Multiscale modelling – 2nd report

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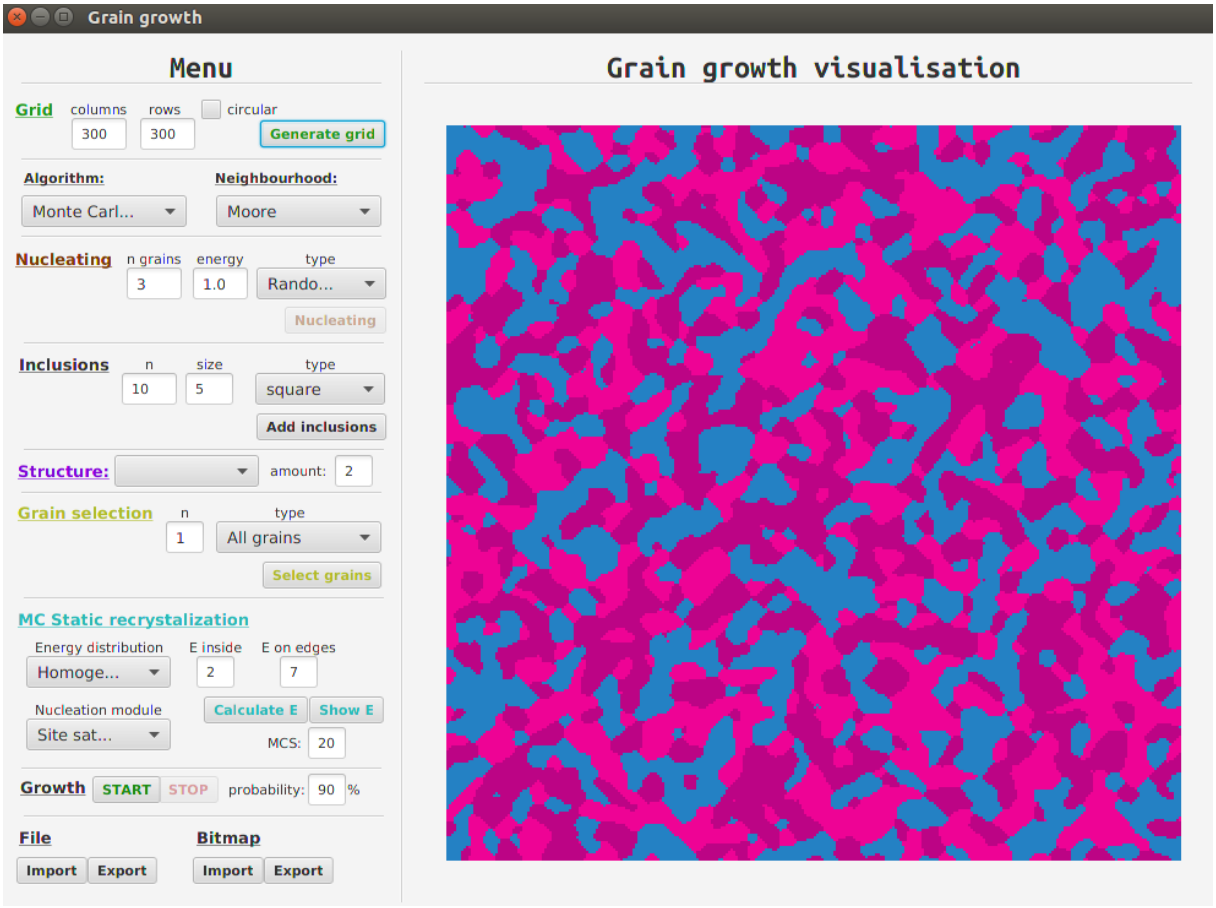
Content

1. Technologies

- Java 8
- JavaFX (user interface)

