Paweł Brzoza
Applied Computer Science
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Report 1 – multiscale modelling

Intro

Project was created to simulate grain growth. Is possible to specify various parameters to own needs and generate plenty of different microstructures. The growth process is carried out in accordance with assumptions of Cellular Automata (finite set of cells, where each cell is described by a set of internal variables describing the state of a cell). Resulted structure is displayed on the right side of the panel.

Technology

For the purpose of building this application I used the C# programming language with WPF framework which resulted easier way creating a GUI [Figure 1].

Main interface

At the beginning we have to specify parameters like:

- Number of grains
- Type of growth (von Neumann, Moore, Moore 2 (with probability)
- Probability [%]
- Inclusions (type, amount, size, time of creation)
- Substructures (last substructures or dual phase)
- Boundaries (type of selecting)

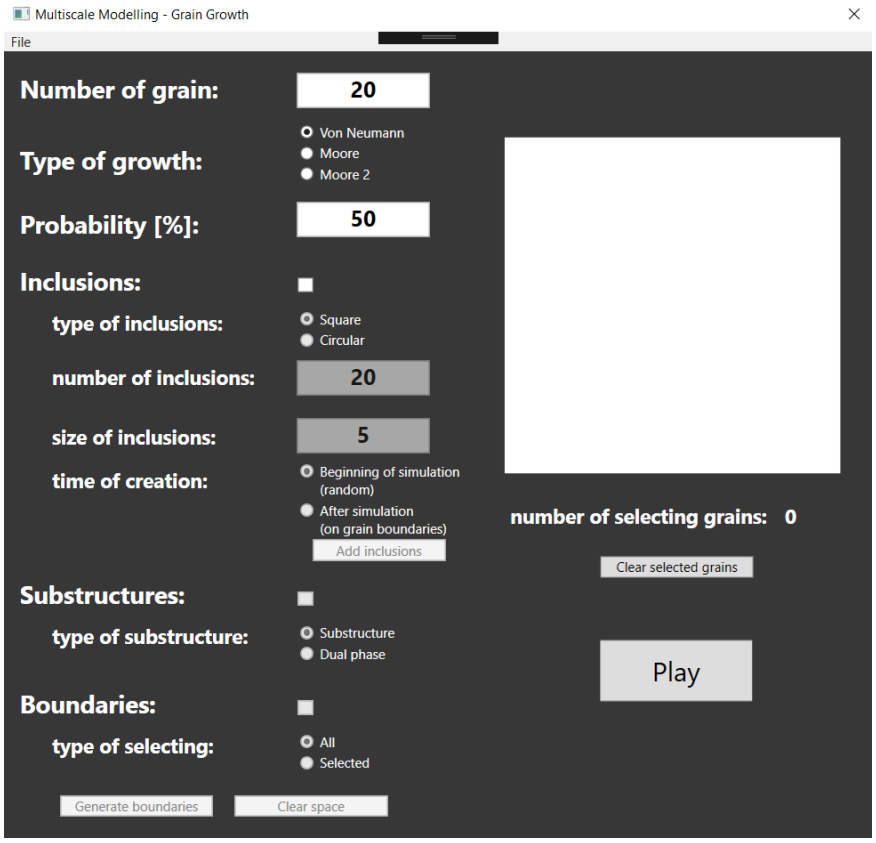

Figure 1 - User Interface

Elements which was implemented in project:

1. Two simple method grain growth cellular automata (von Neumann and Moor methods).
2. Microstructures import/export to/from .txt and .bmp files.
3. Inclusions possible to add at beginning or on the end of simulation.
4. Extended Moore with probability and influence of grain curvature.
5. Creation substructures.
6. Creations specify boundaries.

