \\
0 & 9.28 & 0 & 9.28 & 0 & 0 & 2.32 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 9.28 & 0 \\
9.28 & 0 & 9.28 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 9.28 \\
0 & 0 & 0 & 0 & 0 & 2.32 & 2.32 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
2.32 & 0 & 0 & 0 & 2.32 & 0 & 0 & 2.32 & 2.32 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 2.32 & 0 & 2.32 & 0 & 0 & 0 & 0 & 2.32 & 2.32 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 2.32 & 0 & 0 & 0 & 0 & 0 & 2.32 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 2.32 & 0 & 0 & 0 & 0 & 0 & 0 & 2.32 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 2.32 & 0 & 0 & 0 & 0 & 0 & 2.32 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 2.32 & 0 & 0 & 0 & 0 & 2.32 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 2.32 & 0 & 0 & 2.32 & 0 & 0 & 2.32 & 0 & 0 & 0 & 2.32 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2.32 & 2.32 & 0 & 0 & 0 & 2.32 & 0 & 2.32 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2.32 & 2.32 & 0 & 0 & 0 & 0 & 0 \\
9.28 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 9.28 & 0 & 9.28 \\
0 & 9.28 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2.32 & 0 & 9.28 & 0 & 9.28 & 0 \\
0 & 0 & 9.28 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 9.28 & 0 & 9.28 \\
0 & 0 & 0 & 9.28 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2.32 & 0 & 0 & 9.28 & 0 & 9.28 & 0
\end{bmatrix}$$

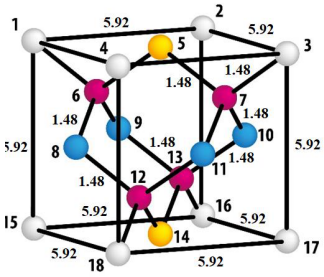

Figure 5. Graph for size of grain 9.30 nm and thermal conductivity 5.92 W/mK

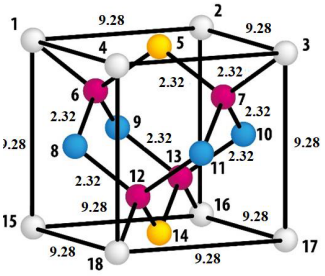

Figure 6. Graph for size of grain 9.80 nm and thermal conductivity 9.28 W/mK

Graph for grain size 12. 30 nm and thermal conductivity 22.35 W/mK, has matrix, fig 7:

$$W = \begin{bmatrix}
0 & 22.35 & 0 & 22.35 & 0 & 5.59 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 22.35 & 0 & 0 & 0 \\
22.35 & 0 & 22.35 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 22.35 & 0 & 0 \\
0 & 22.35 & 0 & 22.35 & 0 & 0 & 5.59 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 22.35 & 0 \\
22.35 & 0 & 22.35 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 22.35 \\
0 & 0 & 0 & 0 & 0 & 5.59 & 5.59 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
5.59 & 0 & 0 & 0 & 5.59 & 0 & 0 & 5.59 & 5.59 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 5.59 & 0 & 5.59 & 0 & 0 & 0 & 0 & 5.59 & 5.59 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 5.59 & 0 & 0 & 0 & 0 & 0 & 5.59 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 5.59 & 0 & 0 & 0 & 0 & 0 & 0 & 5.59 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 5.59 & 0 & 0 & 0 & 0 & 0 & 5.59 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 5.59 & 0 & 0 & 0 & 0 & 5.59 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 5.59 & 0 & 0 & 5.59 & 0 & 0 & 5.59 & 0 & 0 & 0 & 5.59 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 5.59 & 5.59 & 0 & 0 & 0 & 5.59 & 0 & 5.59 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 5.59 & 5.59 & 0 & 0 & 0 & 0 & 0 \\
22.35 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 22.35 & 0 & 22.35 \\
0 & 22.35 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 5.59 & 0 & 22.35 & 0 & 22.35 & 0 \\
0 & 0 & 22.35 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 22.35 & 0 & 22.35 \\
0 & 0 & 0 & 22.35 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 5.59 & 0 & 0 & 22.35 & 0 & 22.35 & 0
\end{bmatrix}$$

