



AGH

**AGH UNIVERSITY OF SCIENCE
AND TECHNOLOGY**

**Multiscale modeling
Report**

I. Application Requirements

1. Simple grain growth CA and Main interface

An board was created in the project, whose dimensions were set by default to 400x500, however, the user can edit the dimensions of the board in the range from 0x0 to 400x500.

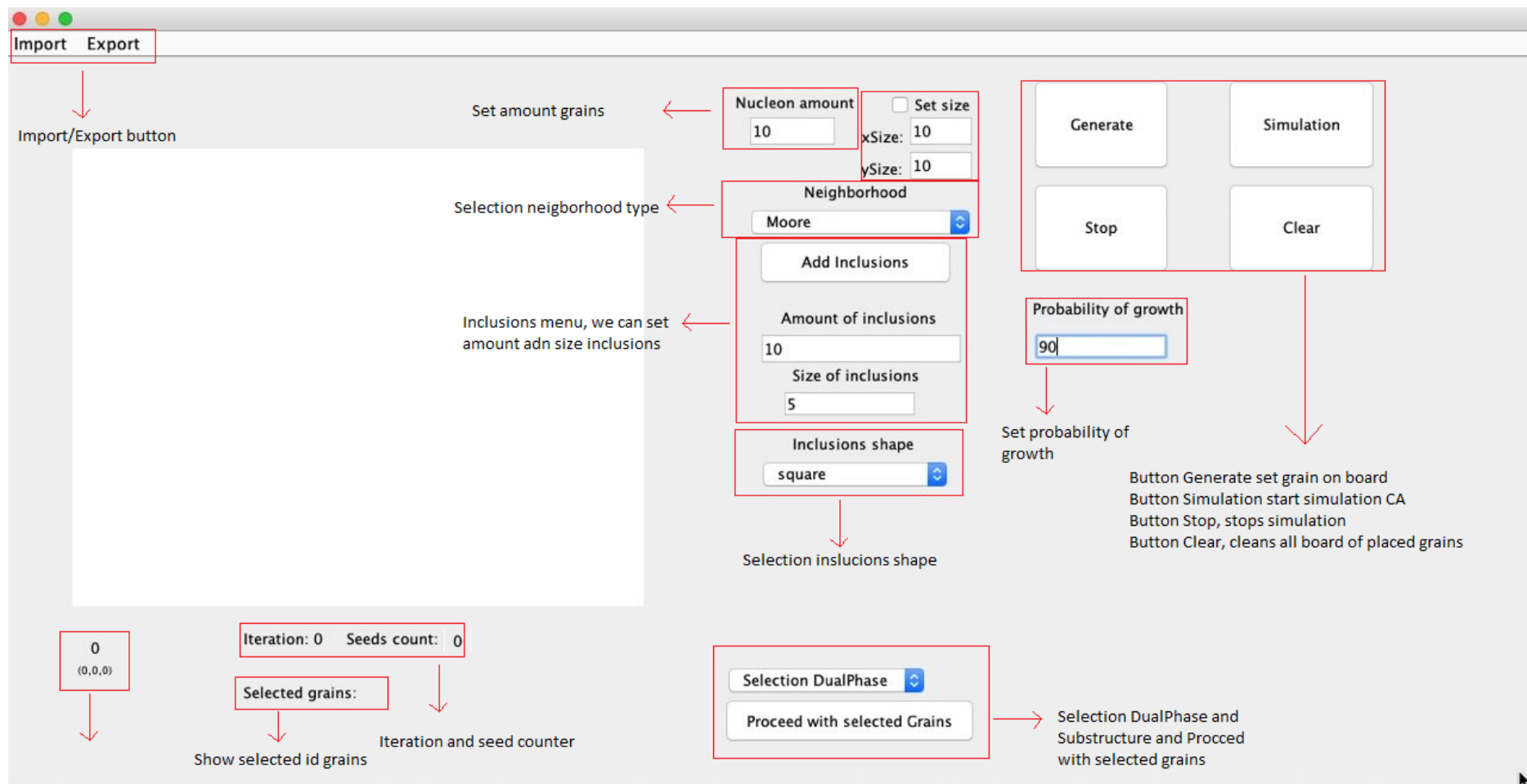
The user can create the first beans, the number of which is selected in the interface, the beans will appear at a random place in the table. After setting the parameters, to view the result, press the Generate button.

