An Overview on a Graph Theory Applications New Frontiers in Electronics Materials

Vojislav V.Mitic, Branislav Randjelovic, Dusan Milosevic, Srdjan Ribar, Ivana Radovic, Markus Mohr and Hans Jorg Fecht

***Abstract* — This paper are new exciting results and an overview in graph theory applications on various problems in electronic materials. This opens new frontiers in this field. There are a lot of scientific efforts, especially during last few years. Our research team made very significant contribution, particulary related to calculation of parameters of BaTiO3 ceramics, calculation of syntetized diamonds electrophysical parameters, modelling of microeletronic intergranular relations and use of materials in medicine, based on biomimetic. We also discuss interesting possibilities for further research.**

***Index Terms* — graph theory; nanostructures; ceramics.**

I. Introduction

Graph theory application in synthesis of ceramic materials with control on phenomena between the grains is very challenging (see [1-5]), especially combined or compared with fractals and neural networks applications. It could enable design of the material with specific functionalities and widen the field and conditions for their application. Properties on the grain boundary can be calculated and analyzed based on the values measured on bulk materials samples (for methods of measurement see [1,3,4,5,8]). Possibility of using graph theory for determination of dielectric properties at the grain boundary of modified $BaTiO_3$ ceramics, based on the properties measured on the bulk samples is shown. This opens completely new perspectives in the area of miniaturization and micropackaging, because electrical-electronic-dielectric parameters values are calculated on a micro level (see [3, 6-9]).

Vojislav V.Mitić is with Faculty of Electrical Engineering, University of Nis, 14 Aleksandra Medvedeva, 18000 Belgrade, Serbia (e-mail: vmitic.d2480@gmail.com).

Branislav M.Randjelović is with Faculty of Electrical Engineering, University of Nis, 14 Aleksandra Medvedeva, 18000 Belgrade, Serbia (e-mail: bane@elfak.ni.ac.rs).

Dusan Milosević is with Faculty of Electrical Engineering, University of Nis, 14 Aleksandra Medvedeva, 18000 Belgrade, Serbia (e-mail: dusan.milosevic@elfak.ni.ac.rs).

Srdjan Ribar is with Faculty of Mechanical Engineering, University of Belgrade, Kraljice Marije 16, 11120 Belgrade Serbia, Belgrade, Serbia (e-mail: srdjanribar@gmail.com).

Ivana Radovic is with Institute of Nuclear Sciences 'VINČA', University of Belgrade, Mike Petrovica Alasa 12-14, 11000 Belgrade, Serbia (e-mail: ivanaradovic.80@gmail.com).

Markus Mohr is with University of Ulm, Institute of Functional Nanosystems, Ulm, Germany (e-mail: markus.mohr@uni-ulm.de).

Hans J. Fecht is with University of Ulm, Institute of Functional Nanosystems, Ulm, Germany (e-mail: hans.fecht@uni-ulm.de).

II. Graph Theory in Intergranular Relations

We have 3D structure of synthesized electronic material that should be presented or modelled using graph theory for calculation of parameters at grain boundary ([2]), shown on Fig.1. Let us consider 1D and 2D case, because this 2D case could be, later, easily generalized and mapped onto some 3D case.

A. Modelling with 1D and 2D graphs

In order to establish appropriate theoretical experiment, through which we will model this sintered plate with graph [2], lets simplify, and instead of 2D case (Fig.2), we will take one of 1D cases (Fig.3):

Fig. 1. Structure of grains (3D case)

Fig. 2. Structure of grains according to 2D case

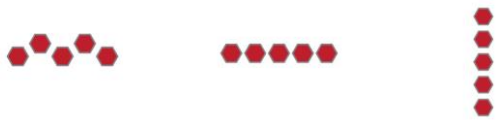

Fig. 3. Structure of grains according to 1D case

Now, let us make graph from one of those cases, for example the last one (vertical arrangement) with n=5 grains. Our goal is to get overall results in change of capacitance, in relation with those (measured) overall results. So, we have graphs, shown on Fig.4 (see [5]).

