Study of the Materials Microstructure using Topological Properties of Complex Networks

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Abstract. A method for mapping a two-dimensional color image of the microstructure of the material to a complex network is proposed. Each image element is assigned to a node network. A weighted combination of distance metrics – the Euclidean distance and the Manhattan distance – defines whether there is or not an edge between corresponding nodes. The first metric is used to calculate the spatial distance between the picture elements (pixels), the second metric takes into account the contrast between the brightness of pixels in the gray scale. On the basis of the topological properties of the constructed network the edge pixels were detected that allows us to identify the border areas in the microstructure of materials. The proposed method can be used in automated systems of materialographic analysis.

1. Introduction
There are many problems from different areas can be solved by the application of algorithmic graph theory. Basic and applied research in material science, engineering and medicine can use a network model as a prototype of a real network. Many studies are conducted on network models in which the number of nodes as well as the number of edges incident to them can be changing in time [1] or at a constant number of nodes of the graph the number of edges changes [2], that affects the network characteristics.

We note a number of studies addressed to image processing in the context of networks with constant topology. In the paper [3] a visualization approach of complex three-dimensional structure of osteocyte networks based on the voxel skeleton was proposed. This network topology includes three entries: nodes, links, and cells. A cell is a connected region with a defined distance and a size restrictions. A node is a cluster of voxels with more than two neighbors each, and a link or branch (if connected to one node only) is a group of connected voxels with two neighbors each. In the paper [4] a model for mapping a grayscale image into weighted undirected network is proposed. The conversion of images into complex networks concentrates mainly on the weight of corresponding edge, and edges in that network depend on both the Euclidean distance and the gray-level difference. This model is based on the weighted combination of the Euclidean distance and gray-level similarity between pixels. In the paper [5] proposed a graph based algorithm of grayscale image processing. Every pixel is represented by one vertex in weighted graph, the weight of each edges is defined by function in which absolute difference of intensities and distance between a pixels pair are taken account.

The aim of this paper is to research the materials microstructure based on complex networks and their topological properties. To achieve the identified aim it is necessary to solve the
following problems: a) to map a color image into a complex network, b) to calculate topological properties of complex network, c) to detect pixels on object boundaries.

2. Network Construction

Suppose we have a color image, characterized by the size of $N$ pixels in width and $M$ pixels in height. Each pixel of a color image is described by a position $(p_x, p_y)$ and a triple of intensities: red $(r)$, green $(g)$, and blue $(b)$. In order to design a model, we will use a spatial distance as well as the contrast between the brightness of picture elements (pixels).

First, in the proposed method we need to convert an image from color to grayscale. There are various ways to convert color images to grayscale image, in our study the weighted average luminosity method was used. We have applied the Rec. 709 coefficients [6] to mapping a color image into grayscale. Thus, the linear luminance $Y$, which is given by:

$$Y = 0.2126 \cdot r + 0.7152 \cdot g + 0.0722 \cdot b.$$ 

Each pixel of the original image corresponds to 8 bits (1 byte) of information that allows us to transfer 256 gray levels. The result of the conversion of color images saves in the bitmap, $N$ is the number of rows and $M$ is the number of columns. Elements of bitmap take values from the interval $[0, 255]$, where the left boundary of the interval 0 corresponds to the black color, and the value 255 – to the white color.

Second, each element of the bitmap is assigned one node of the network. For given image with pixel set $P = \{p_1, p_2, \ldots, p_n\}$, a network can generally be represented as a set $G = (V, E)$, where the node set is given by $V = \{v_1, v_2, \ldots, v_n\}$, $n$ is the total number of nodes; the set of edges is given by $E \subseteq V \times V$. To define the set $E$ we use distance metrics: the Manhattan distance, $d_1$, and the Euclidean distance, $d_2$. To account for the brightness contrast between a pair of pixels $(p, q) \in P$ in gray scale we use the Manhattan distance:

$$d_1(p, q) = |p_g - q_g|,$$

where $p_g$ and $q_g$ are gray level of pixels respectively. The value of Euclidean distance, $d_2$, of the two pixels defines whether there is or not an edge between corresponding nodes $(p, q) \in V$:

$$d_2(p, q) = \sqrt{(p_x - q_x)^2 + (p_y - q_y)^2},$$

where $(p_x, p_y)$, and $(q_x, q_y)$ are coordinates of pixels $p, q \in P$ respectively. Then the set $E$ can be determined as follows: $E = \{e_i = (p, q) \in V \times V : 0 < d_2 \leq R, p, q \in V, i = 1, 2, \ldots\}$, where $R \in [0, max(N, M)/2]$ is a model parameter that is called the radius. If we choose $R = 0$, then zero-graph will be generated, all of whose nodes are isolated. If we set $R = 1$, we will obtain the two-dimensional model of crystal with square lattice. As one should expect, the number of edges $m$ exponentially increases with the radius $R$. In the limiting case we will deal with the complete graph, for which the total number of edges is equal to $m = |E| = n(n - 1)/2$. In practical cases we used $1 < R < max(N, M)/2$. We note that for the Manhattan distance, $d_1$, Eq. (1) the impact of an outlier is reduced as compared with the Euclidean distance, $d_2$, Eq. (2).