Possibility to choose one of the available neighbourhoods types Moore and von Neumann.

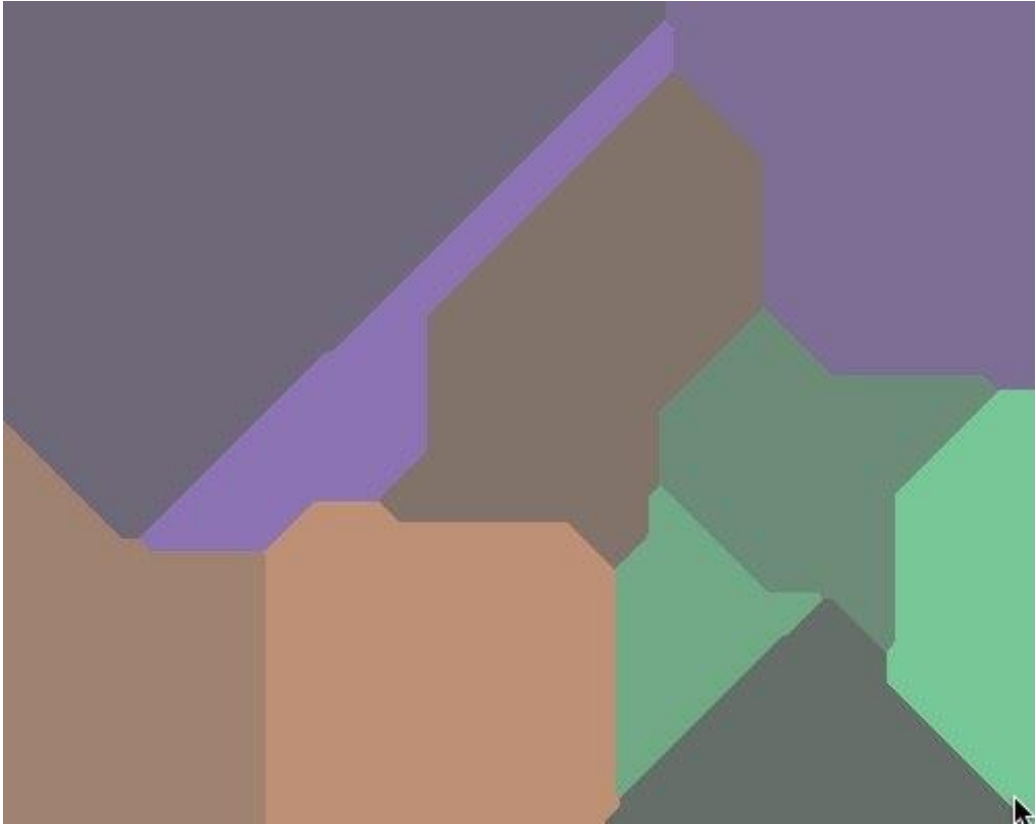
- The simulation button starts the CA simulation.
- The stop button stops the simulation, to restart the CA simulation press the simulation button.
- The clear button cleans board of placed grains.
- The import and export buttons allow you to export the map to a .txt or .bmp file and then open it in the program.
- Neighborhood allows you to choose Neighborhood types Moore, von Neumann and extended Moore.
- In the interface, we can also see the number of grains generated, as well as the number of iterations performed during the simulation.
- Inclusion menu allows you to choose the shape, size, quantity inclusion and generate them on board.
- Also we can see the marked grain which we will use in the selected grain modification DualPhase or Substructure.

In image 1 we can see the main interface with labeled subviews.

In image 2 and 3 we can see simple grain growth CA for choose Neighborhood types Moore, von Neumann.



Img 1. Main inteface with descriptions.



