AGH UNIVERSITY OF SCIENCE AND TECHNOLOGY

Faculty of Metals Engineering and Industrial Computer Science

Multiscale Modelling

Simple grain growth with cellular automata algorithms

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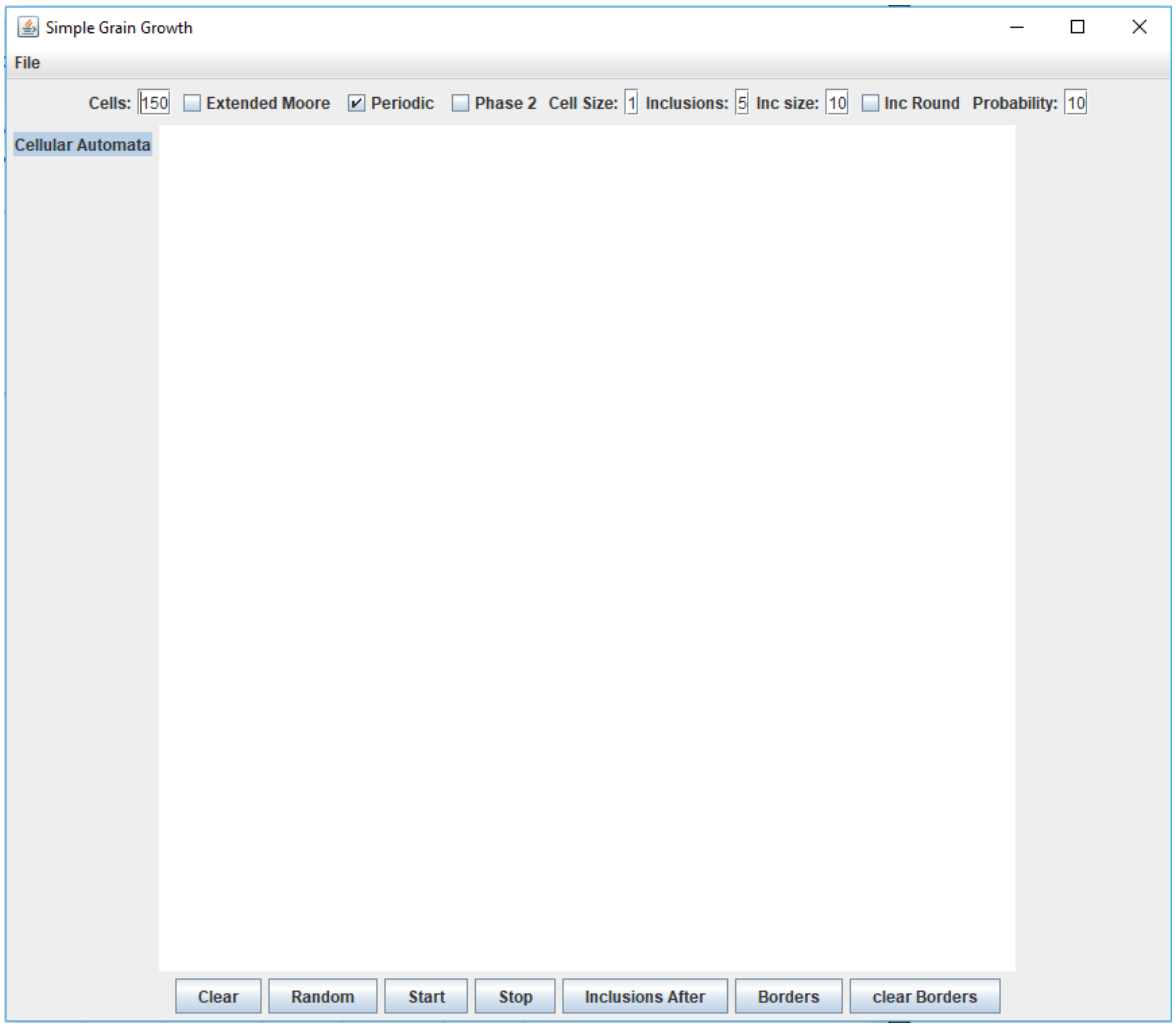
The main assumption of the project was creation a simple grain growth by using Cellular Automata method. The project was made in java using Net-Beans IDE 8.2. During the development I have implemented simple grain growth CA, microstructure import/export: txt/bmp, inclusion with circular and square shape, substructures of cellular automata, control of grain boundary shape (Moor neighbourhood)



