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IM. STANISŁAWA STASZICA W KRAKOWIE

Wydział Inżynierii Metali i Informatyki Przemysłowej

Project: Multiscale modelling

„Grain growth simulation report”

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1. Abstract

Modeling and control of microstructure and grain size during thermal processing operations are essential for tailoring the properties of polycrystalline materials. In the present work, a cellular automaton model. A cellular automaton (CA) is an algorithm that describes the spatial evolution of a complex system by applying local deterministic or probabilistic transformation rules to the cells of a lattice.

2. Technology

Used in the project:

- programming language: **Java**
- Framework: **Swing**
- IDE: **NetBeans 8.2**

Figure 1. Used technology

The above selection let to create a simple window application in easy way. The Swing Application Framework allowed for easier creating graphics components. Also. selected IDE has an easy and user-friendly Swing visual editor, which allows manipulating of GUI components e.g. JPanel position by using a mouse.

The program can be started in NetBeans by pressing the F6 button or by selecting "Run Project" from the "Run" tab. It should be remembered that the computer on which the application is to run should have JAVA SDK and NetBeans version 8.2 or newer.

3. Graphical user interface

3.1.GUI layout

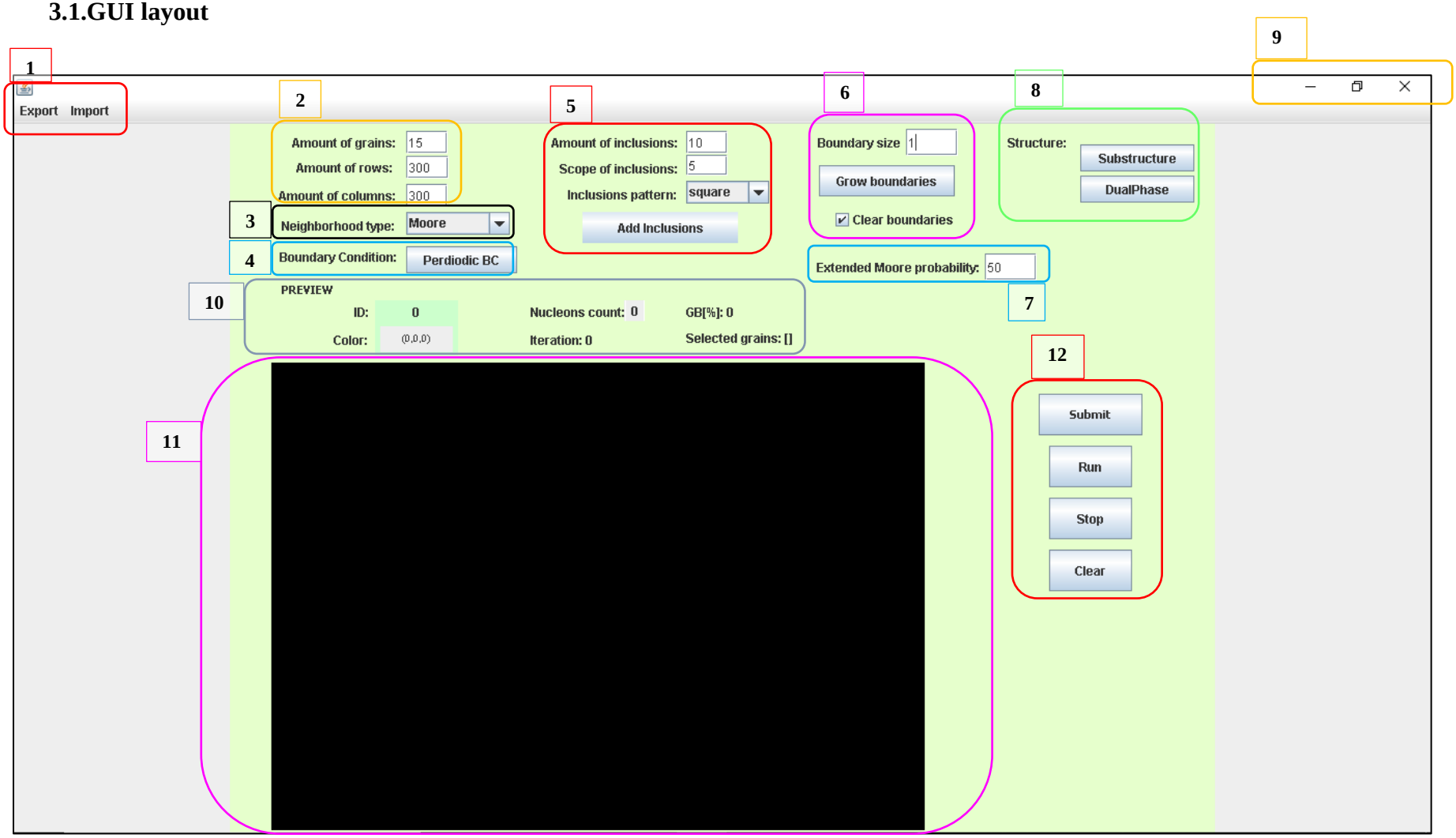

Figure 2. GUI layout

3.2.GUI description

No. 1 – User can export/import the result of the process to .bmp or .txt file. After clicking the selected function, a list will appear with the option of choosing the file type (figure 3). In the case of the export function, you can additionally select or deselect the boundaries between nucleons (figure 4). User can export/import files to/from any place on the computer (figure 5).

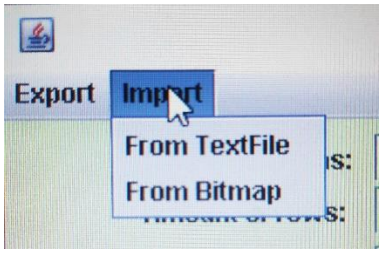

Figure 3. Import option

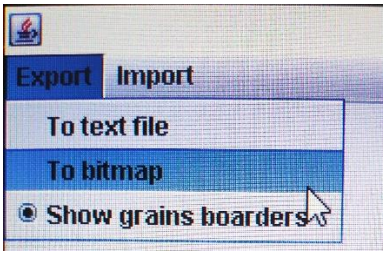

Figure 4. Export option

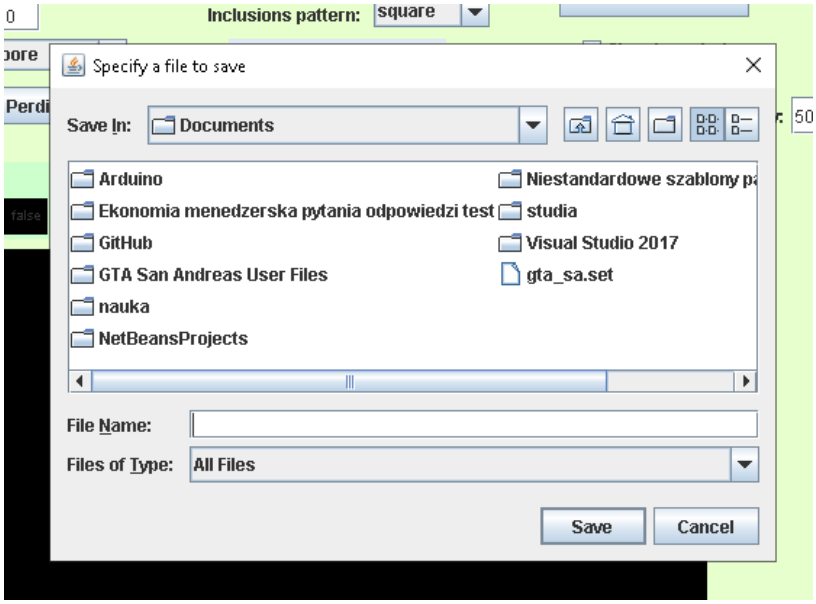

Figure 5. Data export window

No. 2 – User can determine the number of grains and dimensions of cells area or leave the default values unchanged. The unit of rows and columns is a pixel.

