MULTISCALE MODELING

Report 1

„*Application for simple grain growth with cellular automata algorithm*”

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1. Used technologies:

- WPF – Windows Presentation Foundation, subsystem for present user interfaces in Windows applications.
- C# - programming language, functional, generic, object-oriented
- .NET 4.6.1 – framework which included class library Framework Class Library (FCL). Provides language interoperability in several languages.
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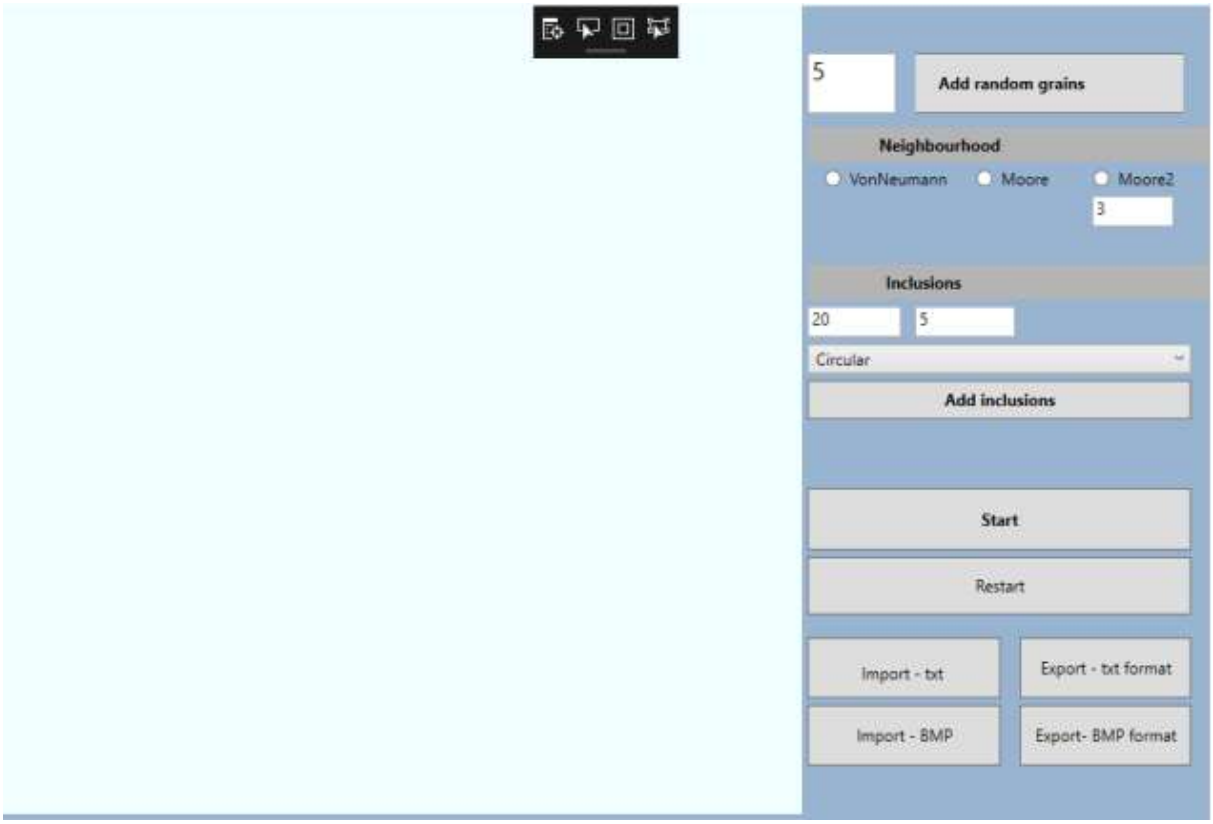
Best option for this project, was used WPF application with .Net framework. WPF provides many prepared controls and events for user interface which speed up time of work.

Program is designed to simulate simple grain growth algorithm based on cellular automata. It provides prospect to manipulate parameters simulation like neighbourhood, inclusions, numbers of grains.