If we use experimental results from [5] and divide overall capacitance change to a local measure, between two grains, for example, for n=5 and for DC bias 25V, we have overall

capacity change 69.45. This means that between neighboring vertices in graph we have capacity change $\frac{\Delta C}{C}$ of

$$\frac{\Delta C}{C} = 69.45 / (n-1) = 69.45 / 4 = 17.3625$$

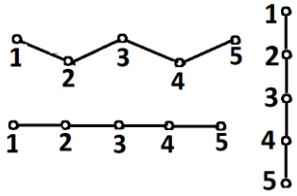

Fig. 4. Modelling with 1D graphs

Appropriate matrix of this graph (for n=5) is

$$A = \begin{bmatrix} 0 & 17.3625 & 0 & 0 & 0 \\ 17.3625 & 0 & 17.3625 & 0 & 0 \\ 0 & 17.3625 & 0 & 17.3625 & 0 \\ 0 & 0 & 17.3625 & 0 & 17.3625 \\ 0 & 0 & 0 & 17.3625 & 0 \end{bmatrix}$$

In that case, we have parallel connection of capacity changes, and overall capacity change is equal to 68.73 (see [10]).

For results in same experiment (see [5]), for n=5 and for DC bias 95V, we have overall capacity change 100.97. This means that between neighboring vertices in graph we have capacity change $\frac{\Delta C}{C}$ of

$$\frac{\Delta C}{C} = 100.97/(n-1) = 100.97/4 = 25.2425$$

Appropriate neighboring matrix of this graph (for n=5) is

$$A = \begin{bmatrix} 0 & 25.2425 & 0 & 0 & 0 \\ 25.2425 & 0 & 25.2425 & 0 & 0 \\ 0 & 25.2425 & 0 & 25.2425 & 0 \\ 0 & 0 & 25.2425 & 0 & 25.2425 \\ 0 & 0 & 0 & 25.2425 & 0 \end{bmatrix}$$

In that case, we have parallel connection of capacity changes, and overall capacity change is equal to 100.97 (see [5]).

Let us make graph from one of 2D cases, for example with n=8 graines (see [5], see Fig.5). So, we have graph with same number of vertices (n=8),

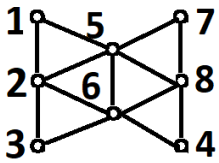

Fig. 5. Modelling with 2D graphs

If we use experimental results from [5] and if we divide overall capacitance change to local measure that characterizes relation between two grains (two vertices in graph). For example, for DC bias of 25V, we have overall capacity change of 69.45. This means that for *n=8, m=13* and for between neighboring vertices in graph we have capacity change $\frac{\Delta C}{C}$ of

$$\frac{\Delta C}{C} = 69.45/(n-1) = 69.45/12 = 5.7875$$

Appropriate neighboring matrix of this graph (see [10]) is

$$A = \begin{bmatrix} 0 & 5.7875 & 0 & 0 & 5.7875 & 0 & 0 & 0 \\ 5.7875 & 0 & 5.7875 & 0 & 5.7875 & 5.7875 & 0 & 0 \\ 0 & 5.7875 & 0 & 0 & 0 & 5.7875 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 5.7875 & 0 & 5.7875 \\ 5.7875 & 5.7875 & 0 & 0 & 0 & 5.7875 & 5.7875 & 5.7875 \\ 0 & 5.7875 & 5.7875 & 5.7875 & 5.7875 & 0 & 0 & 5.7875 \\ 0 & 0 & 0 & 0 & 5.7875 & 0 & 5.7875 & 0 \\ 0 & 0 & 0 & 5.7875 & 5.7875 & 5.7875 & 5.7875 & 0 \end{bmatrix}$$

This results to overall capacitance change equal to 68.73.

B. Modelling with 3D graphs

We will now apply 3D graphs on calculation of breakdown voltage on $BaTiO_3$ sample (see [1]) with some predefined constraints. Relation between grains in sample is established and described and now we have mathematical approach for calculation of breakdown voltage using experimental results. As a result, we introduced mapping between property of sample and grain structure, then between grain structure and mathematical graph, using various crystal structures. The main idea was to apply 3D-graph theory for distribution of electronic parameters between the neighboring grains. We will use simple $BaTiO_3$ sample, shown on Fig.6.

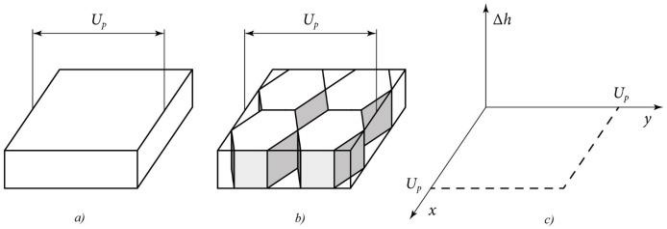

Fig. 6. $BaTiO_3$ sample with 4 grains.