Graph for grain size 12.90 nm and thermal conductivity 13.66 W/mK, fig. 8:

$$W = \begin{bmatrix}
0 & 13.66 & 0 & 13.66 & 0 & 3.415 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 13.66 & 0 & 0 & 0 \\
13.66 & 0 & 13.66 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 13.66 & 0 & 0 \\
0 & 13.66 & 0 & 13.66 & 0 & 0 & 3.415 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 13.66 & 0 \\
13.66 & 0 & 13.66 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 13.66 \\
0 & 0 & 0 & 0 & 0 & 3.415 & 3.415 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
3.415 & 0 & 0 & 0 & 3.415 & 0 & 0 & 3.415 & 3.415 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 3.415 & 0 & 3.415 & 0 & 0 & 0 & 0 & 3.415 & 3.415 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 3.415 & 0 & 0 & 0 & 0 & 0 & 3.415 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 3.415 & 0 & 0 & 0 & 0 & 0 & 0 & 3.415 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 3.415 & 0 & 0 & 0 & 0 & 0 & 3.415 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 3.415 & 0 & 0 & 0 & 0 & 3.415 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 3.415 & 0 & 0 & 3.415 & 0 & 0 & 3.415 & 0 & 0 & 0 & 3.415 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3.415 & 3.415 & 0 & 0 & 0 & 3.415 & 0 & 3.415 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3.415 & 3.415 & 0 & 0 & 0 & 0 & 0 \\
13.66 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 13.66 & 0 & 13.66 \\
0 & 13.66 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3.415 & 0 & 13.66 & 0 & 13.66 & 0 \\
0 & 0 & 13.66 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 13.66 & 0 & 13.66 \\
0 & 0 & 0 & 13.66 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3.415 & 0 & 0 & 13.66 & 0 & 13.66 & 0
\end{bmatrix}$$

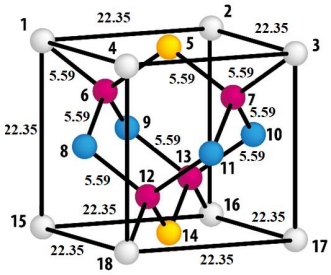

Figure 7. Graph for size of grain 12.30 nm and thermal conductivity 22.35 W/mK

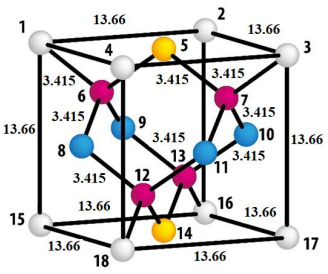

Figure 8. Graph for size of grain 12.90 nm and thermal conductivity 13.66 W/mK

Graph for grain size 13.60 nm and thermal conductivity 27.70 W/mK, fig. 9:

$$W = \begin{bmatrix}
0 & 27.70 & 0 & 27.70 & 0 & 6.925 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 27.70 & 0 & 0 & 0 \\
27.70 & 0 & 27.70 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 27.70 & 0 & 0 \\
0 & 27.70 & 0 & 27.70 & 0 & 0 & 6.925 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 27.70 & 0 \\
27.70 & 0 & 27.70 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 27.70 \\
0 & 0 & 0 & 0 & 0 & 6.925 & 6.925 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
6.925 & 0 & 0 & 0 & 6.925 & 0 & 0 & 6.925 & 6.925 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 6.925 & 0 & 6.925 & 0 & 0 & 0 & 0 & 6.925 & 6.925 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 6.925 & 0 & 0 & 0 & 0 & 0 & 6.925 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 6.925 & 0 & 0 & 0 & 0 & 0 & 0 & 6.925 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 6.925 & 0 & 0 & 0 & 0 & 0 & 6.925 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 6.925 & 0 & 0 & 0 & 0 & 6.925 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 6.925 & 0 & 0 & 6.925 & 0 & 0 & 6.925 & 0 & 0 & 0 & 6.925 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 6.925 & 6.925 & 0 & 0 & 0 & 6.925 & 0 & 6.925 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 6.925 & 6.925 & 0 & 0 & 0 & 0 & 0 \\
27.70 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 27.70 & 0 & 27.70 & 0 \\
0 & 27.70 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 6.925 & 0 & 27.70 & 0 & 27.70 & 0 \\
0 & 0 & 27.70 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 27.70 & 0 & 27.70 \\
0 & 0 & 0 & 27.70 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 6.925 & 0 & 0 & 27.70 & 0 & 27.70 & 0
\end{bmatrix}$$