Img 2. Simple grain growth CA Moore



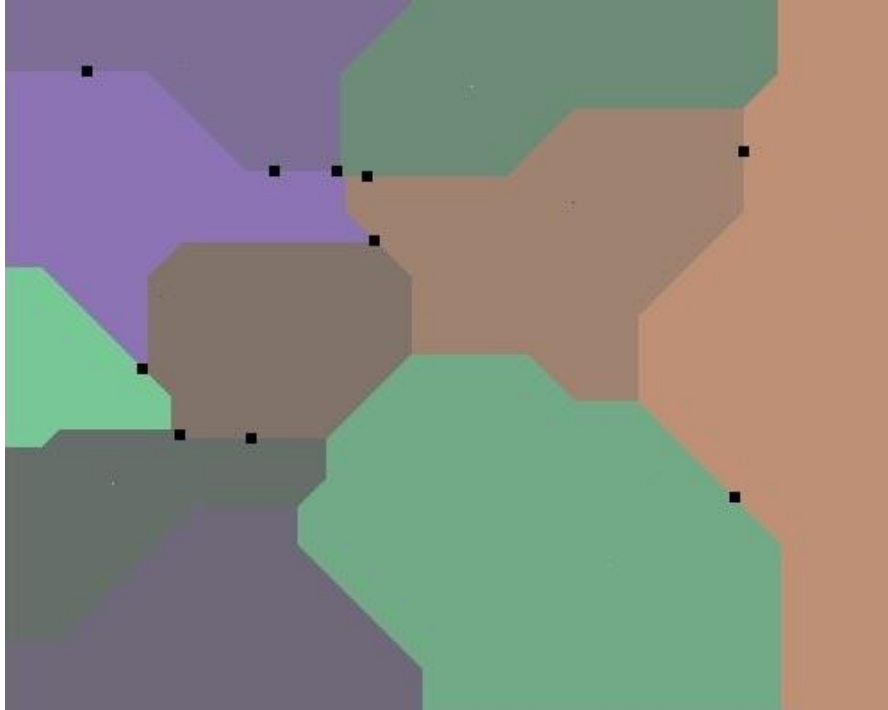
Img 3. Simple grain growth CA von Neumann.

2. Inclusion

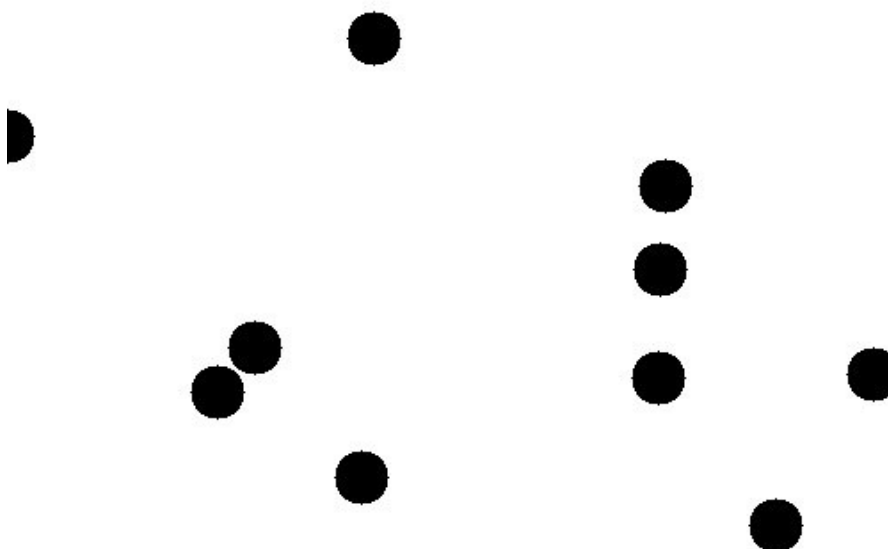
User can determine size, amount and shape of the inclusions. Available shapes: square, circular.