Breakdown voltage U_p is obtained by measuring on whole sample, i.e.it is measured on two opposite sides of this sample. It is same in both directions, along x-axis and along y-axis (Fig. 2). Third dimension will be denoted with Δh, and that is vertical size of this sample, distance between top and bottom of the sample (tom and bottom of the grain).

If we do mapping of this grain sample (see [1]), onto 3D graph with eight vertices, shown on Fig.7. We put vertices on the top of each grain and at the bottom of each grain, assuming that there is also some value of U_p between grain ends. Breakdown voltage is very small and it can be neglected, leaving $U_p = \delta$, ($\delta \approx 0$). Assume that "dimensions" of this problem are now $x = 2$, $y = 2$ and $\Delta h = 2$.

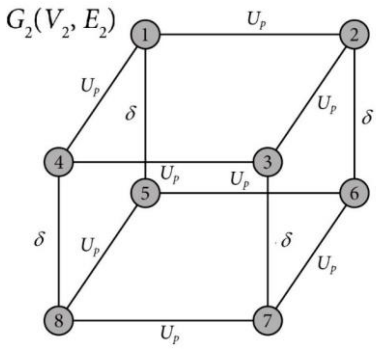

Fig. 7. 3D graph model of 2x2 grain sample, with 8 vertices.

Graph $G_2 = (V_2, E_2)$, has 8 vertices and 12 edges. Corresponding weight matrix of this graph is:

$$W_2 = \begin{bmatrix} 0 & U_p & 0 & U_p & \delta & 0 & 0 & 0 \\ U_p & 0 & U_p & 0 & 0 & \delta & 0 & 0 \\ 0 & U_p & 0 & U_p & 0 & 0 & \delta & 0 \\ U_p & 0 & U_p & 0 & 0 & 0 & 0 & \delta \\ \delta & 0 & 0 & 0 & 0 & U_p & 0 & U_p \\ 0 & \delta & 0 & 0 & U_p & 0 & U_p & 0 \\ 0 & 0 & \delta & 0 & 0 & U_p & 0 & U_p \\ 0 & 0 & 0 & \delta & U_p & 0 & U_p & 0 \end{bmatrix}$$

Each "horizontal" (along x-axis and along y-axis) edge of this graph has the same weight U_p, and each "vertical" edge (between top and bottom of the grain) has the same weight δ. In the case obtained from the experiment in [1], case I-16 $BaTiO_3$ ceramics without additives, we have:

$$W_2 = \begin{bmatrix} 0 & 12.54 & 0 & 12.54 & \delta & 0 & 0 & 0 \\ 12.54 & 0 & 12.54 & 0 & 0 & \delta & 0 & 0 \\ 0 & 12.54 & 0 & 12.54 & 0 & 0 & \delta & 0 \\ 12.54 & 0 & 12.54 & 0 & 0 & 0 & 0 & \delta \\ \delta & 0 & 0 & 0 & 0 & 12.54 & 0 & 12.54 \\ 0 & \delta & 0 & 0 & 12.54 & 0 & 12.54 & 0 \\ 0 & 0 & \delta & 0 & 0 & 12.54 & 0 & 12.54 \\ 0 & 0 & 0 & \delta & 12.54 & 0 & 12.54 & 0 \end{bmatrix}, (\delta \approx 0).$$

After that, we do the mapping of the same grain sample onto 3D graph with nine vertices, shown on next Fig.8. We put vertices on "top" of each grain and also on "bottom" of each grain (see [1]), like in previous case, breakdown voltage between those ends is very small, so we will assume that it is δ. New, ninth vertex is, by BCC principle (body-centered cubic crystal system imaginary point in the middle of this sample, and its appearance rises gives dimension of this problem from 2 to 3. Assume that "dimensions" of problem are $x = 2, y = 2$ and $\Delta h = 3$.

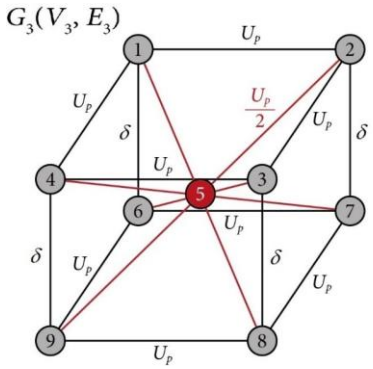

Fig. 8. 3D graph model (Body-centered in crystal system) with 9 vertices.