No. 3 – There are three possibilities for neighborhood type (figure 6). Available options are: Moore, von Neumann and extended Moore. Examples of use will be presented in section 4.

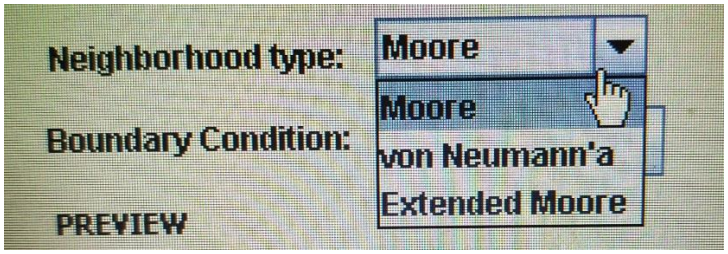

Figure 6. Neighborhood type option

No. 4 – User can determine the type of boundary conditions. If the button is highlighted in dark blue, it means that the absorbing boundary conditions are on (figure 7). In contrast, a lighter button background means periodic boundary conditions are enabled (figure 8).

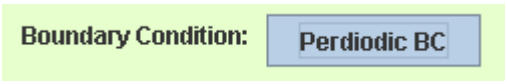

Figure 7. Inactive periodic boundary conditions

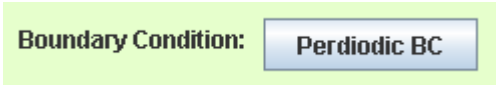

Figure 8. Active periodic boundary conditions

No. 5 - User can determine the numer, size and shape of inclusions. Available shapes of inclusions are: square and circular (figure 9). Size of inclusion is the radius for the circle and half of the diagonal for the square. Unit of size is a pixel. This option is not mandatory. If the user wants to perform a simulation with inclusions from the very beginning, he must confirm their addition by clicking "Add activation" before starting the simulation. Inclusions can be added before grain growth or after grain growth. Examples of use will be presented in section 4.

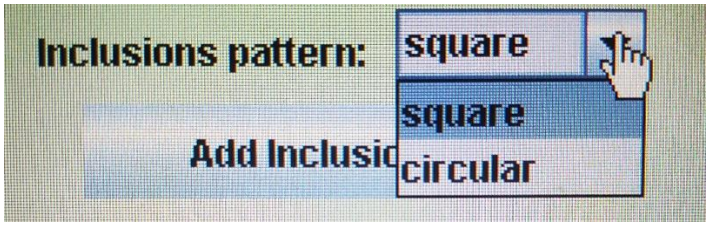

Figure 9. Inclusion shape options

No. 6 – User can mark the boundaries between the nucleons after simulation. The program gives the possibility to set the value of grain boundary size. Default value of the boundary width is 1. Also, there is an option „Clear boundaries". If the option is not marked boundaries during the cleaning canvas (using the „Clean" function) won't disappear. The function is enabled by default. Examples of use will be presented in section 4.

No. 7 – If user will select extended Moore from Neighborhood type, he has to type a value of probability chance to chance which is one of the rules of extended Moore. Default value of the probability is 50%. Examples of use will be presented in section 4.

No. 8 – After grain growth simulation user can select some grains by marking by mouse on them and next he can choose one of the options in the „Structure section". It can be „Substructure" or „DualPhase". Substructure relies on that selected grains from the simulation will stay on the map after clearing the map. When the second simulation is over grains will remains the same, but other nucleons will rise. Dualphase relies on that selected grain will change the phase and stay after clearing the map. After the second simulation, they will cover the rest of the grains. Examples of use will be presented in section 4.

No. 9 – buttons used to minimize, maximize and close the application window.