Inclusions can be added before grain growth or after grain growth

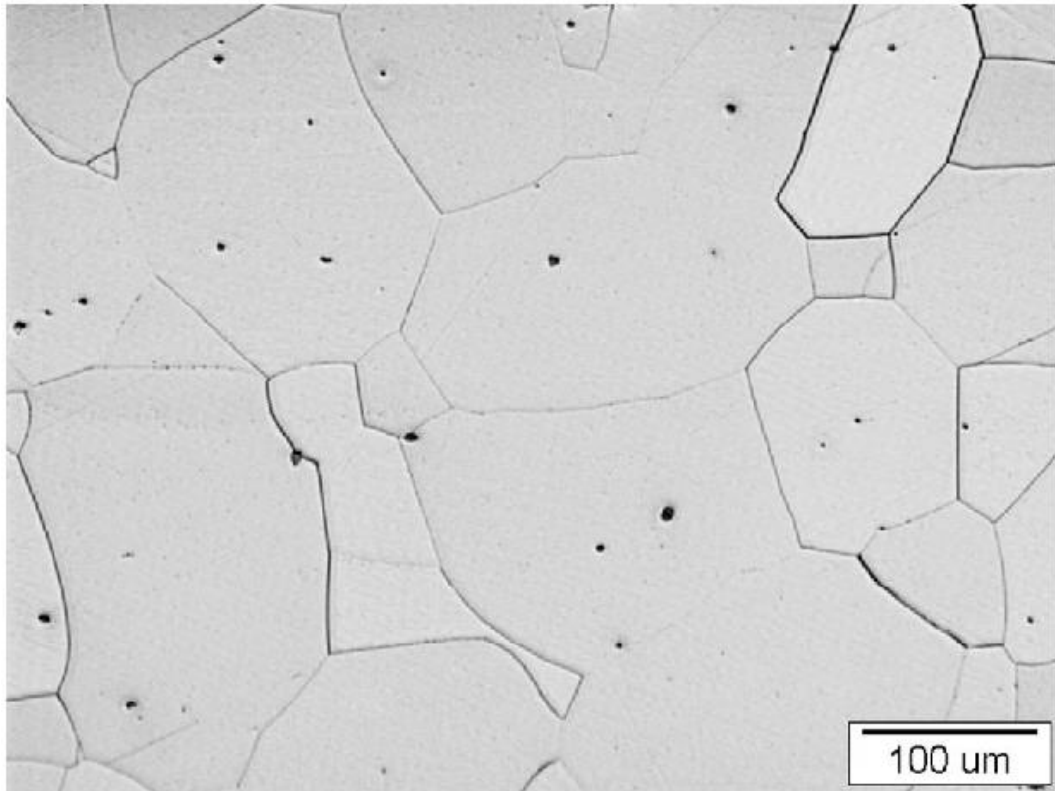
Two types of inclusions are presented to image 4 and 5, in image 6 we can see



Img 4. Square inclusions added after grain growth.



Img 5. Circular inclusions added before grain growth.

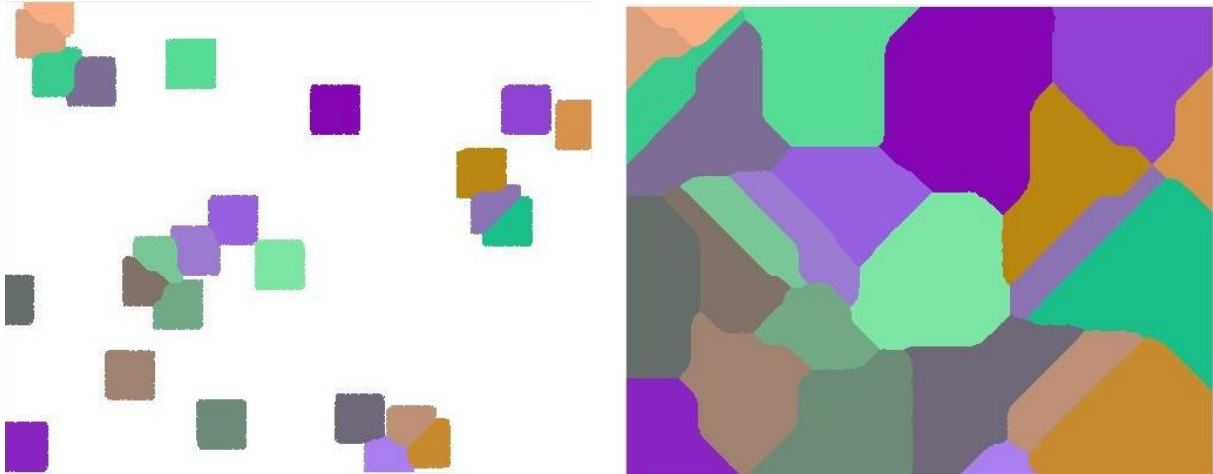


Img 6. Ferrite microstructure of non-oriented, electrical steel sheet exhibiting non-metallic inclusions