2. Interface

The graphic user interface (picture 1) is divided into parts. The first of them is used to set and simulate random grains position. Second one is used to set neighbourhood for simulation. Last one used the method for check all options and parameters and display simulation. The interface contains options:

3. Quantity of nucleons
4. Type of neighbourhood
5. Amount of inclusions
6. Type of inclusions
7. Start/ restart/ make step buttons
8. Save as/ Import buttons for image and txt file



Picture 1 User Interface

3. Features

3.1 Random grains adding:

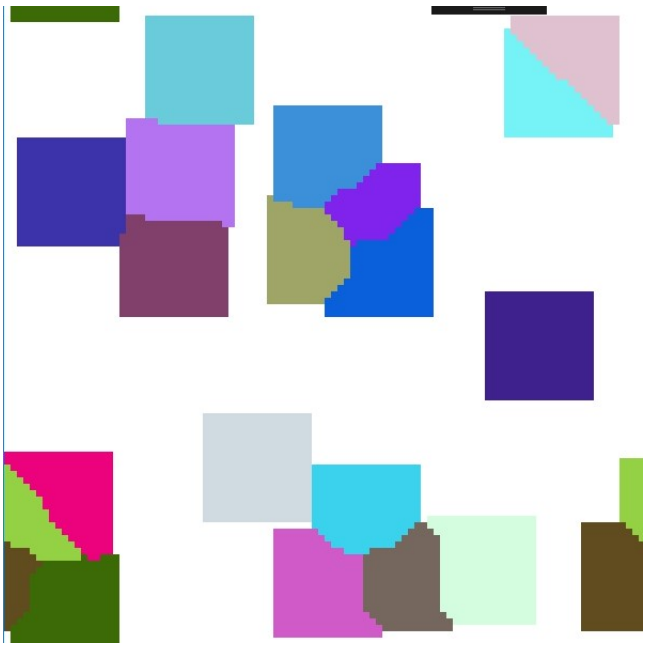
Picture 2 Random grains representation

3.2 Simulation of neighbourhood:

Von Neumann:

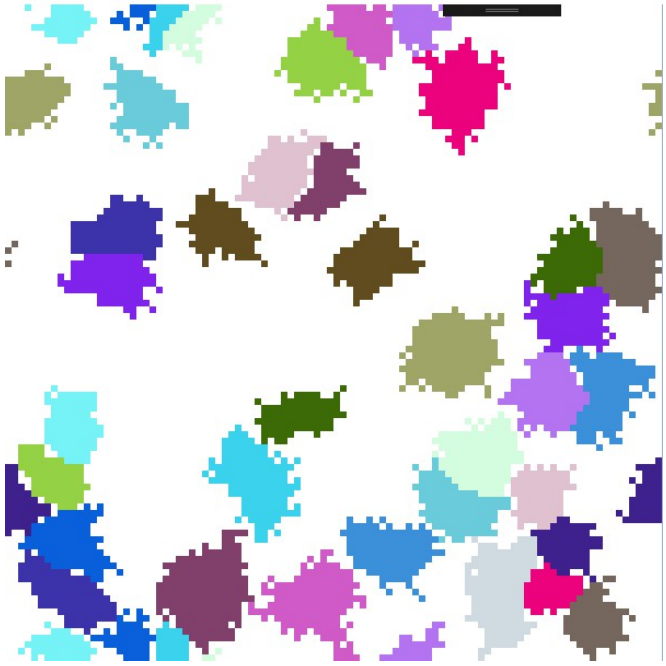
Picture 3 Von Neumman neighbourhood simulation

Moore:



Picture 4 Moore neighbourhood simulation

Moore Extended with shape control:



Picture 5 Moore extended neighbourhood with 20% shape controller

Moore Extended, 300 x 300 matrix, with shape control 80% and 100 grains:

Picture 6 Moore extended, 100 grains, 80% factor

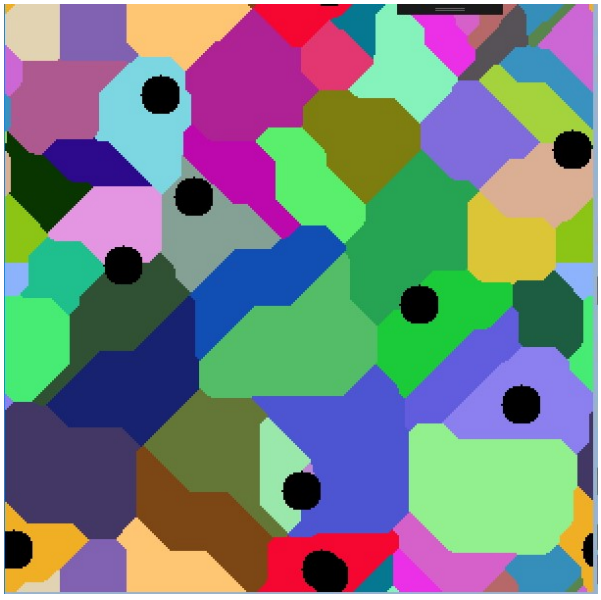
4 Inclusions:

Square:

Picture 7 Moore extended, square inclusions added after simulation

Circle:

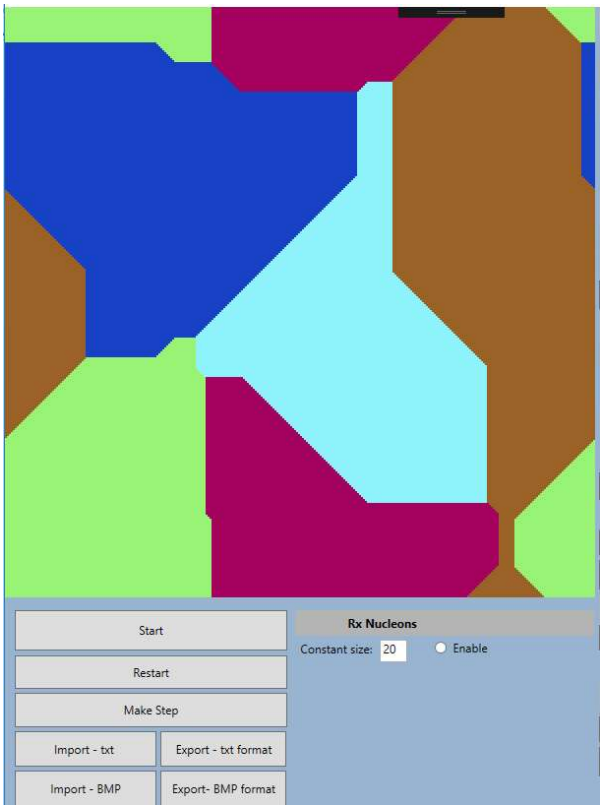
50 grains, Moore neighbourhood, inclusions added before simulation:



Picture 8 Circle inclusion added before simulation

5 Export and import from and to the file:

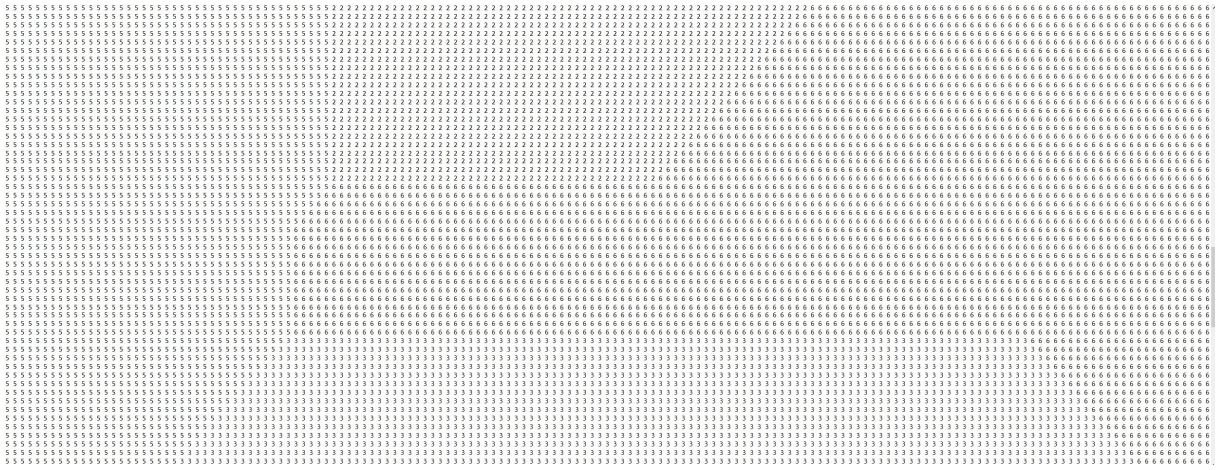
Example of export result to png file:



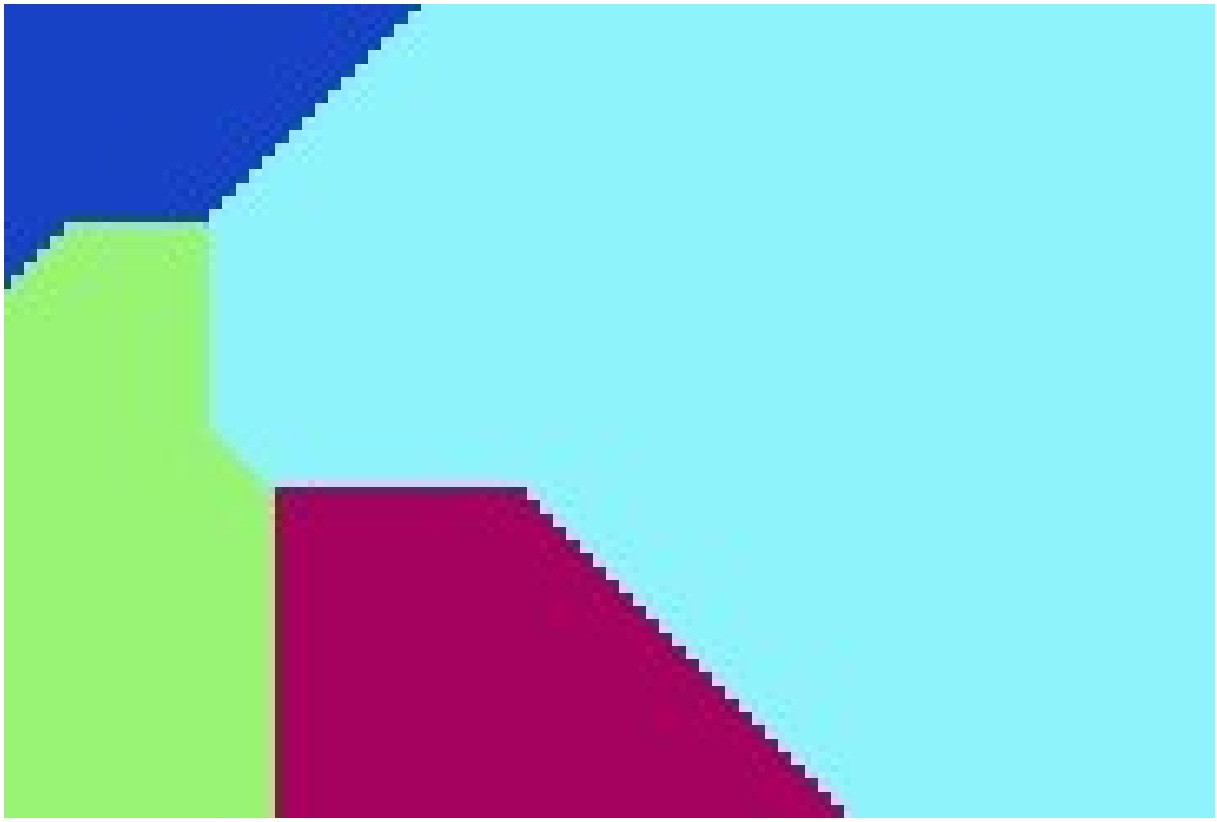
Picture 9 Screen from application

Picture 10 Exported result

Peace of exported result to txt file:

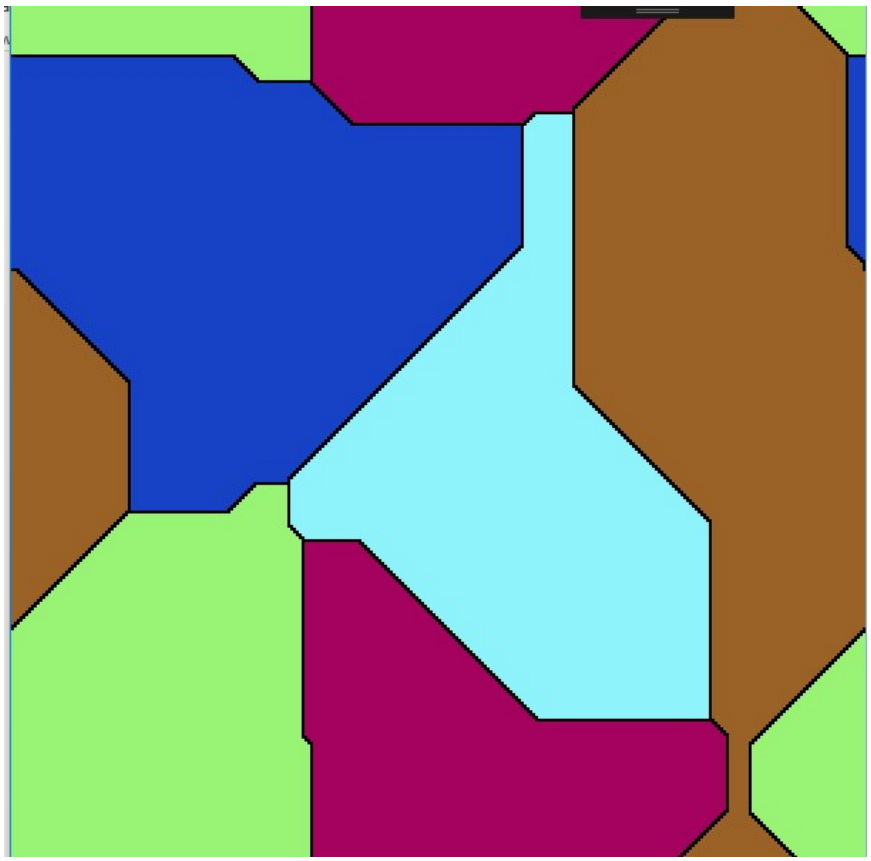


Picture 11 Txt number representation of colors

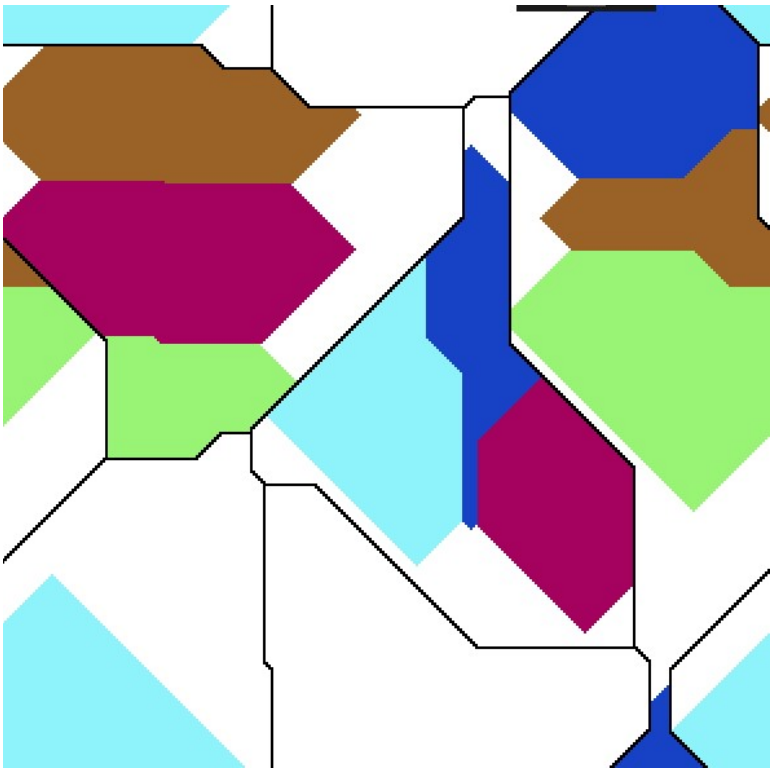


Picture 12 Same part of picture in application result

6 Borders implementation:



Picture 13 Example of simulation with borders added after simulation