Graph $G_3 = (V_3, E_3)$, has a set of 9 vertices and a set of 20 edges (see [1]). Corresponding weight matrix of this graph is:

$$W_3 = \begin{bmatrix} 0 & U_p & 0 & U_p & U_p/2 & \delta & 0 & 0 & 0 \\ U_p & 0 & U_p & 0 & U_p/2 & 0 & \delta & 0 & 0 \\ 0 & U_p & 0 & U_p & U_p/2 & 0 & 0 & \delta & 0 \\ U_p & 0 & U_p & 0 & U_p/2 & 0 & 0 & 0 & \delta \\ U_p/2 & U_p/2 & U_p/2 & U_p/2 & U_p/2 & U_p/2 & U_p/2 & U_p/2 & U_p/2 \\ \delta & 0 & 0 & 0 & U_p/2 & U_p & 0 & U_p & 0 \\ 0 & \delta & 0 & 0 & U_p/2 & 0 & U_p & 0 & U_p \\ 0 & 0 & \delta & 0 & U_p/2 & U_p & 0 & U_p & 0 \\ 0 & 0 & 0 & \delta & U_p/2 & 0 & U_p & 0 & U_p \end{bmatrix}$$

Each "horizontal" edge of this graph has the same weight U_p, and each "vertical" edge, that goes "through" the grain have same weight δ. In case obtained from the experiment (see [1]), we have:

$$W_3 = \begin{bmatrix} 0 & 12.54 & 0 & 12.54 & 6.27 & \delta & 0 & 0 & 0 \\ 12.54 & 0 & 12.54 & 0 & 6.27 & 0 & \delta & 0 & 0 \\ 0 & 12.54 & 0 & 12.54 & 6.27 & 0 & 0 & \delta & 0 \\ 12.54 & 0 & 12.54 & 0 & 6.27 & 0 & 0 & 0 & \delta \\ 6.27 & 6.27 & 6.27 & 6.27 & 6.27 & 6.27 & 6.27 & 6.27 & 6.27 \\ \delta & 0 & 0 & 0 & 6.27 & 12.54 & 0 & 12.54 & 0 \\ 0 & \delta & 0 & 0 & 6.27 & 0 & 12.54 & 0 & 12.54 \\ 0 & 0 & \delta & 0 & 6.27 & 12.54 & 0 & 12.54 & 0 \\ 0 & 0 & 0 & \delta & 6.27 & 0 & 12.54 & 0 & 12.54 \end{bmatrix}, (\delta \approx 0).$$

Now, we can discuss same grain sample, mapped onto 3D graph, but now with twelve vertices, shown on Fig.9. New imaginary vertices are pointed in the middle of each surface of this sample, except upper surface and bottom surface. "Dimensions" of problem are $x = 2, y = 2$ and $\Delta h = 3$.

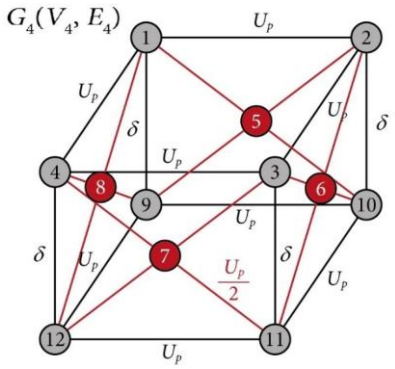

Fig. 9. 3D graph model (Face-centered in crystal system) with 12 vertices.