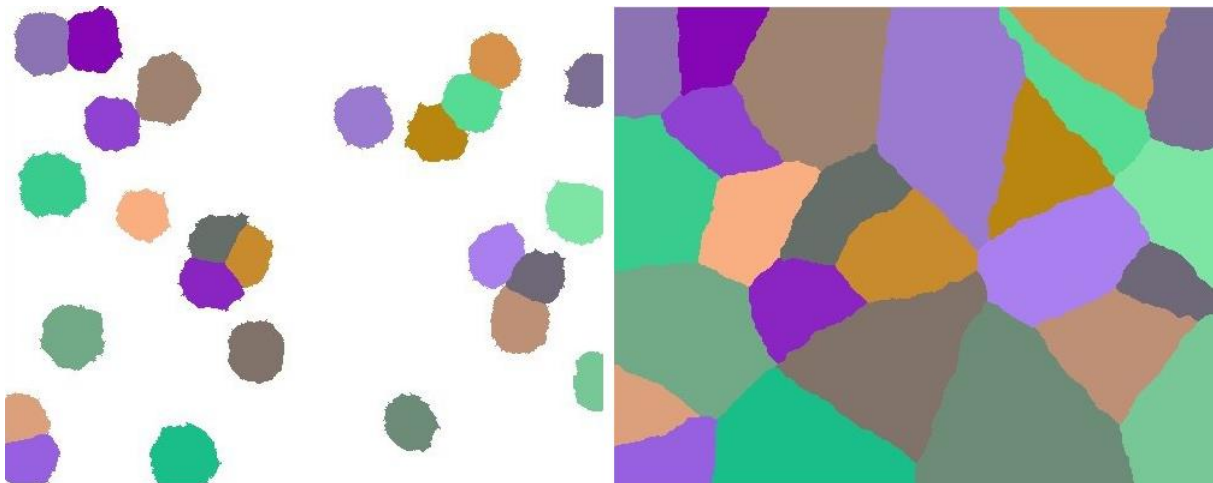
If only we properly choose a properties of our grain growth, it will be close to the real structure The ability to select parameters is useful for simulating grain growth, because in practice this process is not free from any inclusions.

3. Control of grain boundary shape: Extension of Moore neighbourhood

The user can choose the grain growth CA with the option controlling of grain boundary shape, i.e Extension of Moore type neighbourhood. In image 7 and 8 shows result for settings simulation where probability is 10% and 90% during and at the end of the simulation.



Img 7. Extended Moore, 90% probability.



Img 8. Extended Moore, 10% probability.

4. Different microstructure type: Substructure and Dualphase

The next part of the project was devoted to generation the substructure and double phase structures. In both cases, the selected grains become solid after simulation.

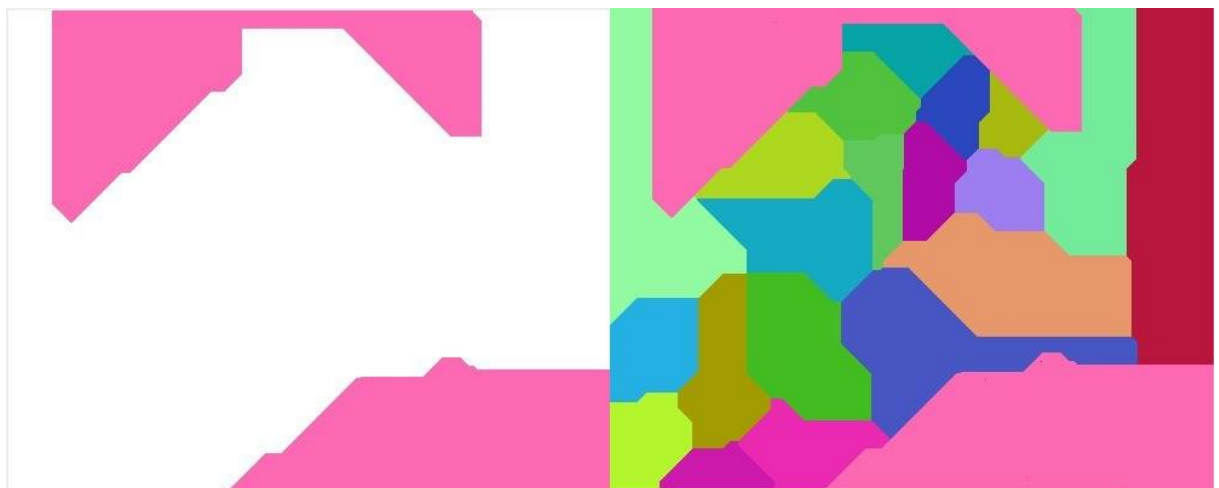
The rest of the structure is removed and simulations can be repeated. Selected grains do not change their structure. We can see this in image 9 substructure and image 10 Dualphase.