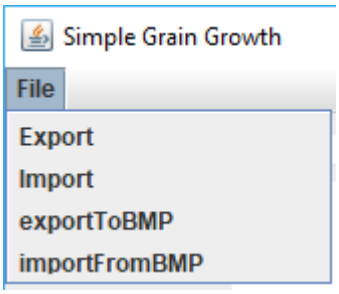
Picture 1 Grafic user interface

The window of application (Picture 1) is divided into sections. The first of them is used to display simulation of grain growth. The second part is panel with options dedicated to different features.

The interface contains options:

1. Quantity of cells
2. Type of neighborhood
3. Control of grain boundary shape (Moor)
4. Cell size

5. Quantity of inclusions
6. Inclusion size
7. Type of inclusions
8. Probability for 4 rule in shape control
9. Clear/Random/Start/Stop button
10. Inclusion button
11. Boundary button

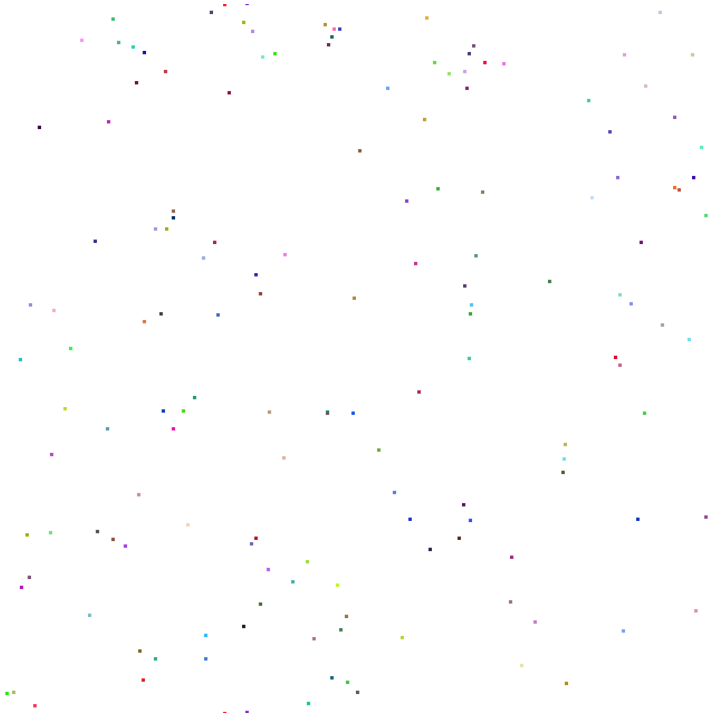


Picture 2 Context file menu

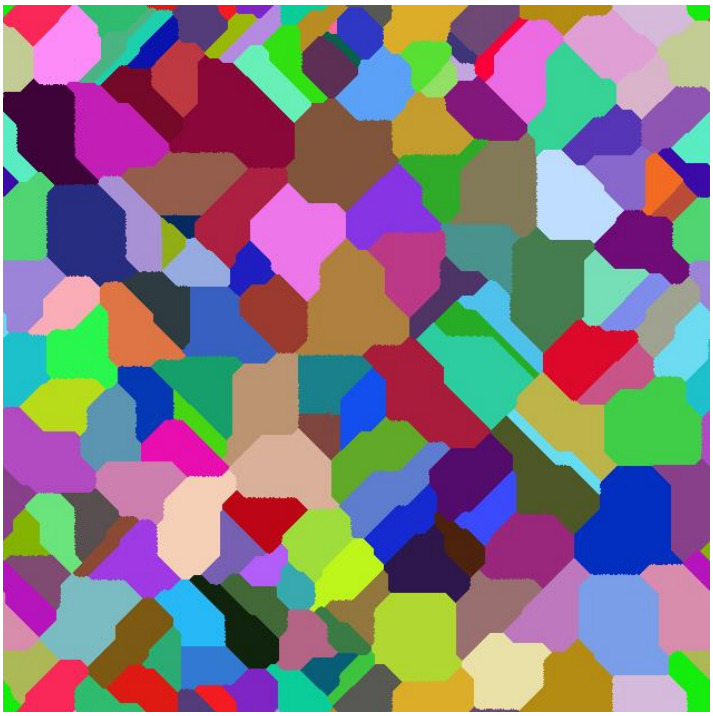
Context File menu contains:
1. Export to txt
2. Import to txt
3. Export to bmp
4. Import from bmp

1. SIMPLE GRAIN GROWTH CA + VISUALIZATION

In picture 3 we can see random generated microstructure. User can define periodic or absorbing boundary conditions and number od grains with is factor in the calculation is to define neighbourhood. It affects the shape of obtained grains and hence final microstructure.