Corresponding weight matrix (see [1]) of this graph is

$$W_4 = \begin{bmatrix}
0 & U_p & 0 & U_p & U_p/2 & 0 & 0 & U_p/2 & \delta & 0 & 0 & 0 \\
U_p & 0 & U_p & 0 & U_p/2 & U_p/2 & 0 & 0 & 0 & \delta & 0 & 0 \\
0 & U_p & 0 & U_p & 0 & U_p/2 & U_p/2 & 0 & 0 & 0 & \delta & 0 \\
U_p & 0 & U_p & 0 & 0 & 0 & U_p/2 & U_p/2 & 0 & 0 & 0 & \delta \\
U_p/2 & U_p/2 & 0 & 0 & 0 & 0 & 0 & 0 & U_p/2 & U_p/2 & 0 & 0 \\
0 & U_p/2 & U_p/2 & 0 & 0 & 0 & 0 & 0 & 0 & U_p/2 & U_p/2 & 0 \\
0 & 0 & U_p/2 & U_p/2 & 0 & 0 & 0 & 0 & 0 & 0 & U_p/2 & U_p/2 \\
U_p/2 & 0 & 0 & U_p/2 & 0 & 0 & 0 & 0 & U_p/2 & 0 & 0 & U_p/2 \\
\delta & 0 & 0 & 0 & U_p/2 & 0 & 0 & U_p/2 & 0 & U_p & 0 & U_p \\
0 & \delta & 0 & 0 & U_p/2 & U_p/2 & 0 & 0 & U_p & 0 & U_p & 0 \\
0 & 0 & \delta & 0 & 0 & U_p/2 & U_p/2 & 0 & 0 & U_p & 0 & U_p \\
0 & 0 & 0 & \delta & 0 & 0 & U_p/2 & U_p/2 & U_p & 0 & U_p & 0
\end{bmatrix}$$

Each "horizontal" edge of this graph has same weight U_p, and each "vertical" edge, that goes "through" the grain have same weight δ. For $BaTiO_3$ ceramics (see [1]) without additives, we have:

$$W_4 = \begin{bmatrix}
0 & 12.54 & 0 & 12.54 & 6.27 & 0 & 0 & 6.27 & \delta & 0 & 0 & 0 \\
12.54 & 0 & 12.54 & 0 & 6.27 & 6.27 & 0 & 0 & 0 & \delta & 0 & 0 \\
0 & 12.54 & 0 & 12.54 & 0 & 6.27 & 6.27 & 0 & 0 & 0 & \delta & 0 \\
12.54 & 0 & 12.54 & 0 & 0 & 0 & 6.27 & 6.27 & 0 & 0 & 0 & \delta \\
6.27 & 6.27 & 0 & 0 & 0 & 0 & 0 & 0 & 6.27 & 6.27 & 0 & 0 \\
0 & 6.27 & 6.27 & 0 & 0 & 0 & 0 & 0 & 0 & 6.27 & 6.27 & 0 \\
0 & 0 & 6.27 & 6.27 & 0 & 0 & 0 & 0 & 0 & 0 & 6.27 & 6.27 \\
6.27 & 0 & 0 & 6.27 & 0 & 0 & 0 & 0 & 6.27 & 0 & 0 & 6.27 \\
\delta & 0 & 0 & 0 & 6.27 & 0 & 0 & 6.27 & 0 & 12.54 & 0 & 12.54 \\
0 & \delta & 0 & 0 & 6.27 & 6.27 & 0 & 0 & 12.54 & 0 & 12.54 & 0 \\
0 & 0 & \delta & 0 & 0 & 6.27 & 6.27 & 0 & 0 & 12.54 & 0 & 12.54 \\
0 & 0 & 0 & \delta & 0 & 0 & 6.27 & 6.27 & 12.54 & 0 & 12.54 & 0
\end{bmatrix},$$

where $\delta \approx 0$.

III. SINTETIZED DIAMONDS AS BIOMIMETIC MATERIALS

Materials science is spreading into all fields of basic and applied science. One of the biggest influence on everydays life in bioceramics materials is the application of these substrates for medical engineering (see [4]). The most prominent bio-relevant properties of a biomaterial are chemical inertness and bio-durability, so submicro diamond is coming into the center of our research interest. This diamond structure is an unique biomaterial with specific compatible characteristics, which are not exactly only one based on its bio-chemical properties. Physical-chemical biocompatibility directions, including data from nano interface water layers could be defined on nanodiamond substrates (see [4]). If we, theoretical, split diamond surface into small particles, we can implement similar approach like with grains in [5]. If we take a small part of diamond surface, of "dimension" 2x2x1 (Fig.6), we can detect and assign graph vertices in upper surface of diamond, shown on Fig.10.

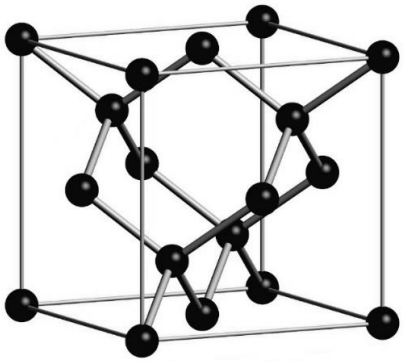

Fig. 10. Syntetized diamond internal structure.