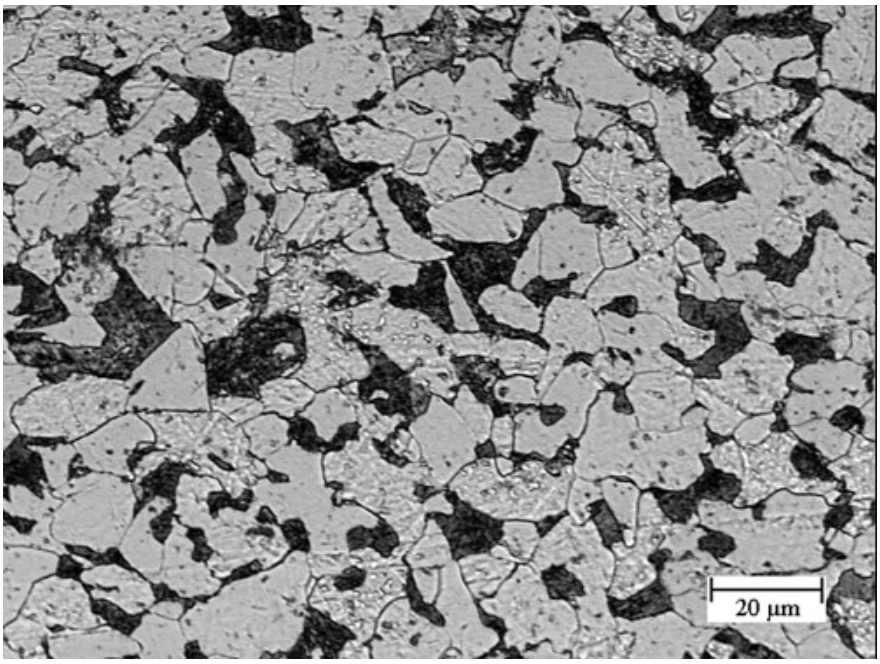


Picture 14 Example with erase simulation and second simulation with constant borders

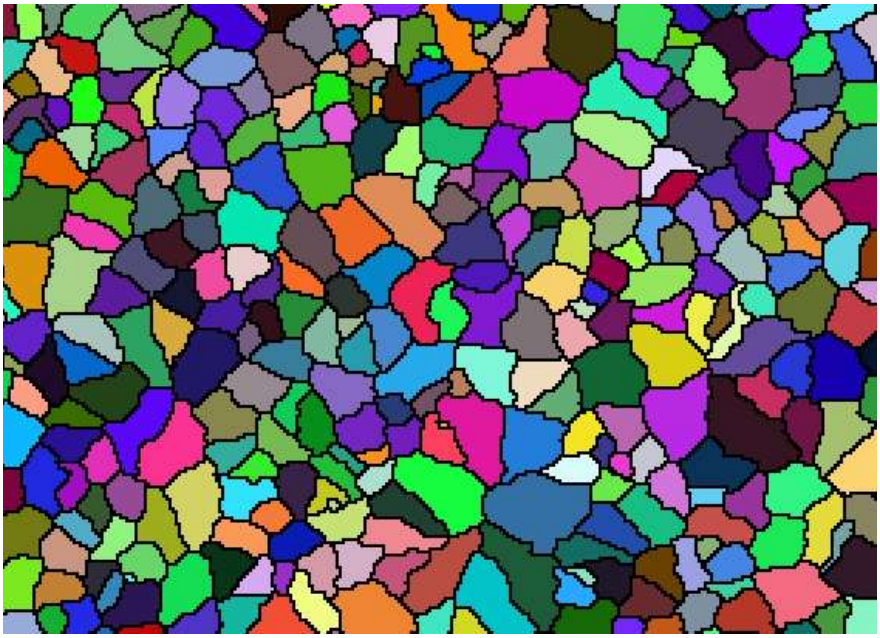
7 Comparison of simulation and real structures:

Grain growth simulation should contains predictions of phenomenon in real materials.