No. 10 – This is an auxiliary section. Informs the user about the properties of the grains, their color, the total number of iterations after the simulation and the number of nucleons. In addition, it presents the percentage content of grain boundaries and a list of selected grains for the "Substructure" and "DualPhase" processes. Examples of use will be presented in section 4.

No. 11 – Canvas indicates the graphic area visualizing the result of the simulation.

No. 12 – This part of the GUI contains the main application buttons. Namely:

- „Submit” - allows user to generate new nucleons on the map
- „Run” – allows to running the simulation
- „Stop”- allows to stopping the simulation
- „Clear” – allows you to clean the canvas, but if the "Clear borders" checkbox is not selected and the boundaries lines have been drawn then the borders remain in the drawing. Examples of use will be presented in section 4.

4. Results

Simulations were carried out for the same area dimensions and number of grains.

Amount of grains = 50 Amount of rows = 300 Amount of colums = 300

4.1.Grain growth simulation using Moore neighborhood method

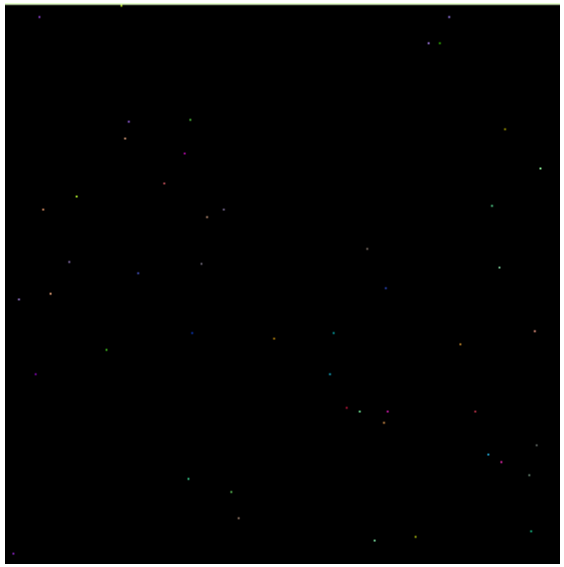

Figure 10. Generated area

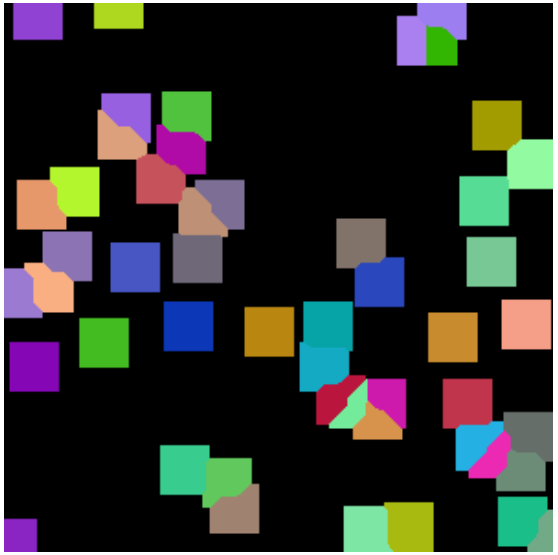

Figure 11. After 14 iterations

Figure 12. Result of simulation

4.2.Grain growth simulation using von Neumann neighborhood method

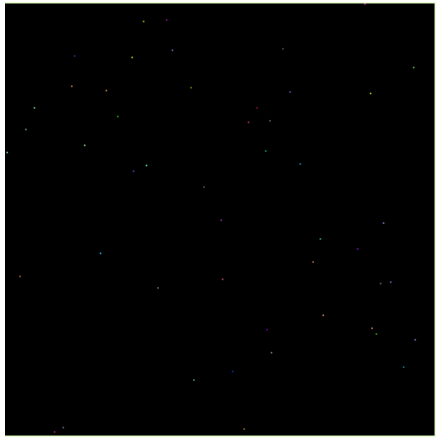

Figure 13. Generated area

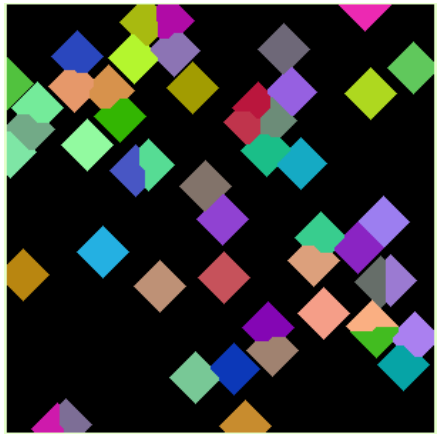

Figure 14. After 19 iterations

Figure 15. Result of simulation

4.3.Grain growth simulation using extended Moore neighborhood method

Probability was assumed in the simulation equal 50%.