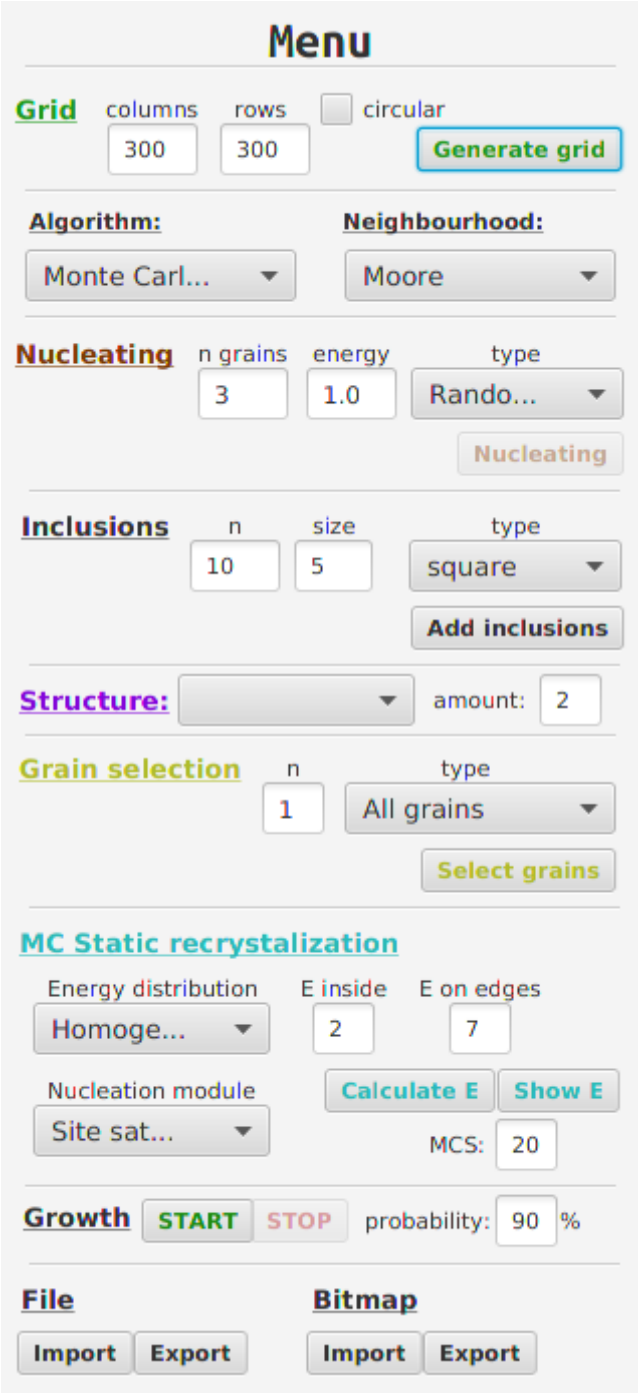
I used Java and JavaFX to continue next part of application in the same technologies. Next options and algorithms where added to existing ones in whole project.

2. User interface



Img 1: Main app view

In the Img 1 we can see main app view. On the left, there is main menu where we can start simulation, import and export microstructure or set some options. On the right we have the main part of the application – microstructure visualization. We can start/stop simulation from every step also it's associated with import from file or bitmap. There are some options for MC static recrystallization algorithm like calculate energy or show energy distribution.



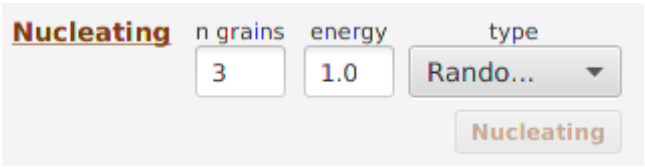
Img 2: Main menu

Img 2 shows main menu available in app. Menu was divided into sections to group it by functionalities. Some options are set when we generate grid for example algorithm or neighbourhood but not all of them. Structure or grain selection are available after microstructure is fully generated. Additional options are: grain boundary energy and new section with MC static recrystallization.

Main menu - options:

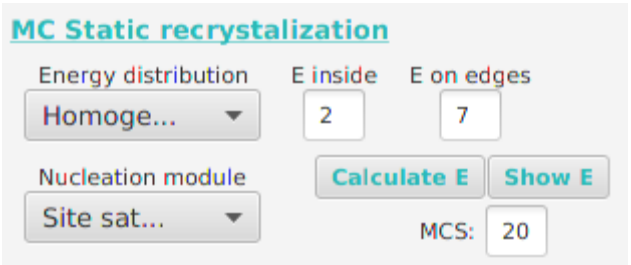
Here will be shown only these options which were added to program during second part of implementation.