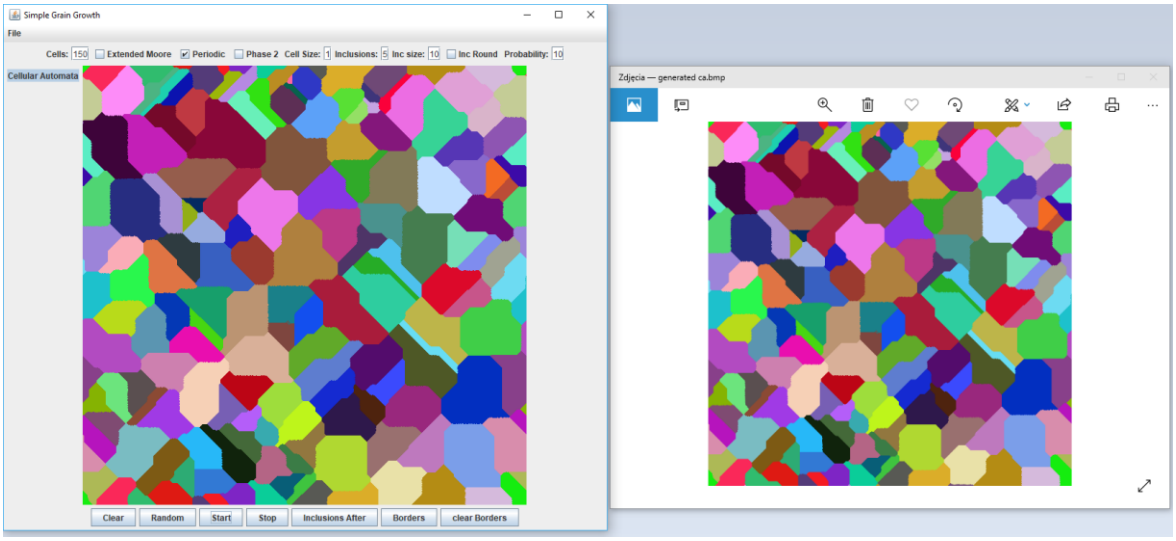
Picture 3 Random selection of grains



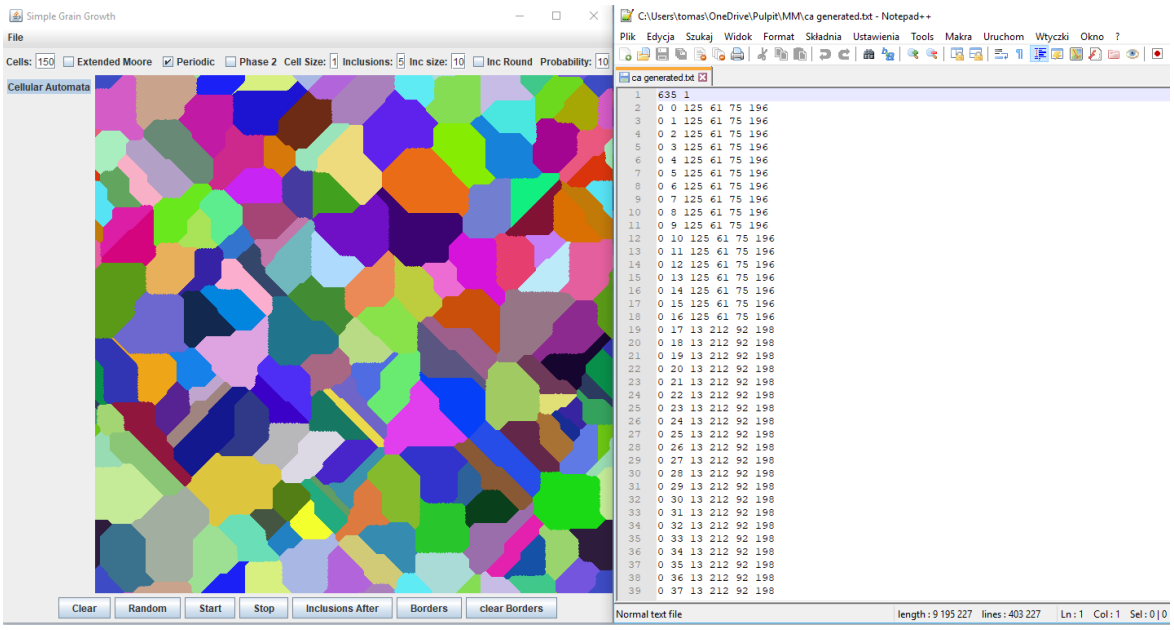
Picture 4 Random generated microstructure