Uses neighborhoods types – describes the closest neighbors of a particular cell:

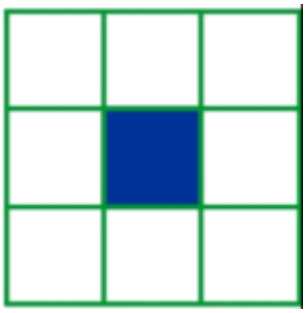

Figure 2 - Moore's method

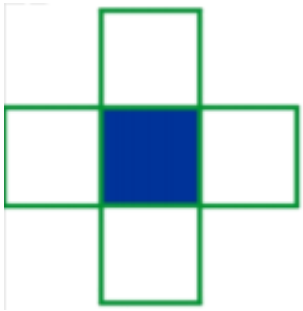

Figure 3 - von Neuman's method

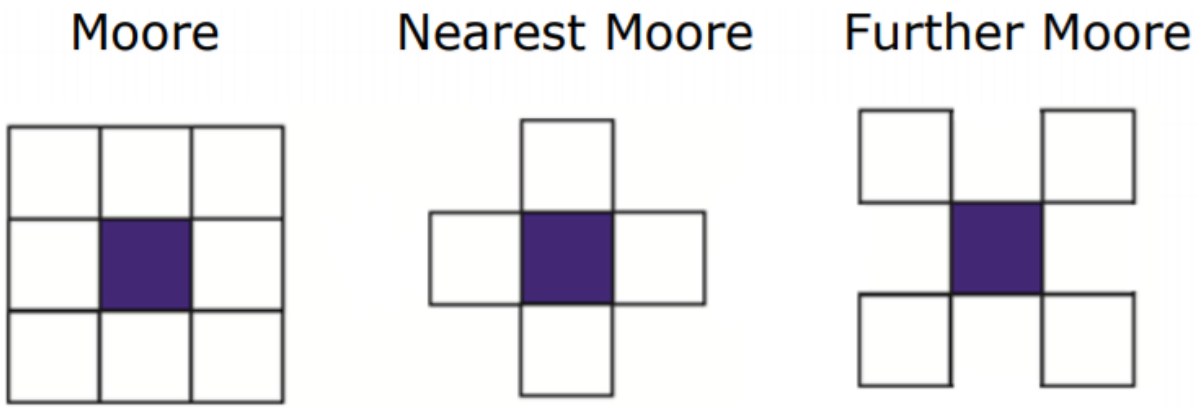

Figure 4 - Extended Moore's method

The following illustrations [Figure 5 – 20] shows resulted structures created with specify parameters configuration:

Figure 5 - generated microstructure (Number of grains: 5; Type of neighborhood: von Neumann)

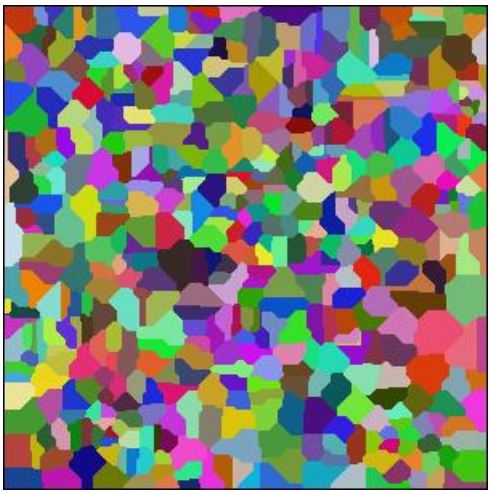

Figure 6 - generated microstructure (Number of grains: 500; Type of neighborhood: von Neumann)

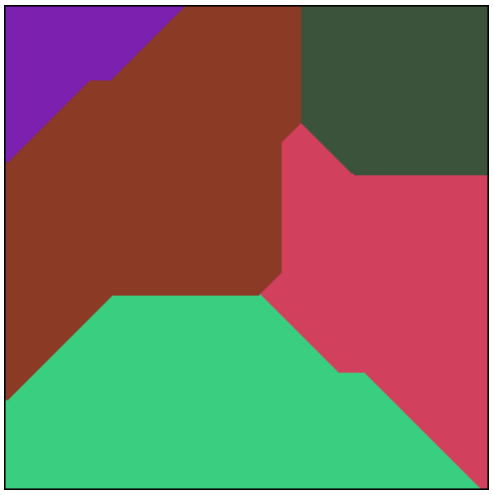

Figure 7 - generated microstructure (Number of grains: 5; Type of neighborhood: Moore)