Nucleating (Img 3) – there is two type options – random nucleating which seed grains randomly on the grid. We can also specify how many grains generate. Second option is random nucleating on the edges. This option is used for SRXMC algorithm to set recrystallized nucleons on the grain boundaries or anywhere.



Img 3: Nucleating section

Nucleating (Img 4) – in this section we can select energy distribution type: homogeneous or heterogeneous. Moreover we can define energy inside grains and on their edges. Thanks to nucleation module we can specify how SRXMC have to work – how new nucleons will be added on each step of simulation and in which way. Finally there are two buttons: calculate energy which set energy distribution for microstructure and show energy toggle button which is responsible for energy distribution visualization. This button might be used on every step of simulation to switch between two views.

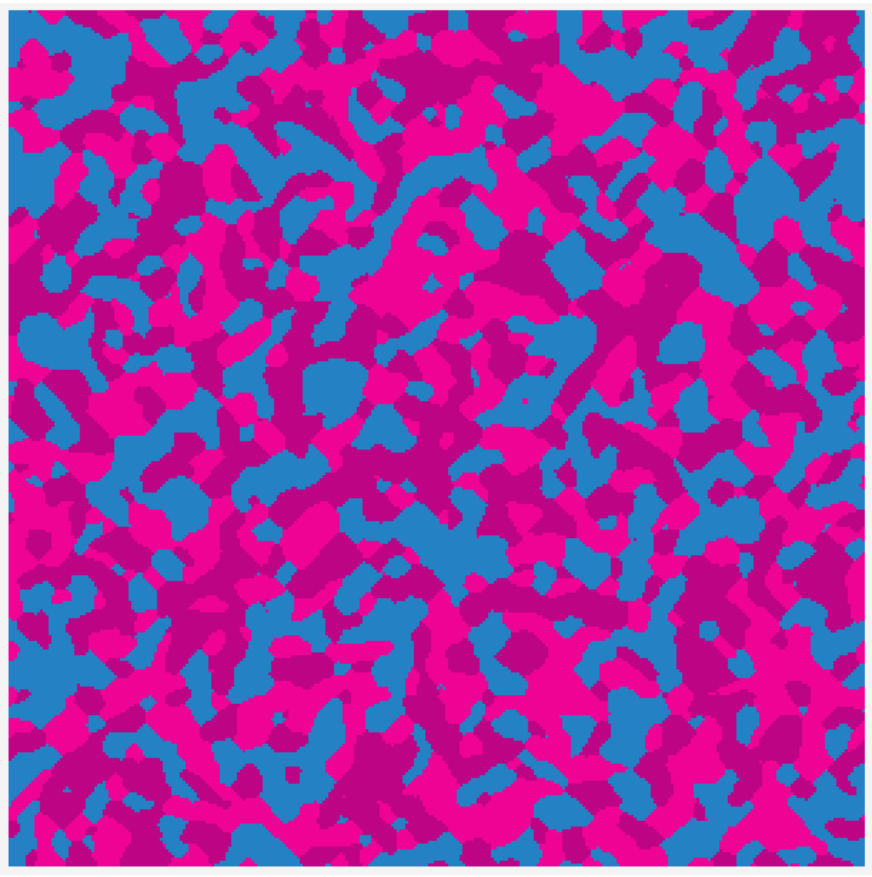


Img 4: MC Static recrystallization section

3. App operating

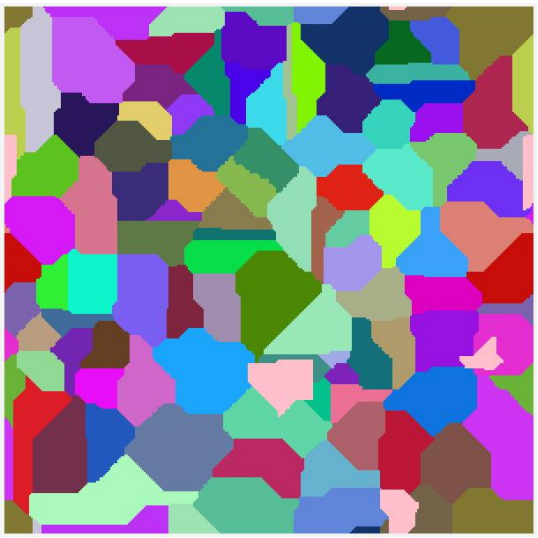
Below there is exemplary microstructure generated by application:

- Algorithm: Monte Carlo grain growth
- Neighbourhood: Moore
- Number of grains: 3
- MCS: 20

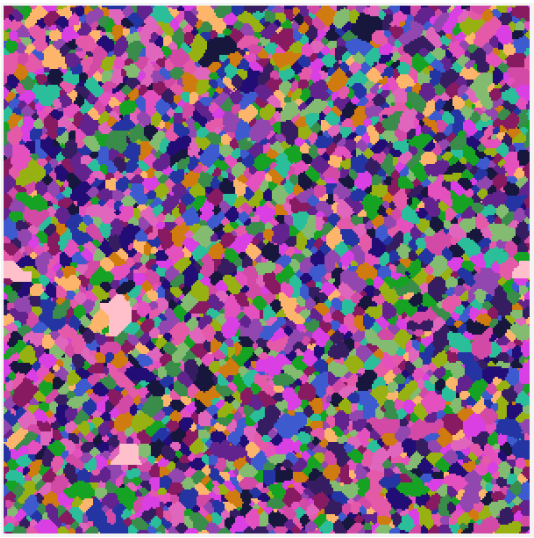


Img 5: Exemplary microstructure generated by application

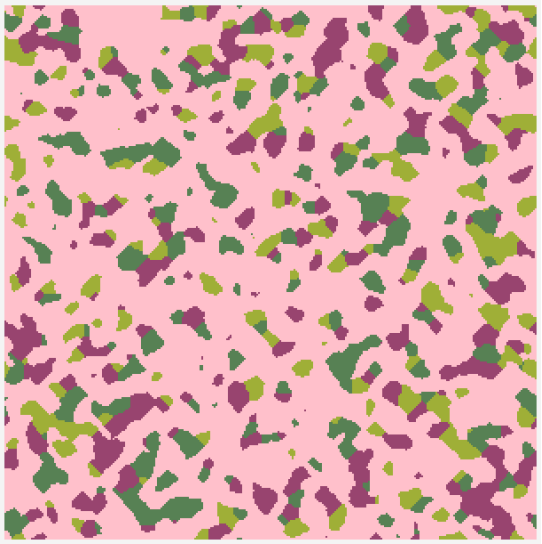
Next example shows dual phase microstructure:



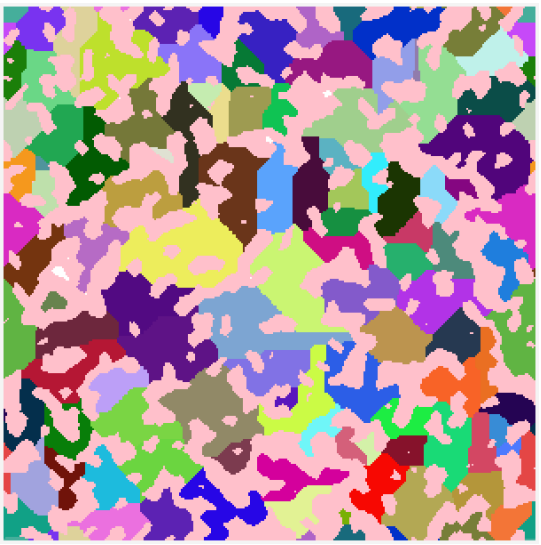
Img 6: CA -> CA



Img 7: CA -> MC

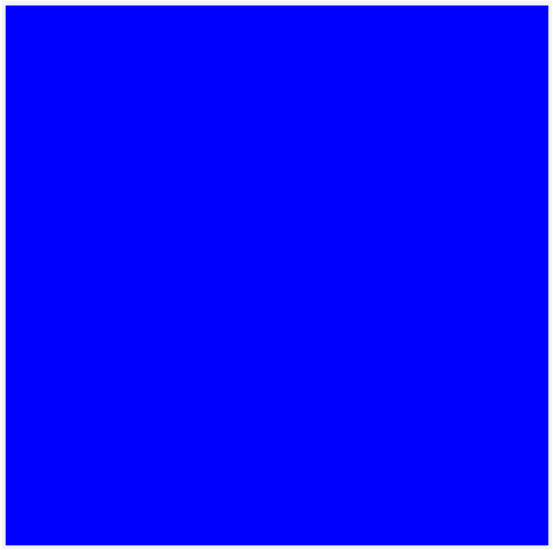


Img 8: MC -> MC

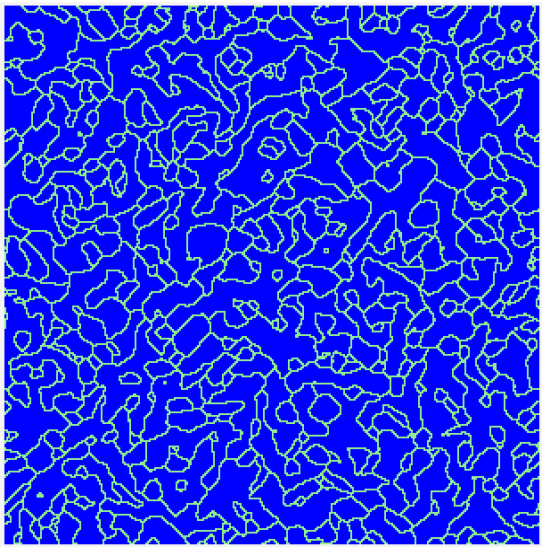


Img 9: MC -> CA

This example shows two types of energy distribution:

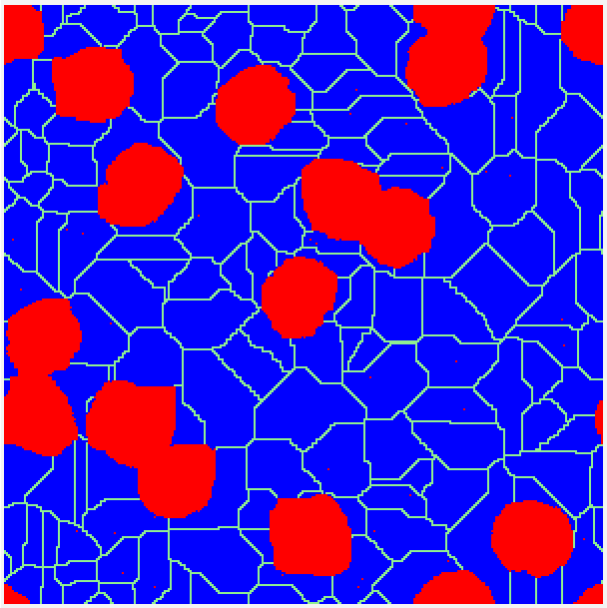


Img 10: Homogeneous



Img 11: Heterogeneous

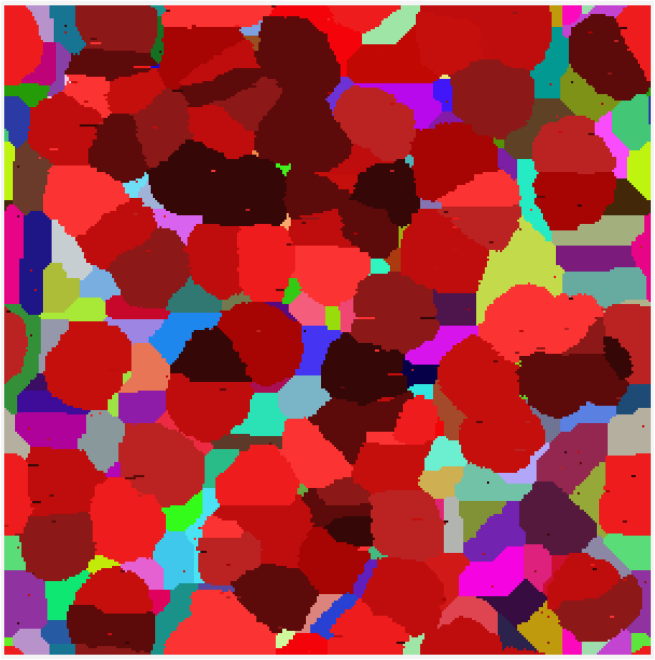
Additionally example below show energy distribution with recrystallized grains:



Img 12: Heterogeneous with recrystalized grains

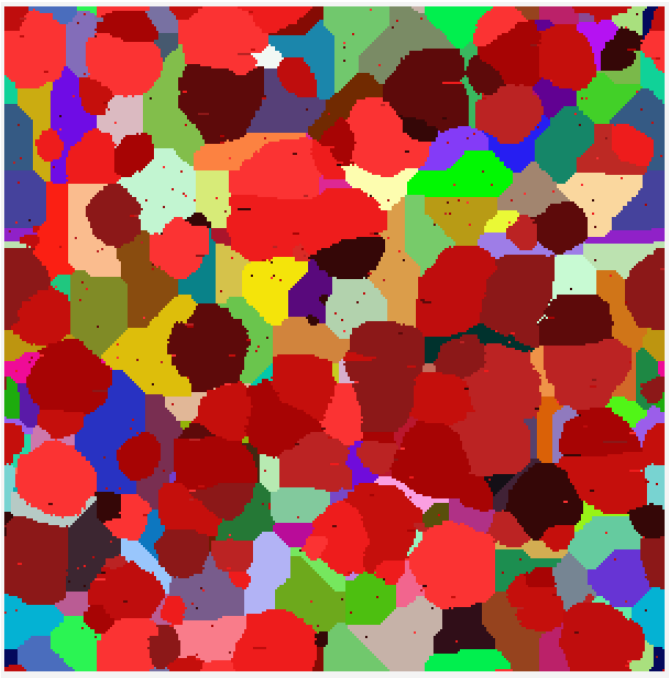
Finally, we have Monte Carlo static recrystallization algorithm:

- Number of nucleons: 20
- Nucleation module: Site saturated
- MCS: 20



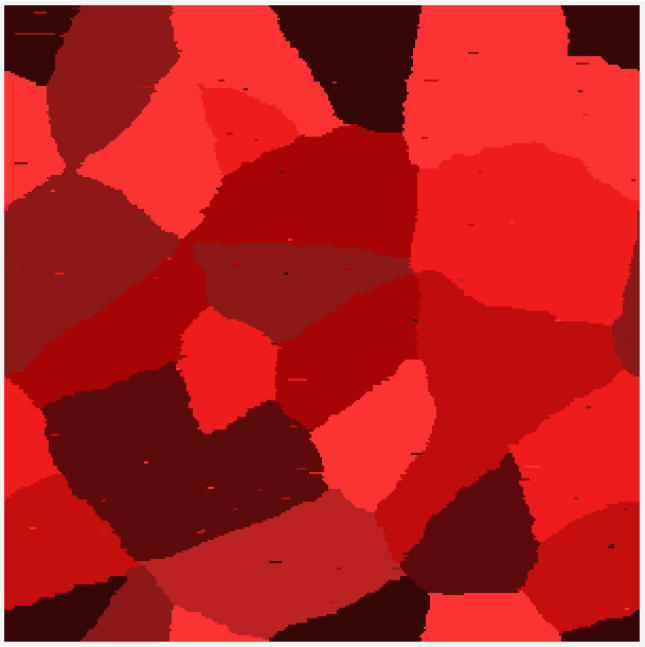
Img 13: SRXMC – Site saturated

- Number of nucleons: 20
- Nucleation module: Constant
- MCS: 20



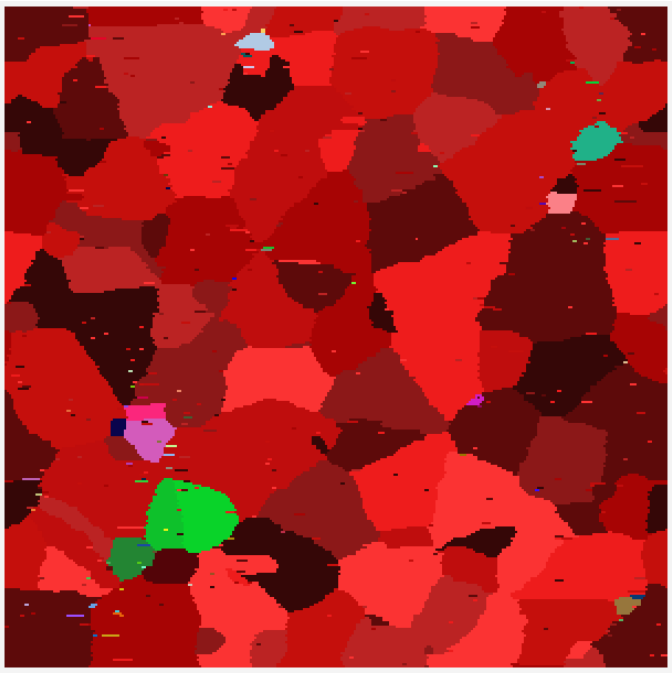
Img 14: SRXMC – Constant

- Number of nucleons: 20
- Nucleation module: Site saturated
- MCS: Full recrystallization



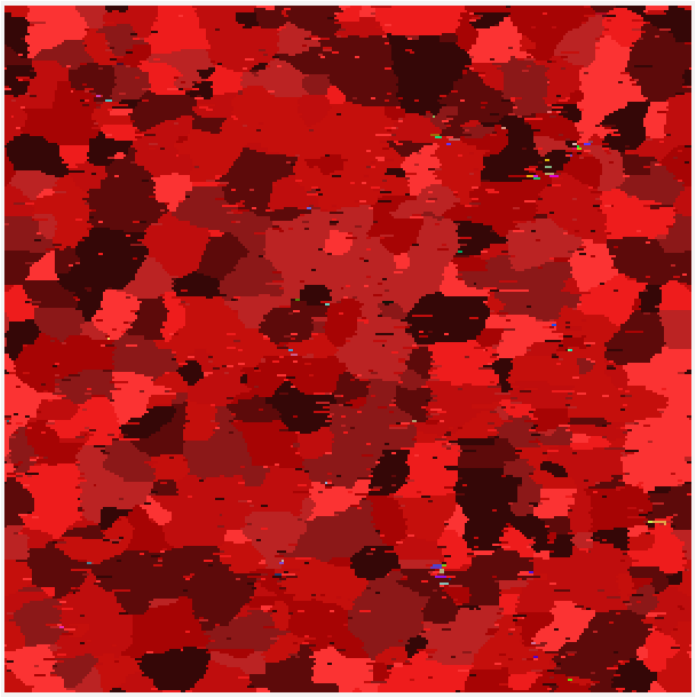
Img 15: SRXMC – Site saturated - Full

- Number of nucleons: 20
- Nucleation module: Constant
- MCS: Full recrystallization



Img 16: SRXMC – Constant - Full

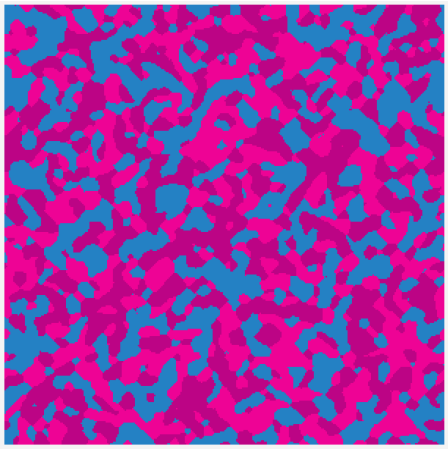
- Number of nucleons: 20
- Nucleation module: Increasing
- MCS: Full recrystallization



