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ORIGINAL ARTICLE

2D ceramic grains images manipulations: A simple geometrical characterization and grain domain recreation algorithm

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ABSTRACT

The precision and accuracy of certain simulations in nanoscience, fluid dynamics and biotechnology in the analyses of boundary conditions problems with real experimental results are in general related to the characteristics of numerical approach used and subsequently to the morphological structure of lattices used along these calculations. The more the lattice used approximates to the original boundary or initial condition problem more precise the simulation would be. This work shows a simple algorithm that can be used to build huge lattices containing the main geometrical structures statistically similar to experimental 2D image data of ceramic grains by using some freeware software.
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1. Introduction

In the area of nano-science, biotechnology, fluid dynamics and other scientific research branches the investigation of the main characteristics or nature of the interactions on each system can be developed by means of computational simulations [1–7]. In general, these approaches involve the solution of partial differential equations or ordinary differential equations and a big amount of these set of equations are boundary value problems.

Particulary, the matching between solution of the Dirichlet and Neumann boundary condition problems that emerge on these analyses and the real system are strictly correlated to the right choose of the lattice used to solve the differential equations [8–11].

Besides the numerical solution of differential equations there are the stochastic models [12], classical molecular dynamics simulations [13] and the cellular automata modeling [14,15] that are strongly dependent on the lattice used to role the simulations. Hence, the determination of geometrical structures of these lattices are very important for the correct accuracy of the models investigated.

One of the branches in applied physics research that requires the accurate description of the lattice is the analyses of superconductors junctions [16,17]. At these theoretical studies, part of them developed using percolation theory [18–20], the similarity between real grains morphology and the simulated ones are suitable important. For example, the area of the grains and the linear size of a junction can determine the behaviour of the current density associated with the Cooper pairs [21–23].

The present article develops an algorithm based on freeware software capable of characterize qualitatively the distributions of area and linear length of a grain edge per site of a scanned electronic microscopy image of a ceramic material containing the grains edges. Consequently, with all the statistical information obtained a modified Voroni diagram algorithm is proposed to reconstruct the original grain image with great similarity and determine exactly the connectivity of the grains.

2. Thecnique and results

The algorithm here proposed here is similiar to the one developed by Tuan et al. [24], and is useful to deal with any kind of source image, otherwise, a scanned electronic microscopy image have a gray scale pattern of colors. Due to the quality of the original image used at the example here shown, modifications on the color contrast was performed in order to clarify the grain edges and the resulting image is represented in Fig. 1. This previous processing of the image can be performed using any manipulation software, here *GIMP* [25] was used.

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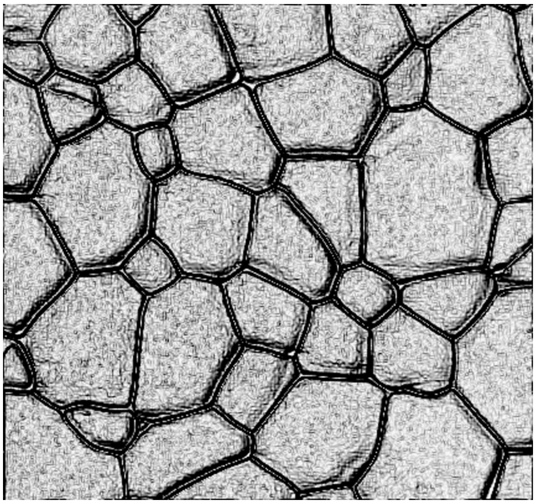

Fig. 1. Processed image is in gray scale format the original doped TiO_2 SnO_2 based electronic ceramics micrography using GIMP v.2.8. The original image is the Fig. 6 of Ref. [26].