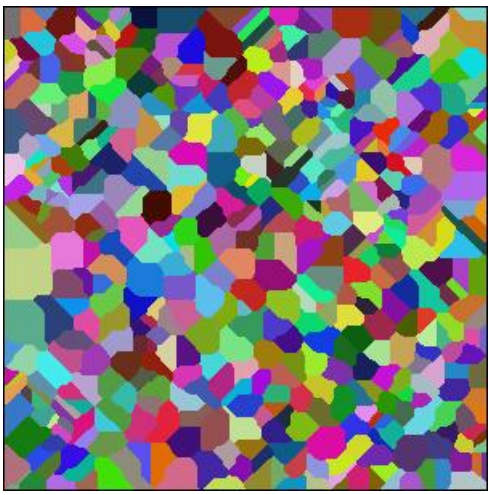

Figure 8 - generated microstructure (Number of grains: 500; Type of neighborhood: Moore)

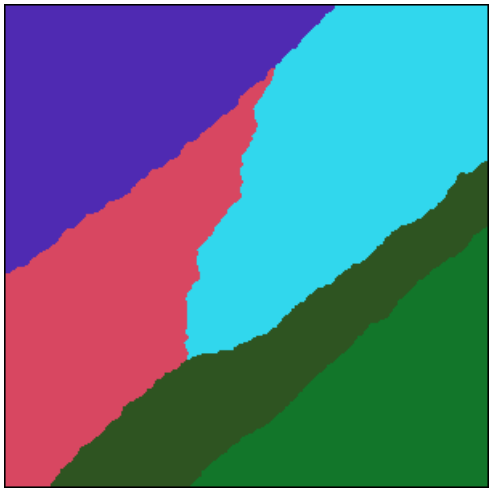

Figure 9 - generated microstructure (Number of grains: 5; Type of neighborhood: Moore 2; Probability: 50%)

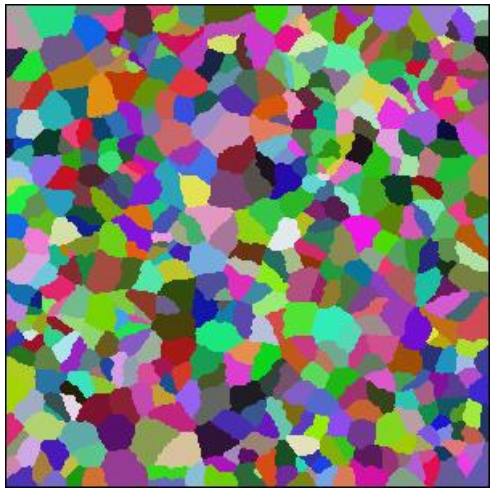

Figure 10 - generated microstructure (Number of grains: 500; Type of neighborhood: Moore 2; Probability: 50%)

Figure 11 - generated microstructure (Number of grains: 5; Type of neighborhood: Moore 2; Probability: 10%)

Figure 12 - generated microstructure (Number of grains: 500; Type of neighborhood: Moore 2; Probability: 10%)

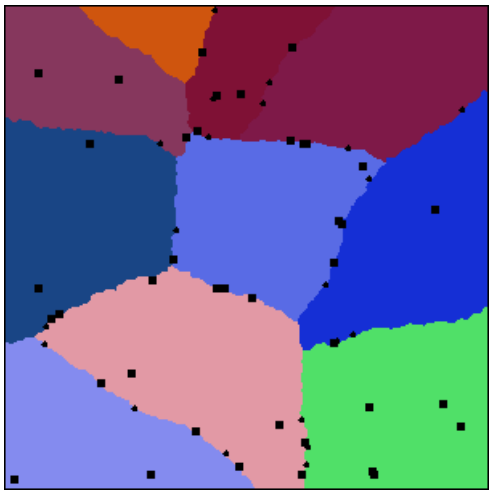

Figure 13 - generated microstructure (Number of grains: 10; Type of neighborhood: Moore 2; Probability: 50%; Inclusion: square at the beginning and square/circle after on boundaries)

Figure 14 - generated microstructure (Number of grains: 10; Type of neighborhood: Moore 2; Probability: 50%; Inclusion: circle on boundaries)