2. MICROSTRUCTURES EXPORT/IMPORT TO/FROM TXT FILES

The second part of the project was to make the software available to import and export data. I used two formats files: .txt and .bmp



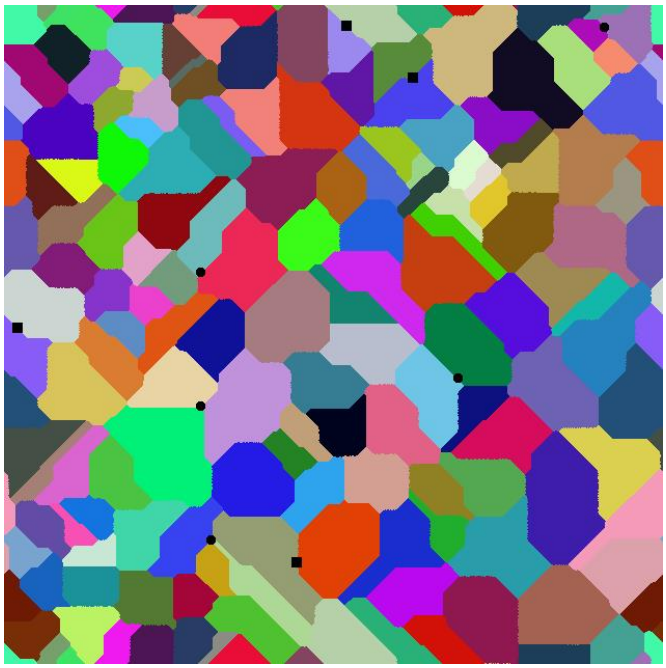
Picture 5 Example of export to bmp



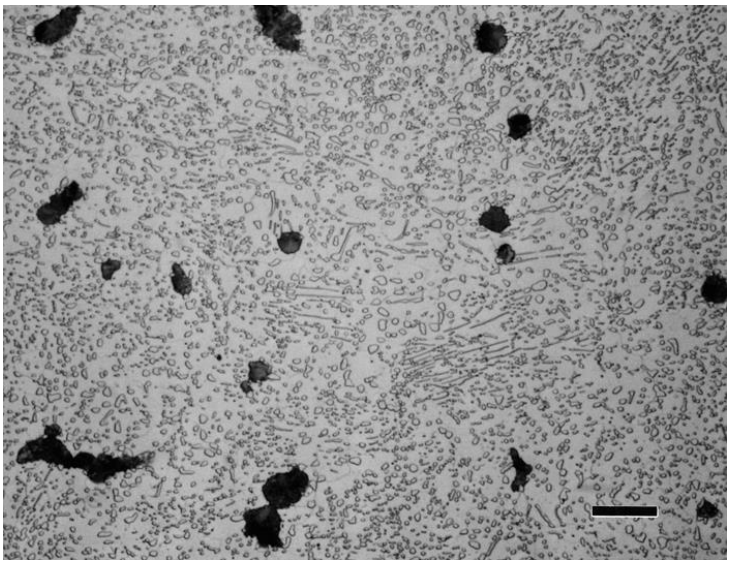
Picture 6 Example of export to txt

3. MODIFICATION OF CA – INCLUSIONS

The next part of the project was to generate inclusions. The inclusions are treated as cells that are not empty, but does not belong to the grain. Inclusions can be added before and after grain growth and may take the form of a square or circle