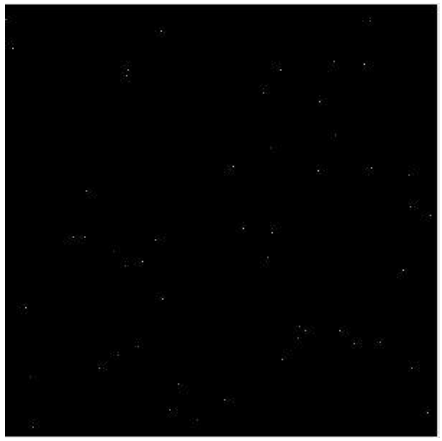

Figure 16. Generated area

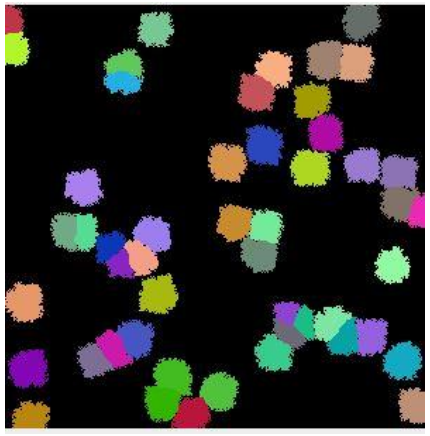

Figure 17. After 15 iterations

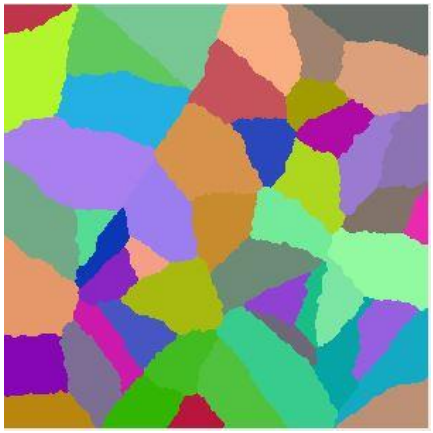

Figure 18. Result of simulation

4.4.Inclusions

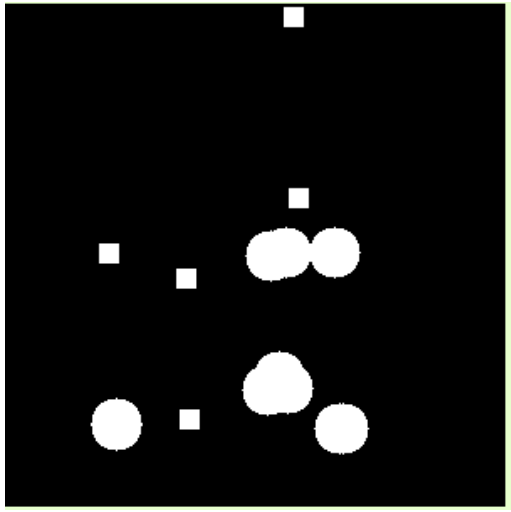

Figure 19. Inclusion shapes

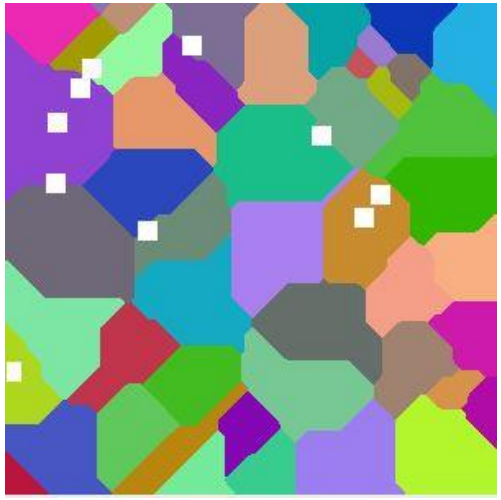

Figure 20. Inclusions added before simulation

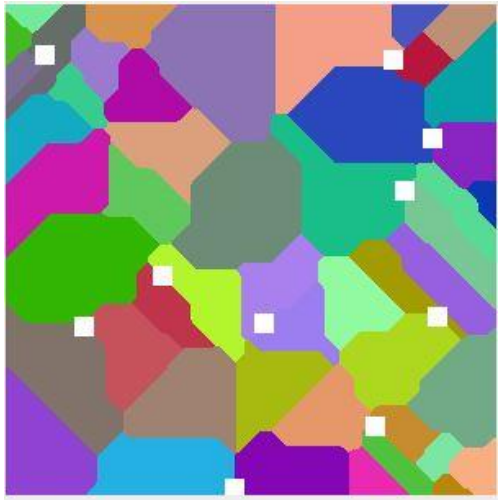

Figure 21. Inclusions added after simulation

4.5.Structure

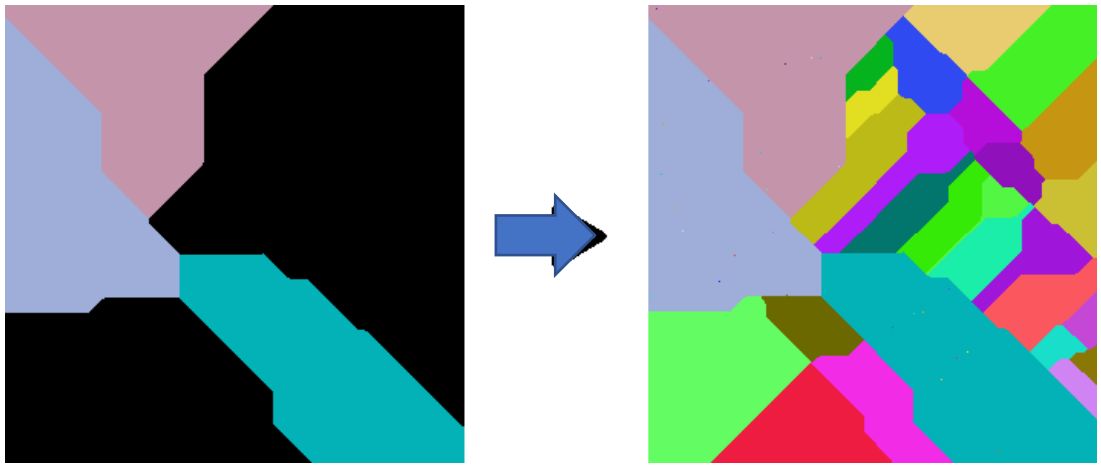

Figure 22. Subtraction of structure

Figure 23. Dual phase of structure

4.6.Grain boundaries

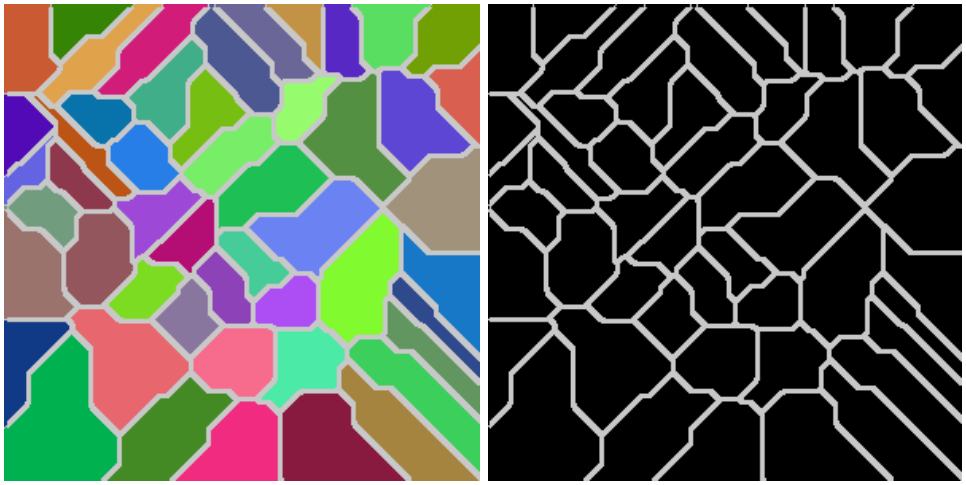

Figure 24. Grain boundaries

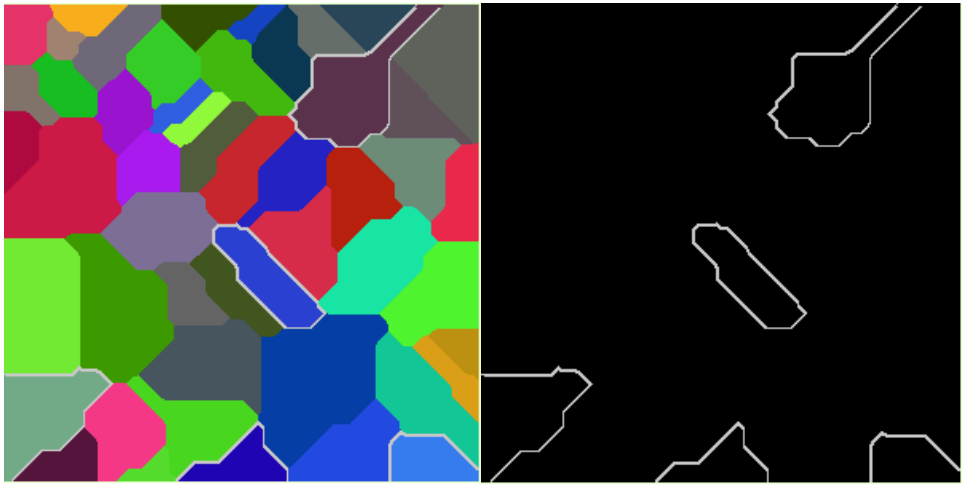