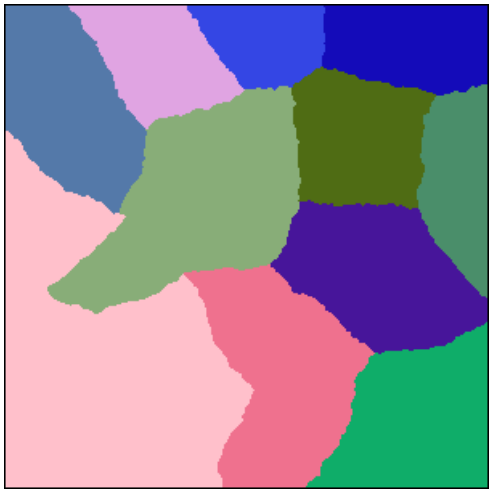

Figure 15 - generated microstructure (Number of grains: 10; Type of neighborhood: Moore 2; Probability: 50%; Substructures: Dual phase)

Figure 16 - generated microstructure (Number of grains: 10; Type of neighborhood: Moore 2; Probability: 50%; Substructures: last substructure)

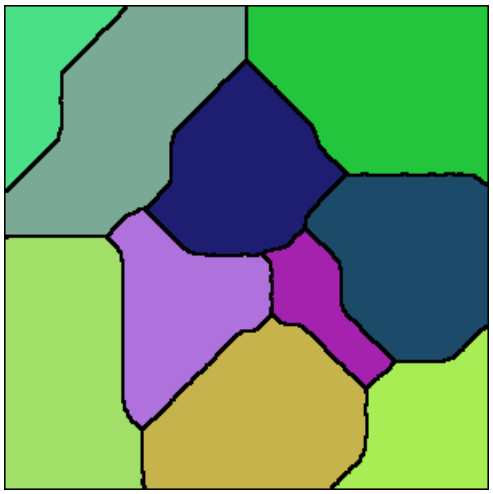

Figure 17 - generated microstructure (Number of grains: 10; Type of neighborhood: Moore 2; Probability: 90%; Boundaries: All)

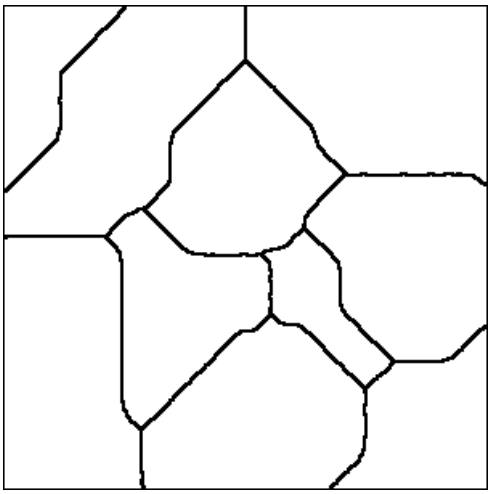

Figure 18 - generated microstructure (Number of grains: 10; Type of neighborhood: Moore 2; Probability: 90%; Boundaries: All and space clear)

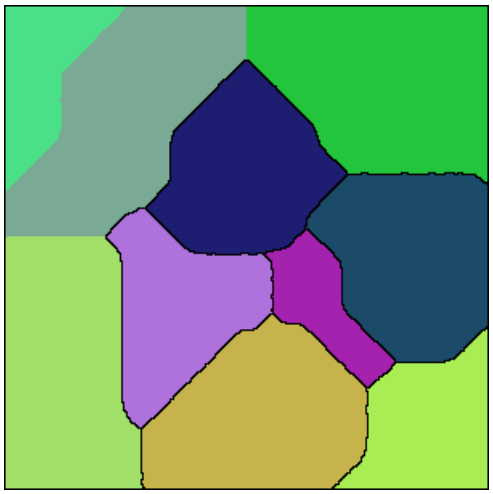

Figure 19 - generated microstructure (Number of grains: 10; Type of neighborhood: Moore 2; Probability: 90%; Boundaries: Selected)