Graph for grain size 14.60 nm and thermal conductivity 38.21 W/mK, fig. 10:

$$W = \begin{bmatrix}
0 & 38.21 & 0 & 38.21 & 0 & 9.552 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 38.21 & 0 & 0 & 0 \\
38.21 & 0 & 38.21 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 38.21 & 0 & 0 \\
0 & 38.21 & 0 & 38.21 & 0 & 0 & 9.552 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 38.21 & 0 \\
38.21 & 0 & 38.21 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 38.21 \\
0 & 0 & 0 & 0 & 0 & 9.552 & 9.552 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
9.552 & 0 & 0 & 0 & 9.552 & 0 & 0 & 9.552 & 9.552 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 9.552 & 0 & 9.552 & 0 & 0 & 0 & 0 & 9.552 & 9.552 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 9.552 & 0 & 0 & 0 & 0 & 0 & 9.552 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 9.552 & 0 & 0 & 0 & 0 & 0 & 0 & 9.552 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 9.552 & 0 & 0 & 0 & 0 & 0 & 9.552 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 9.552 & 0 & 0 & 0 & 0 & 9.552 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 9.552 & 0 & 0 & 9.552 & 0 & 0 & 9.552 & 0 & 0 & 0 & 9.552 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 9.552 & 9.552 & 0 & 0 & 0 & 9.552 & 0 & 9.552 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 9.552 & 9.552 & 0 & 0 & 0 & 0 & 0 \\
38.21 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 38.21 & 0 & 38.21 & 0 \\
0 & 38.21 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 9.552 & 0 & 38.21 & 0 & 38.21 & 0 \\
0 & 0 & 38.21 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 38.21 & 0 & 38.21 \\
0 & 0 & 0 & 38.21 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 9.552 & 0 & 0 & 38.21 & 0 & 38.21 & 0
\end{bmatrix}$$

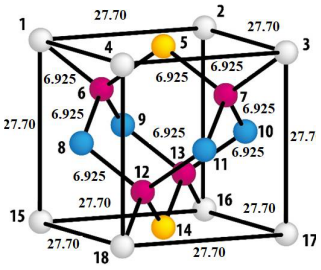

Figure 9. Graph for size of grain 13.60 nm and thermal conductivity 27.70 W/mK

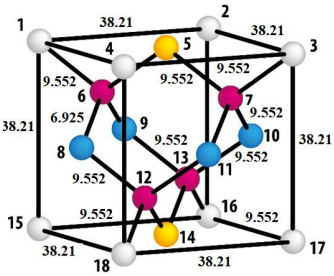

Figure 10. Graph for size of grain 14.60 nm and thermal conductivity 38.21 W/mK

Outlook

In the future research, we plan to correlate graph theory application on electrical conductivity in correlation with thermal conductivity. Also, we assume that is very interesting to compare the results based on neural networks and graph application, simultaneously.

Conclusion

The nanocrystalline synthetized diamonds are very advanced materials for high tech applications esspecially in medicine, electronic and space research. In our research we applied the graph theory with thermal conductivity in synthetized diamonds. In this paper we present the complex relation between graph theory and consolidated nanodiamond thermophysical parameters. We presented related experimental procedure with corresponding results. This novelty as graph applications, have the great importance in creating the additional ideas in thermal conductivity phenomena analysis, better understanding. Before the graph and neural network theories applications, we have used different experimental methods for measurements and collecting the physical parameters from the samples surfaces. Now we can define values directly at the level of the grains and pores, and, also, between them. Based on this method we provided way for defining the thermophysical parameters on micro and nanograins and pores constituents, what is important for advance predicting microelectronic structures and related parameters.