Substructure:



Img 9. Generated Substructure selected grains an new simulation.

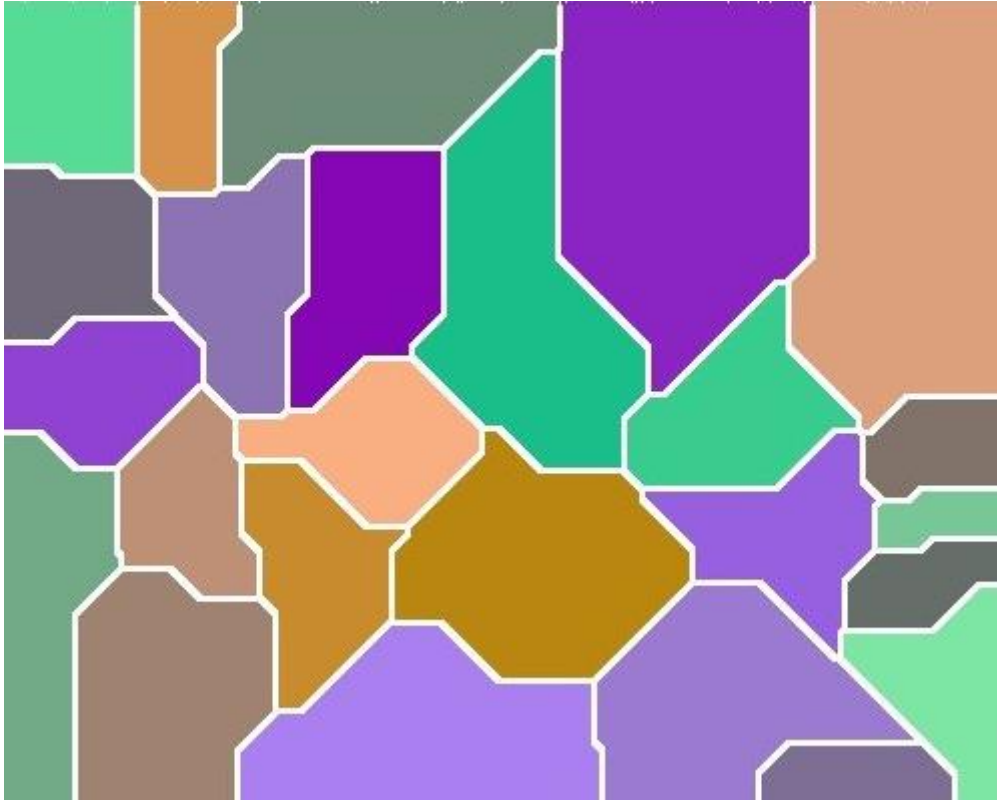
Dualphase:



Img 10. Generated Dualphase selected grains an new simulation.