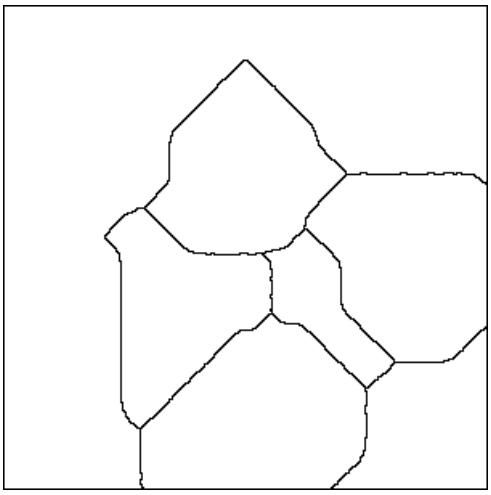

Figure 20 - generated microstructure (Number of grains: 10; Type of neighborhood: Moore 2; Probability: 90%; Boundaries: Selected and space clear)

Comparing with real structures:

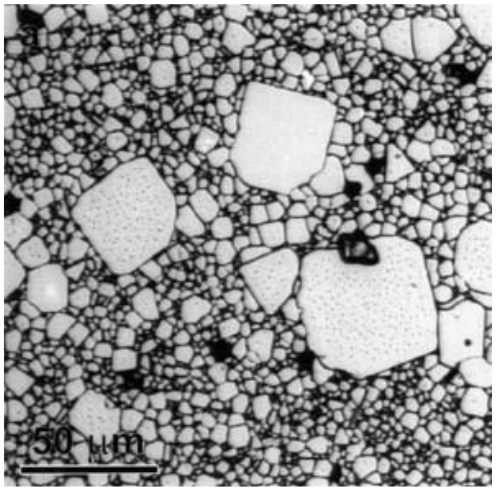

Figure 21 - exaggerated grain growth in polycrystalline[1]

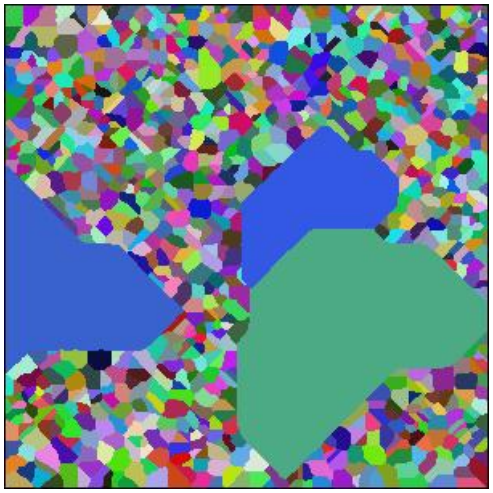

Figure 22 – grain growth in created program with substructures (Number of grains: 10 / 1000; Type of neighborhood: Moore 2; Probability: 90%)

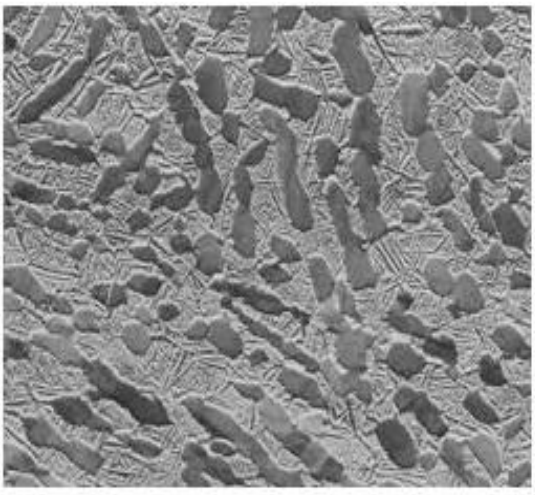

Figure 23 - microstructures of DP Steel[2]