Picture 7 Microstructure from generated application with inclusion (round and square) after growth



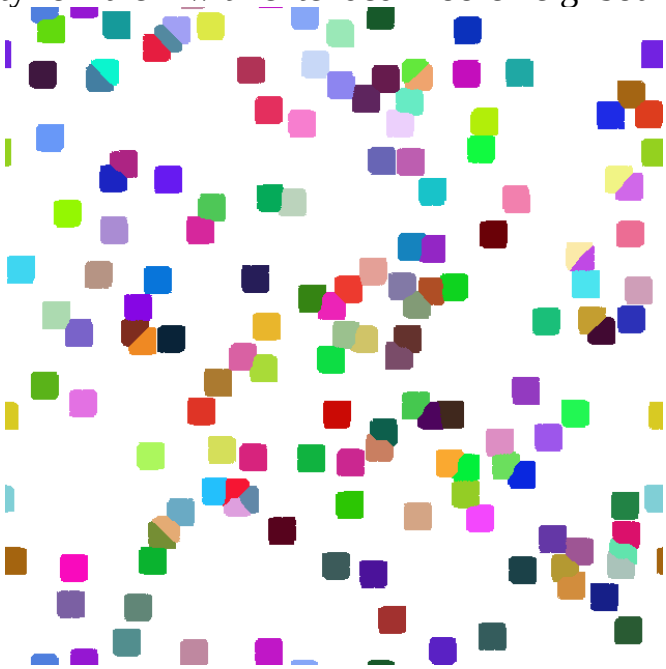
Picture 8 Annealed microstructure of type O6 graphitic tool steel with inclusions

Picture 7 and 8 show a comparison between microstructure generated by application and real microstructure of annealed microstructure of type O6

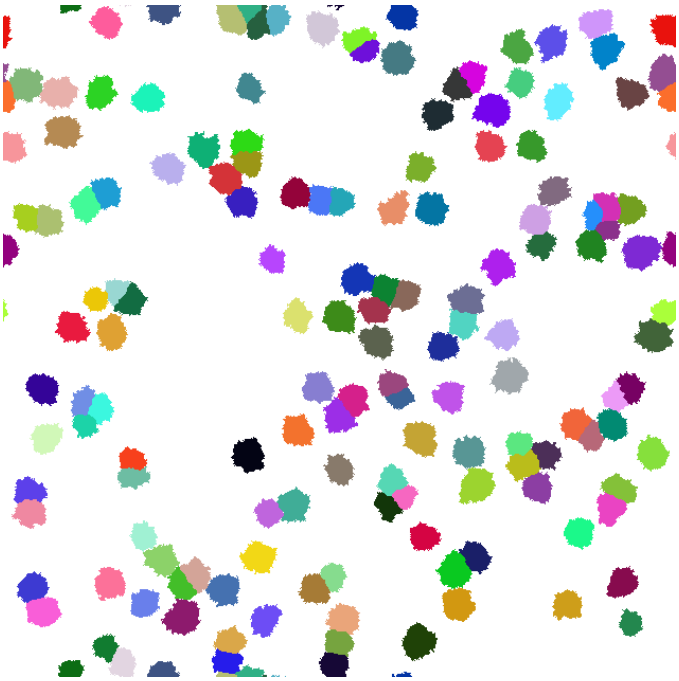
graphitic tool steel. If only we properly choose a property of our grain growth, it will be close to the real structure.

4. MODIFICATION OF CA GRAIN GROWTH ALGORITHM (MOOR EXTENDED NEIGHBOURHOOD

In the picture number 9 and 10 we can see the difference between 20% and 80% probability for rule 4 with extended Moore neighbourhood.