Finally, the weighted undirected network $G$ is denoted by a symmetric weight $n \times n$ matrix, $W = [w_{pq}]$, where $w_{pq} = (\alpha \cdot d_1(p, q))^2 + (\beta \cdot d_2(p, q))^2$, if there is an edge between nodes $p$ and $q$ and $w_{pq} = 0$ otherwise, where $\alpha, \beta > 0$ are the scaling parameters of gray-level difference and spatial distance respectively.

Thus, based on the symmetric weight matrix $W$ we constructed the weighted undirected network $G = (V, E)$, with one connectivity component.
3. Calculation of Local Node Dimension

Authors [4] using the measure of dimensionality of individual nodes to the image of edge detection. Following the study [7] the local node dimension $D_i(r)$ can be obtained by the angular coefficient (slope) of the $B_i(r)$ curve on the interval $[0, R]$, where $B_i(r)$ is number of nodes at different topological distances $r \in [0, R]$ from a focal node $p$. $R$ is radius in the proposed model. For defining the local node dimension $D_i(r)$ the $B_i(r)$ curve was approximated with a linear regression. It is necessary to note, for a small number of points the role of the chosen regression method becomes important to the resulting values. Currently, authors [7] addressed this problem by using the least squares method defined directly for the logarithmic scales.

In figure 1 there are shown three circles ($r = 1, 2, 3$) of the fragment of a two-dimensional model with square lattice. For any pair of nodes $(p, q) \in V$, we shall use the $(X, Y)$ coordinate system whose axis are run through the corresponding nodes that are denoted by squares. In the case of the nearest and third neighbors in the coordinate system the axes are respectively denoted by $X_{1,3} \times Y_{1,3}$, and for second neighbors – $X_2 \times Y_2$ [8].

In order to observe the distribution of node dimension, the set of node dimension $D(R) = \{d(p_i) : i = 1, 2, \ldots, n\}$ can be mapped to a grayscale image. Gray level in the grayscale image responds to the value of the node dimension [4]. We applied a contrast enhancement technique to obtain the grayscale image. A linear scaling transform has been used in order to improve the pixel contrast for output image: $g = a \cdot f + b$, where $a$ and $b$ are the transform parameters which can be determined based on the required change of the dynamic range. As a result of the image processing we get the scale $[g_{\text{min}} = 0, g_{\text{max}} = 255]$, then

\[
\begin{align*}
g_{\text{min}} &= a \cdot f_{\text{min}} + b, \\
g_{\text{max}} &= a \cdot f_{\text{max}} + b.
\end{align*}
\]

Here $f_{\text{min}}$ and $f_{\text{max}}$ are extreme values of node dimension interval.

4. Detection of Pixels on Object Boundaries

In the paper [4] the authors carried out the computational experiments and found that pixels on object boundaries have a lower node dimension. The node dimension interval directly depends on the original image. To determine the pixels on object boundaries, we suggest using a $p$-quantile of the node dimension distribution. A pixel of output image, $p$, can be obtained by values of node dimension interval $[f_{\text{min}}, f_{\text{max}}]$ as follows:

\[
p \text{ is } \begin{cases} 
\text{edge pixel, } d(p) < p\text{-level quantile}, \\ 
\text{non-edge pixel, } d(p) \geq p\text{-level quantile.}
\end{cases}
\]
5. Computational Experiments

To conduct the computational experiment, we chosen the picture from the related paper [9], which is shown in figure 2. Square $55 \times 55$ pixels part has been selected from the picture, in figure 2 borders of chosen picture are marked with red line (top left corner).

In order to design the complex network $G$ we used the following values of the model parameters: $\alpha = \beta = 1$, and $R = 2$. Then we calculated the local node dimension, the first, second and third $4$-quantiles are $\{0.005, 0.013, 0.0269\}$ respectively, and the extreme values are $\{0, 0.0421\}$. To determine the boundary pixels, we varied the value of $p$-quantile as thresholds. The original image and images with different thresholds of edge pixel are shown in figure 3, colors were inverted. The part of original network $G$, containing $10 \times 10$ numbered nodes, is shown in figure 4. In our experiment, based on the identified borders the original network $G$ (figure 4a) was divided into two networks $G_1$ and $G_2$ (figure 4b, c). The density, average path length and degree distribution were calculated for each network $G, G_1,$ and $G_2$: graph density are $\{0.92, 0.82, 1.00\}$, average path length are $\{1.07, 1.17, 1.00\}$, and average degree are $\{91.64, 52.67, 34.0\}$ respectively.

6. Conclusion

To study the material microstructure a model of a complex network is proposed. On the basis of the topological properties of the constructed network the local node dimension was calculated, and pixels on object boundaries were defined. The proposed approach allows us to apply the algorithmic graph theory to the image processing. The outcome of the designed network is therefore that basic characteristics of a network can be calculated. Thus our approach can be used in automated systems materialographic analysis.

References