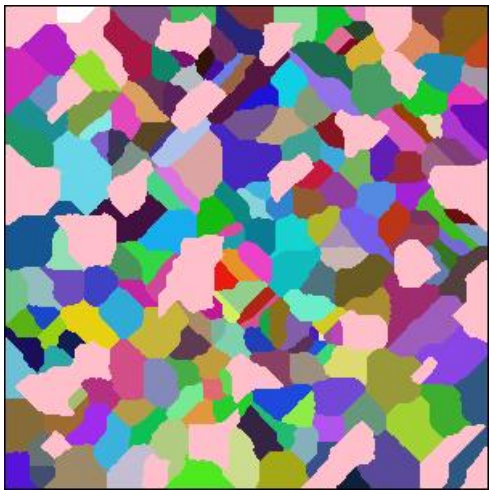

Figure 24 - generated microstructure with Dual Phase (Number of grains: 200; Type of neighborhood: Moore 2; Probability: 80%)

[1] https://www.sciencedirect.com/science/article/abs/pii/S0955221901001844 , 20.11.2018
[2] https://www.worldautosteel.org/steel-basics/steel-types/dual-phase-dp-steels/, 20.11.2018

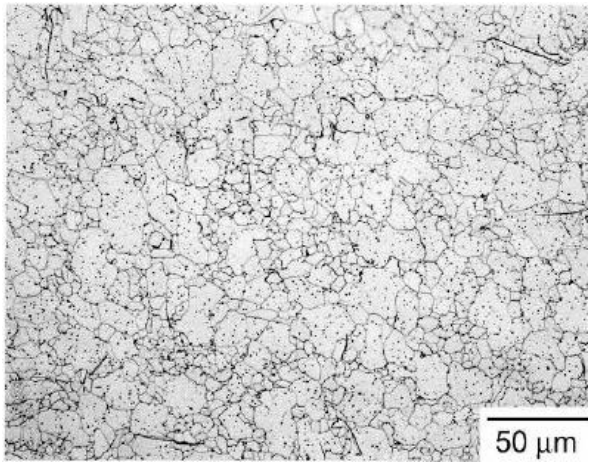

Figure 25 - CP titanium[3]

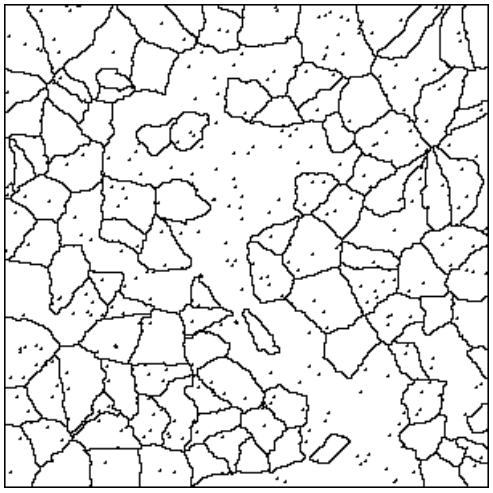

Figure 26 - generated microstructure with selected boundaries, inclusion and without content / color (Number of grains: 150; Type of neighborhood: Moore 2; Probability: 50%; Inclusions: type: circle, size 3, amount: 300)

Conclusion

The presented program made it possible to generate structures with strictly defined parameters. Which make it possible to adjust parameters in such a way that they accurately reproduce the actual state of a given microstructure as accurately as possible. As you can see in the presented bitmaps, the structure of the grains growth is similar to the real ones.

Three methods have been implemented that have enabled the generation of structures in various ways. Everything depended on the type of the neighborhood list. For the Moor's method, the neighborhood list contained all the cells around the grain, the von Neumann's method only had only 4 neighbors, while the Moor's 2 contained combinations of the simple Moor method, von Neumann, Further Moor and additionally the probability with which the proliferation for established assumptions is to be determined.

It is easy to see that the appearance of the boundaries of the first two methods is less ragged due to the established probability of growth. The lower the probability, the grain grows in a more unpredictable way.

When selecting the "All" option, all boundaries on the generated microstructure, will be thicker (double drawn) than those generated with the second "Selected" options. This is because have been used two different algorithms. The first one only checks whether there are other grains in the neighborhood list, while the second additionally includes the color that is marked.

[3] https://www.researchgate.net/figure/Initial-microstructure-of-CP-titanium-longitudinal-direction_fig1_267406005, 22.11.2018