Picture 9 Extended Moor Neighbourhood with 80% probability



Picture 10 Extended Moor Neighbourhood with 10% probability

5. MODIFICATION OF CA GRAIN GROWTH ALGORITHM – SUBSTRUCTURES CA

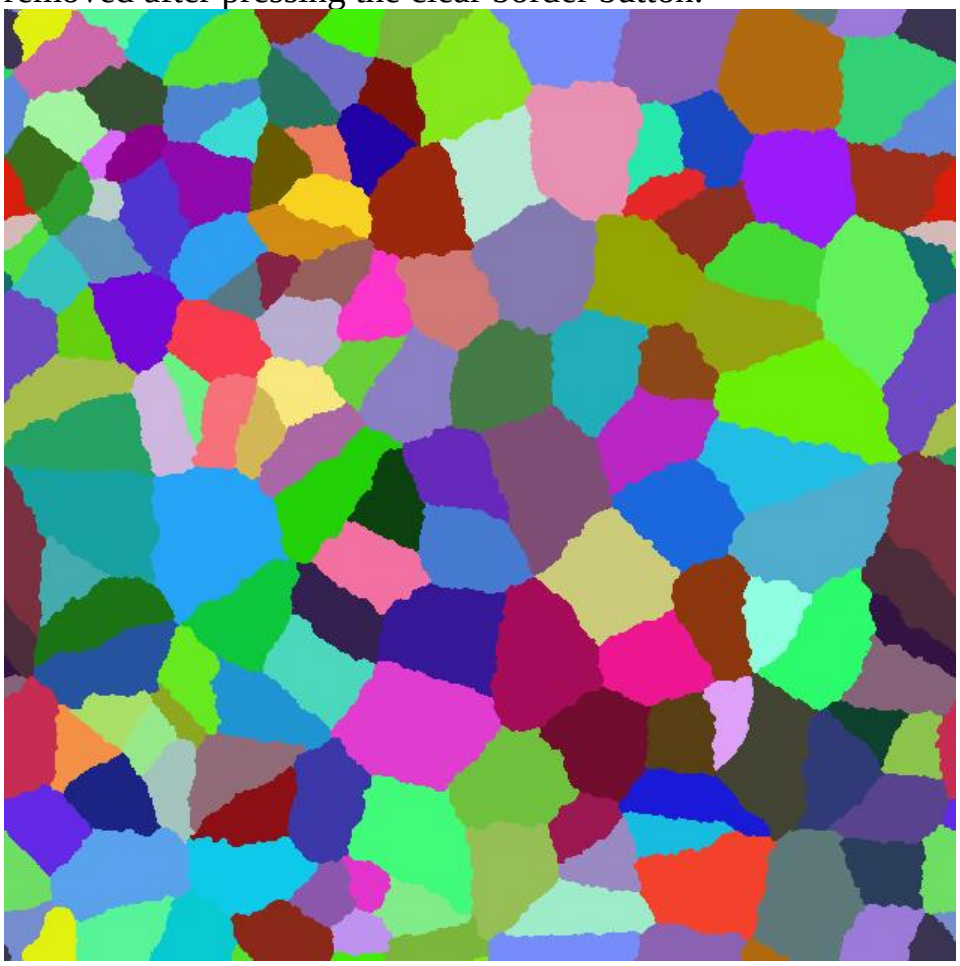
After generate microstructure when we check the Phase2 checkbox and then click random we randomly choose the grain. Next, we can generate microstructure with grain that left.

Picture 11 Microstructure before dualphase

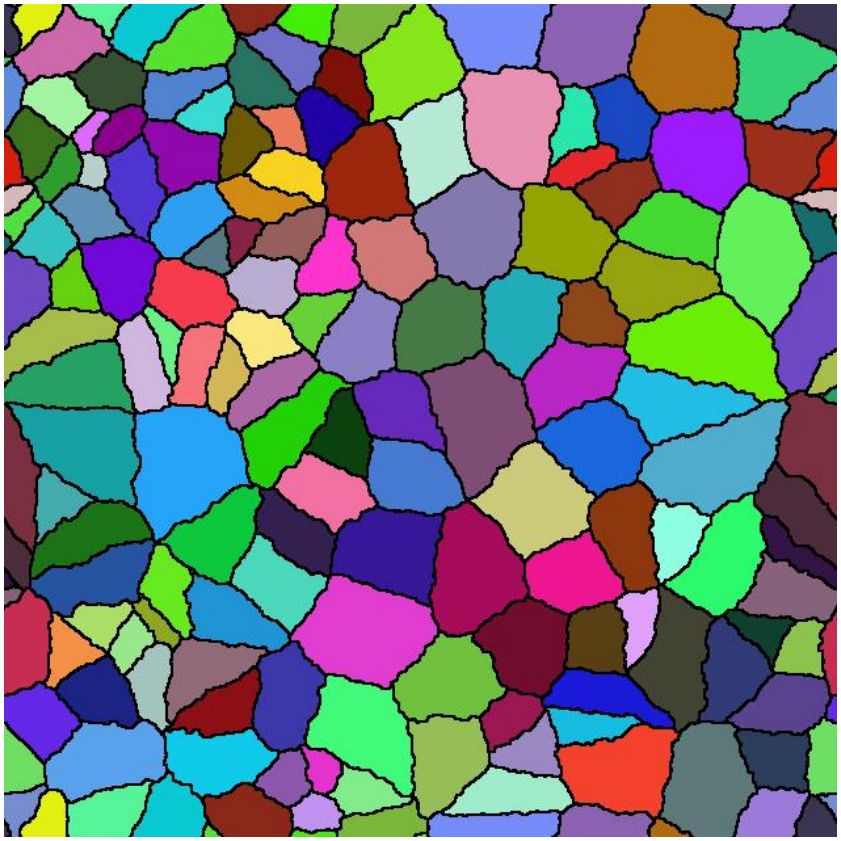
Picture 12 Microstructure after dualphase