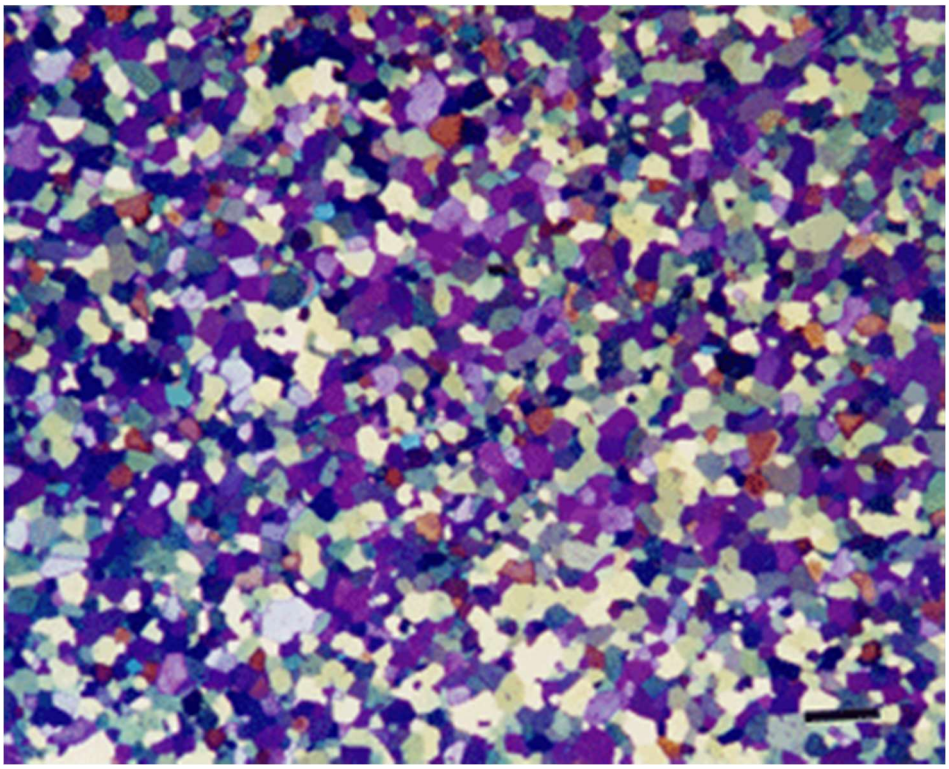
After choose right simulation parameters we should generate structure which is like real material.



Picture 15 The microstructure of ASTM A36 steel showing ferrite and pearlite. The mean grain diameter is 26.173 µm. Etchant is 2% Nital.