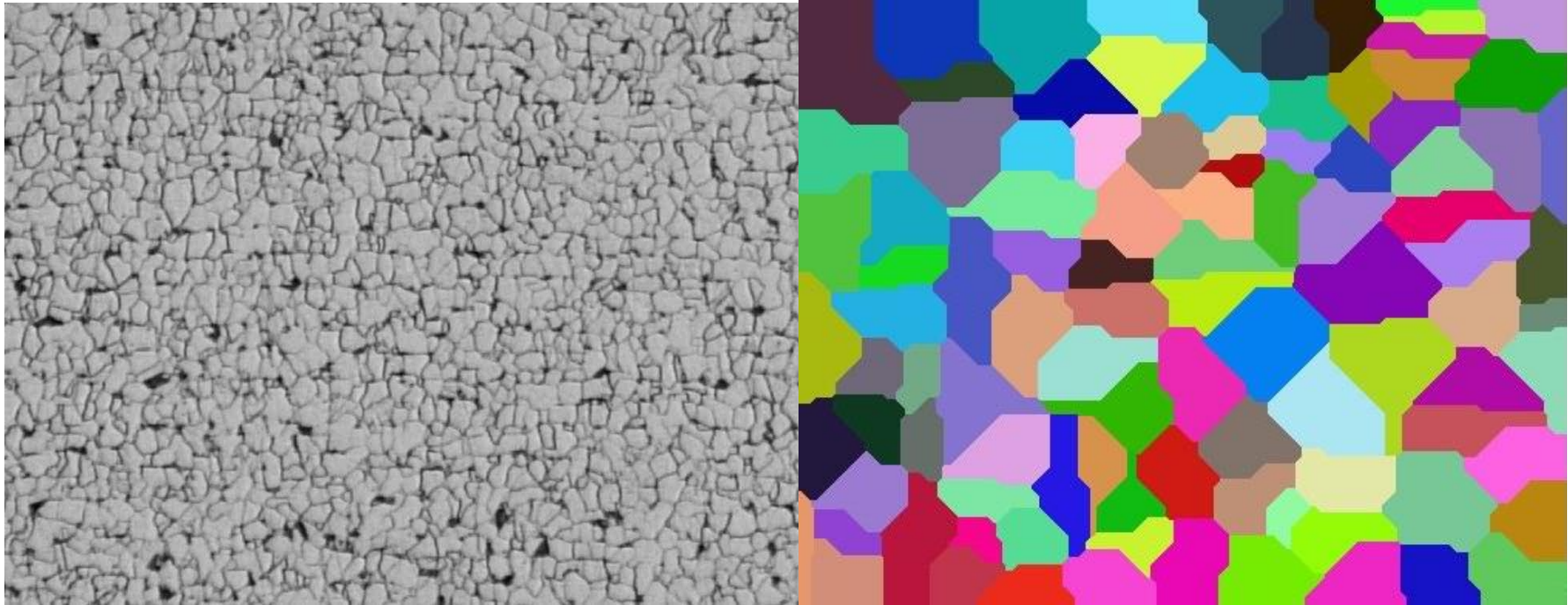
5. Grain boundaries selectio

The last part is the display of grain boundaries.



Img 11. Simple grain growth CA with grain boundaries.

Comparison with real microstructures



Img 12.Comparison Simple grain growth CA with real microstructures steel.

In real microstructure it can be noticed that there are several grayish colors that represent different grains. In the structure generated by the project the grains are much more distinguishable.

Real microstructure always has inclusion i compare generated in application simple grain growth CA with inclusion in image 4 and 6

II. Technology and Installation proces

Application is language in **Java**. Java has GUI femework SWING is a lightweight Graphical User Interface (GUI) toolkit that includes a rich set of widgets. It includes package lets you make GUI components for your Java applications, and It is platform independent.

To write aplication I used **NetBeans** is an integrated development environment (IDE).

III. Conclusion

Created software tool to make modeling of grain growth. Methods of grain growth modeling were implemented: cellar automata method.

Thanks to the program, we can generate many structures, and with properly selected parameters we can get results similar to the real microstructure.

This program can generate any initial microstructure further modeling on the example of dynamic modeling.

Microstructure Source

1. https://www.researchgate.net/figure/Ferrite-microstructure-of-non-oriented-electrical-steel-sheet-exhibiting-non-metallic_fig6_272653336
2. <https://arivinghome.wordpress.com/2015/11/25/wednesday-woody-wednesday-understanding-shrinkage/steel-microstructure/>