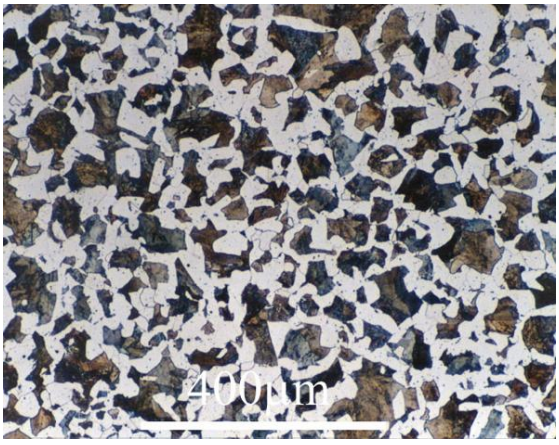
Img 17: SRXMC – Increasing - Full

4. Microstructure comparison

First of all I took these two microstructures to compare them. First microstructure comes from my application, second microstructure is Allotriomorphic ferrite in a Fe-0.4C [1]. Both of them are shown below.

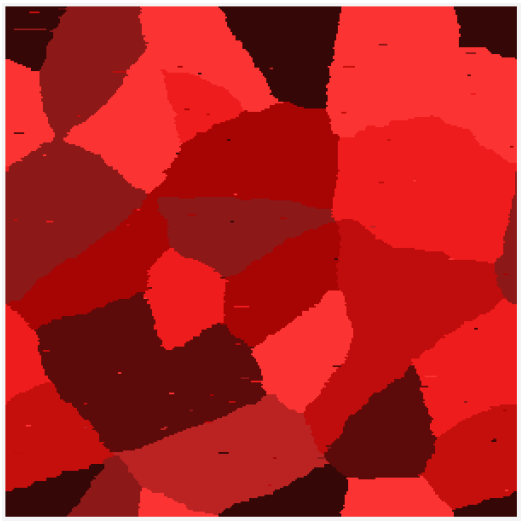


Img 18: Microstructure generated with MC

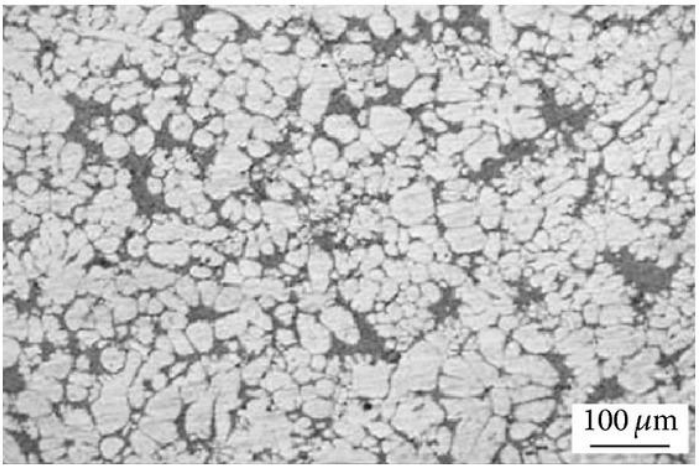


Img 19: Allotriomorphic ferrite in a Fe-0.4C [1]

For the last example I took these two microstructures to compare them. First microstructure comes from my application, second microstructure is Microstructure of 356 aluminum alloy obtained by the GISS method [2]. Both of them are shown below.



Img 20: Microstructure generated with SRXMC



Img 21: Microstructure of 356 aluminum alloy [2]

Conclusions from the comparison:

- Microstructure generated by app (Img 18) is very similar to the real microstructure taken to comparison (Img 19) when it comes to the for example shape of the grains,
- There could be more similar if we manipulate number of grains (Img 18, Img 19),
- Difference is between Microstructure of 356 aluminum alloy representation, generally in app (Img 20) the grains are bigger than in real microstructure (Img 21). It's just an approximation and in this case these two microstructures are not quite similar to each other. It depends on how many grains are recrystallized and their location in the space.

5. Conclusions

- Simulations give results which are similar to real microstructures,
- Application can be used to solve real problems, is expandable if new functionalities will be needed,
- Two parts of application were done and working as I expected before process of implementation.

6. Images

1. https://www.phase-trans.msm.cam.ac.uk/2008/Steel_Microstructure/SM.html, access: 16.12.2018
2. https://www.researchgate.net/figure/Microstructure-of-356-aluminum-alloy-obtained-by-the-GISS-method-50_fig23_258316014, access: 16.12.2018