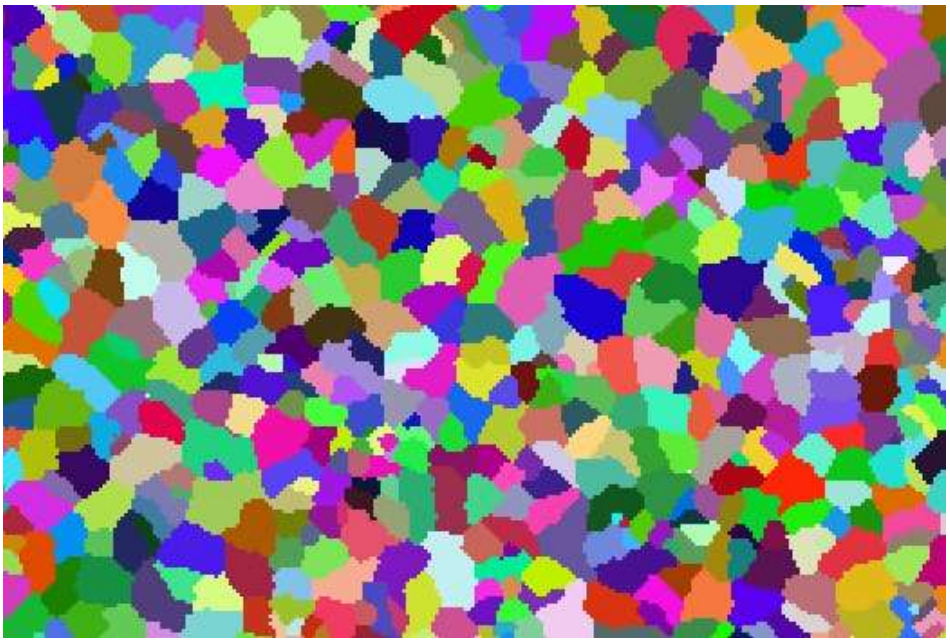


Picture 16 500 grains with Moore extended neighbourhood, X = 40%

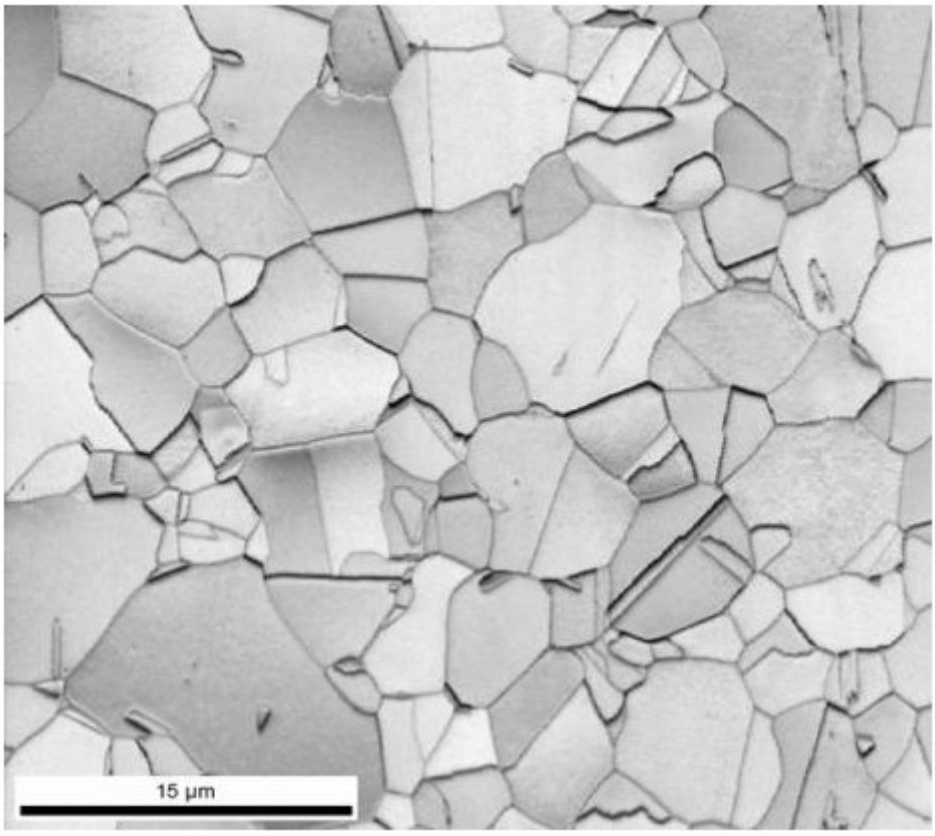


Picture 17 Commercial purity titanium, ASTM F67

After added 1000 random grains, choose Moore extended with 90% shape control.

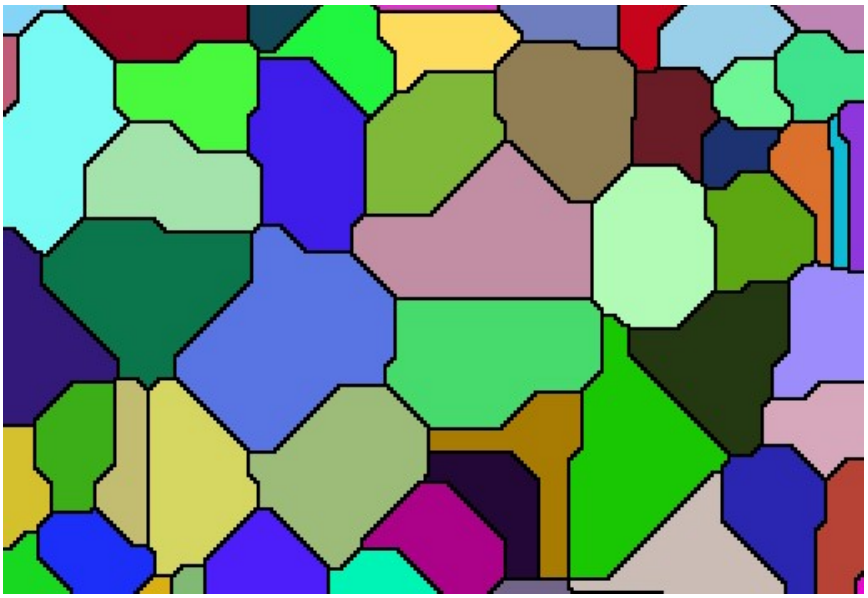


Picture 18 Moore extended, 1000 grains, X = 90%



Picture 19 Photomicrograph of TWIP steel as annealed

Simulation of that structure was quiet easy. The shapes of nucleons are similar to simulation with Von Neumann neighborhood.



Picture 20: 90 growing nucleons and Von Neumman simulation

Sources:
Picture 15: https://www.tms.org/pubs/journals/JOM/9801/Felkins-9801.fig.3.lg.gif

Picture 17: https://vacaero.com/wp-content/uploads/2015/03/2-c_sm.gif

Picture 19: http://worldautosteel.org/wp-content/uploads/2012/03/Fig2-16_TWIPphotomicro.png