References

[1] Mitić, V. V., *et al.*, Fractal Microeletronic Frontiers and Graph Theory Applications, *Proceedings*, Int. Conf. MS&T 2019, Portland, Ore., USA, 2019
[2] Mitic, V. V., *et al.*, Graph Theory Applied to Microelectronic Intergranular Relations, *Ferroelectrics*, *570* (2021), 1, pp. 145-152
[3] Randjelovic, B, *et al.*, Ceramics, Materials, Microelectronics and Graph Theory new Frontiers, *Modern Physic Lett. B*, *34* (2020), 34, pp. 2150-2159
[4] Randjelovic, B. M., *et al*., The 3D-Graph Approach for Breakdown Voltage Calculation on $BaTiO_3$-Ceramics, *Int. J. of Modern Physic B*, *35* (2021), 6, 2150103
[5] Randjelović, B., Nikolić, Z., Graph Theory Applied to Modelling and Simulation of Mevolution in Sintering, Advanced Ceramics and Applications VIII, in: *New Frontiers in Multifunctional Material Science and Processing*, Invited Lecture, Book of Abstracts, (Eds. V. Mitić, *et al*.), Belgrade, Serbian Ceramic Society, Vol. 23-25, 2019, p. 38
[6] Randjelovic, B. M., *et al*., Graph Theory Approach in Synthetized Diamonds Electrophysical Parameters Defining, in: *Biocompatible and Biomimetic Features of Materials for Biomedical Applications – New Insights*, Springer, Heiberberg, Germany, 2021
[7] Mitić, V. V., *et al*., Entropy and Fractal Nature, *Thermal Science*, *24* (2020), 3, pp. 2203- 2212
[8] Mitić, V. V., *et al*., Butler-Volmer Current Equation and Fractal Nature Correction in Electrochemical Energy, *Thermal Science*, *25* (2021), 3A, pp. 1837-1848
[9] Mitic, V. V., *et al*., Fractal Frontiers in Microelectronic Ceramic Materials, *Ceramics International*, *45* (2019), 7, Part B, pp. 9679-9685
[10] Mitic, V. V., *et al*., Electronic Ceramics Fractal Microstructure Analysis-Minkowski Hull and Grain Boundaries, *Ferroelectrics*, *545* (2019), 1, pp. 184-194
[11] Mitic, V. V., *et al*., Neural Networks and Microelectronic Parameters Distribution Measurements Depending on Sinthering Temperature and Applied Voltage, *Modern Physic Letters B*, *34* (2020), 35, 2150172
[12] Mitic, V. V., *et al*., Structures, Fractals and Energy. Nanotechnology for Energy Sustainability, (Eds. Baldev, R., *et al*.), Wiley-VCH Verlag GmbH & Co. KGaA, Germany, 2017, Vol. 3
[13] Randjelovic, B., *et al*., Model for Simulation of Intergranular μ-Capacitance as a Function of Neck Growth in Ceramic Sintering (Eds, Daras N., Rassias T.), in: *Computational Mathematics and Variational Analysis*, Springer Opt. and Its Appl. 159, Springer, Heiberberg, Germany, 2020, pp. 403-420
[14] Ilić, I., Weak Convergence of Product of Sums of Independent Variables with Missing Values, *Filomat*, *24* (2010), 3, p p. 73-81

[15] Ilić, I., Veličković, V., Simple Tail Index Estimation for Dependent and Heterogeneous Data with Missing Values, *Brazilian Journal of Probability and Statistics*, *33* (2019), 1, pp. 192-203
[16] Cahill, D. G., Pohl, R. O., Thermal Conductivity of Amorphous Solids Above the Plateau, *Phys. Rev. B*,. *35* (1987), 8, pp. 4067-4073
[17] Mohr, M., *et al.*, Influence of Grain Boundaries on Elasticity and Thermal Conductivity of Nanocrystalline Diamond Films, *Acta Materiali*a, *122* (2017), Jan., pp. 92-98
[18] Mohr, M., *et al*., *Neuartige Nanostrukturierte Diamantschichten Mit Optimierten Mechanischen*, Elektrischen und Thermischen Eigenschaften (in German), Diss. Universit At Ulm, uLM, Germany, 2017
[19] Wiora, N., *et al*., Grain Boundary Dominated Electrical Conductivity in Ultrananocrystalline Diamond, *Journal Appl. Phys*., *145102* (2017), 122
[20] Mitic, V. V., *et al.*, Exploring Fractality of Microcrystalline Diamond Films, *AIP Advances*, *8* (2018), 075024

Paper submitted: April 22, 2021
Paper revised: July 21, 2021
Paper accepted: July 30, 2021