Figure 25. Selected grain boundaries

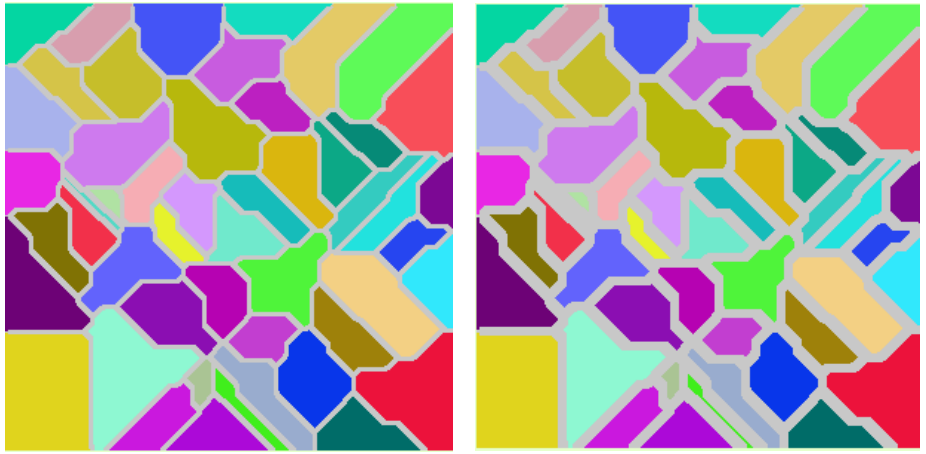

Figure 26. Comparison of grain boundaries size

5. Result comparison

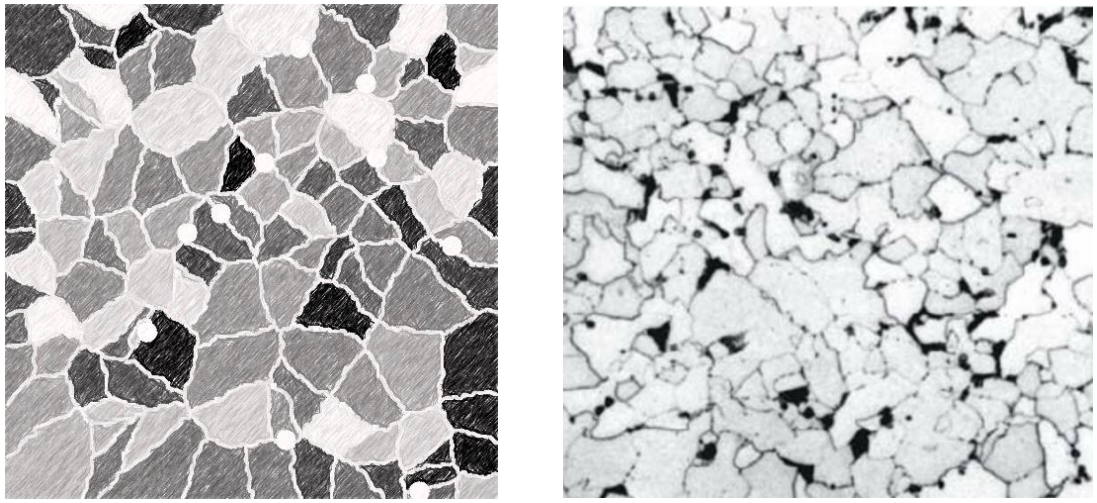

Figure 26. Comparison of simulation result with real steel microstructure[1]

Figure 26 compares the result of the application simulation with the actual steel microstructure . On the left is result of simulation. The image has been rotated. colors have been changed to shades of gray to get closer to the colors of the real photo (right image). The simulation was made using the extended Mora method. Based on the analysis of the above photos, it can be concluded that the shape of the microstructures is similar to each other. The differences are visible in the number of grains and their size.

6. Conclusions

The created application helps us generate multiple variants of microstructures. Understanding and predicting grain growth in Metallurgy is meaningful. Grain growth simulation is especially attractive as:

- ✓ the statistical behawior of the grains is properly reproduced;
- ✓ microstructural evolution depends only on the real topology of the grains and not on any kind of geometric simplification.

Computer simulation has the advantage of allowing the user to visualize graphically the procedures.

The application is very easy to use for new users. All of the attributes which the user can set are in the application GUI like defining the microstructure dimensions stetting, number of nucleons, grain growth method. Nucleons are inserted randomly. One of the main advantages is the assumption of finite sizes of cell grids, whose states change synchronously in a discretely defined time step.

In summary, all the goals of this project have been achieved. A comparison of the simulation results with the actual steel microstructure can be considered satisfactory.

7. Bibliography

[1] Thomas Neville Baker, „The Effects of Vanadium, Niobium, Titanium and Zirconium on the Microstructure and Mechanical Properties of Thin Slab Cast Steel”, https://www.researchgate.net/publication/29814367_The_Effects_of_Vanadium_Niobium_Titanium_and_Zirconium_on_the_Microstructure_and_Mechanical_Properties_of_Thin_Slab_Cast_Steels (accessed: 17.01.2020)