6. MODIFICATION OF CA GRAIN GROWTH ALGORITHM – BOUNDARIES

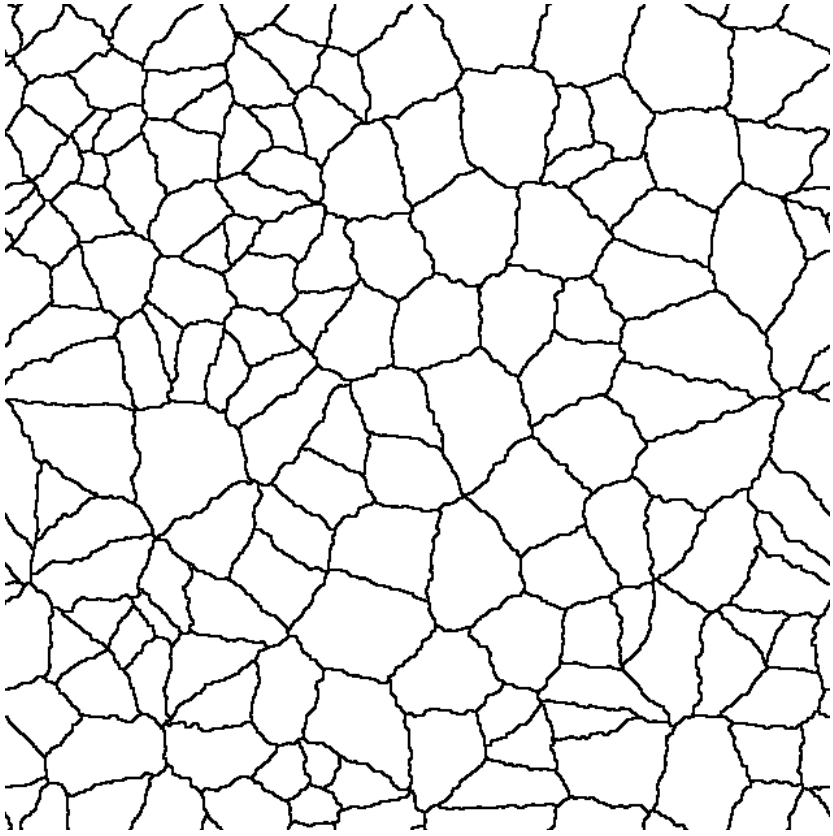
The last part of the project consisted of displaying the grain boundaries and later cleaning the grain color. After pressing the border button, the grain border is determined and is marked in black, after which the color of the grains is removed after pressing the clear border button.



Picture 13 Microstructure before displaying the grain boundaries



Picture 14 Microstructure after displaying the grain boundaries



Picture 15 Microstructure after displaying the grain boundaries and clear the colour of the grains

Picture 16 Example of a polycrystalline metallic sample with grain boundaries

7. CONCLUSIONS

A simple grain growth algorithm and cellular automata is a matrix of coloured points (cells) on a picture box. It come in a variety of shapes and varieties depend of rules based on the states of neighbouring cells. Those rules are applied in intervals for as many time steps as desired to fill the whole grid. There is an option to achieve wanted simulate microstructure by manipulating those rules. Development of this type of application helps in understanding how the microstructure of materials is shaped.