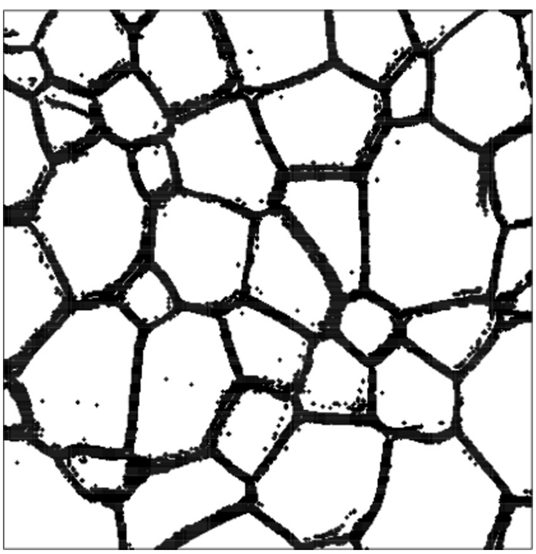

Fig. 2. The black dots represents the pixels associated with specific black color.

In order to scan the ceramic image the software *Imagemagick* [27] was used to convert the *.jpeg* image file into a *.txt* file. The output file obtained is a text file that contains the pixels coordinates as integer numbers and the color associated with each pixel described by a *srgb* color code presented in three formats being one of them the corresponding hexadecimal format code for each kind of color.

The next step of the technique is a clean-up procedure. The pixels coordinates (i,j) and the hexadecimal color code must be selected from the original text file, and all other symbols and information removed. Now, is possible to scan the image inside in an array **A** of integer numbers and associate a number to each color code.

The most important color at this array is black because it was the color associated with the ceramic grains edges. From the point of view of array elements, we create a 2-D vector of integer values called $\mathbf{A}_{n,m}$ with 0 to black pixels and 1 for all other kinds of colors. Here, m, n are the size in pixels of the original picture $(n \times m)$ and represent the dimensions of the vector **A**. Computing only the black pixels the result obtained from the processing of Fig. 1 is shown in Fig. 2.

Fig. 3. Dendritic formation near the ceramic grain edge that can generate some virtual labels associated with the determination of element label. Black box represents the grain edge and other color represents the grains areas.

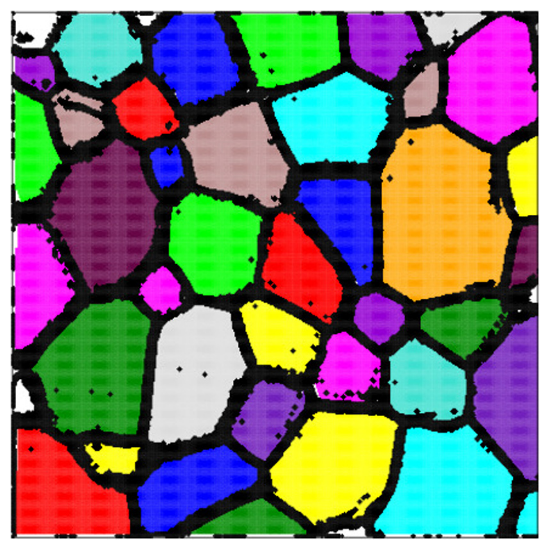

Fig. 4. Determination of each grain associating to them a unique label, for the picture of Fig. 3. Each color is related to a specific grain/label.

As observed some pixels inside the ceramic grains are black, due to the inhomogeneity of the original image. To remove part of these black pixels that do not belong to grain edges, a line search across the array considering it as a rectangular regular lattice was performed a couple of times. Along the search, each black element $\mathbf{A}_{i,j}$ surrounded by more than 3 white first nearest neighbors was changed from 0 to 1. Given the huge number of pixels determining each grain edge, the boundary of the grains was not affected by this process.

The most difficult step was to determine the region/area of the array **A** that belongs to each ceramic grain. To perform it, the array **A** containing only two kinds of elements 0 and 1 was scanned, going from line 1 up to m and from column 1 up to n. Every time that the forward element $\mathbf{A}_{i,j+1} \neq 0$ and the instant element $\mathbf{A}_{i,j} \neq 0$ or 1, then the operation $\mathbf{A}_{i,j+1} = \mathbf{A}_{i,j}$ was evaluated. Doing that, if $\mathbf{A}_{i,j+1} \neq 0$ or 1 but $\mathbf{A}_{i,j} = 0$ then $\mathbf{A}_{i,j+1} = k$ where k is an integer number and is the label associated with the grain where the proposed pixel belongs. The determination of k must be done

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