Appropriate graph is shown on Fig.11. We can assume some property (any electrical, dielectrical or magnetic property), noted with v, and we can assign values on those graph edges, we can represent this graph (see [4]) with weight matrix W.

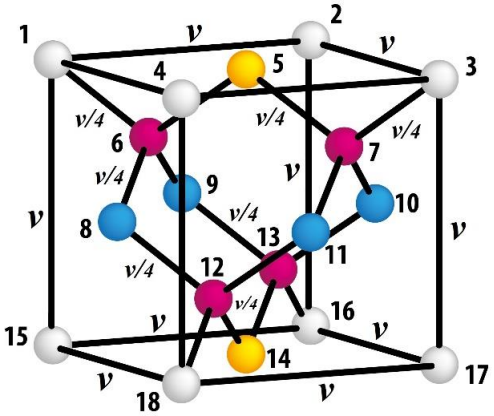

Fig. 11. 3D graph model of syntetized diamond

Weight matrix of this graph (see [4]) is:

$$W = \begin{bmatrix}
0 & v & 0 & v & 0 & v/4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & v & 0 & 0 & 0 \\
v & 0 & v & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & v & 0 & 0 \\
0 & v & 0 & v & 0 & 0 & v/4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & v & 0 \\
v & 0 & v & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & v \\
0 & 0 & 0 & 0 & 0 & v/4 & v/4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
v/4 & 0 & 0 & 0 & v/4 & 0 & 0 & v/4 & v/4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & v/4 & 0 & v/4 & 0 & 0 & 0 & 0 & v/4 & v/4 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & v/4 & 0 & 0 & 0 & 0 & 0 & v/4 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & v/4 & 0 & 0 & 0 & 0 & 0 & 0 & v/4 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & v/4 & 0 & 0 & 0 & 0 & 0 & v/4 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & v/4 & 0 & 0 & 0 & 0 & 0 & v/4 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & v/4 & 0 & 0 & v/4 & 0 & 0 & v/4 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & v/4 & v/4 & 0 & 0 & 0 & v/4 & v/4 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & v/4 & v/4 & 0 & 0 & 0 & 0 \\
v & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & v & 0 & v \\
0 & v & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & v/4 & 0 & v & 0 & v & 0 \\
0 & 0 & v & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & v & 0 & v & 0 \\
0 & 0 & 0 & v & 0 & 0 & 0 & 0 & 0 & 0 & 0 & v/4 & 0 & 0 & v & 0 & v
\end{bmatrix}$$

Each "horizontal" edge of this graph has weight v, direct "vertical" edge also has weight v, and "skew" edges, through structure has weight $v/4$. Why divided with 4? Because in this model every algebraic path through this graph, starting from upper surface down to lower surface, consist of 4 edges, length of algebraic path is 4 (see [4]).

The ultra-nanocrystalline synthetized diamonds are very advanced materials for biomedical and other applications. We pointed out to a complex relation between graph theory and electrophysical parameters of the consolidated nano-diamonds is presented. We performed and explained related experimental procedure with results data (see [4]). By this method we provided way for defining the electrophysical parameters on micro and nano level of grains and pores, what is important for further designing microelectronic structures and advance miniaturization.

IV. Outlook

In the future research, it is possible to correlate graph theory application on some other ceramic materials characteristics and to use it for some other values calculation on microlevel, for example electrical conductivity, thermal conductivity, etc. Also, it could be very important to compare the results based on neural networks and graph application, simultaneously. The nanocrystalline synthetized diamonds are very advanced materials for high-tech applications especially in medicine, electronic and space research. Further application of the graph theory decelopment could make some new and unexpected contributions in this field.

V. Conclusion

In this research paper we intended to make an overview on a complex relation between graph theory, BaTiO3-ceramics and synthetized diamonds electrophysical parameters calculations, and also designed microeletronic intergranular relations. Before the graph and neural network theories (see [10-14]), we have used different experimental methods for global measurements and collecting the physical parameters from the sample surfaces, based mostly on the statistic distribution.

Now we can define values directly at the level of the grains and pores, and, also, between them. Based on this approacch we provided a way for defining other parameters on micro and nano grains and pores constituents, what is important for advance predicting microelectronic structures and related parameters, in electronic material sciences in general.

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