Rafał Szyszka, laboratory group 2.

Multiscale modeling – Application implementation report – report 2.

1. Application user interface.

The application has been extended with amount of new features which forced rearranging position of GUI controls. The main view changes of the application's GUI is shown in figure 1.

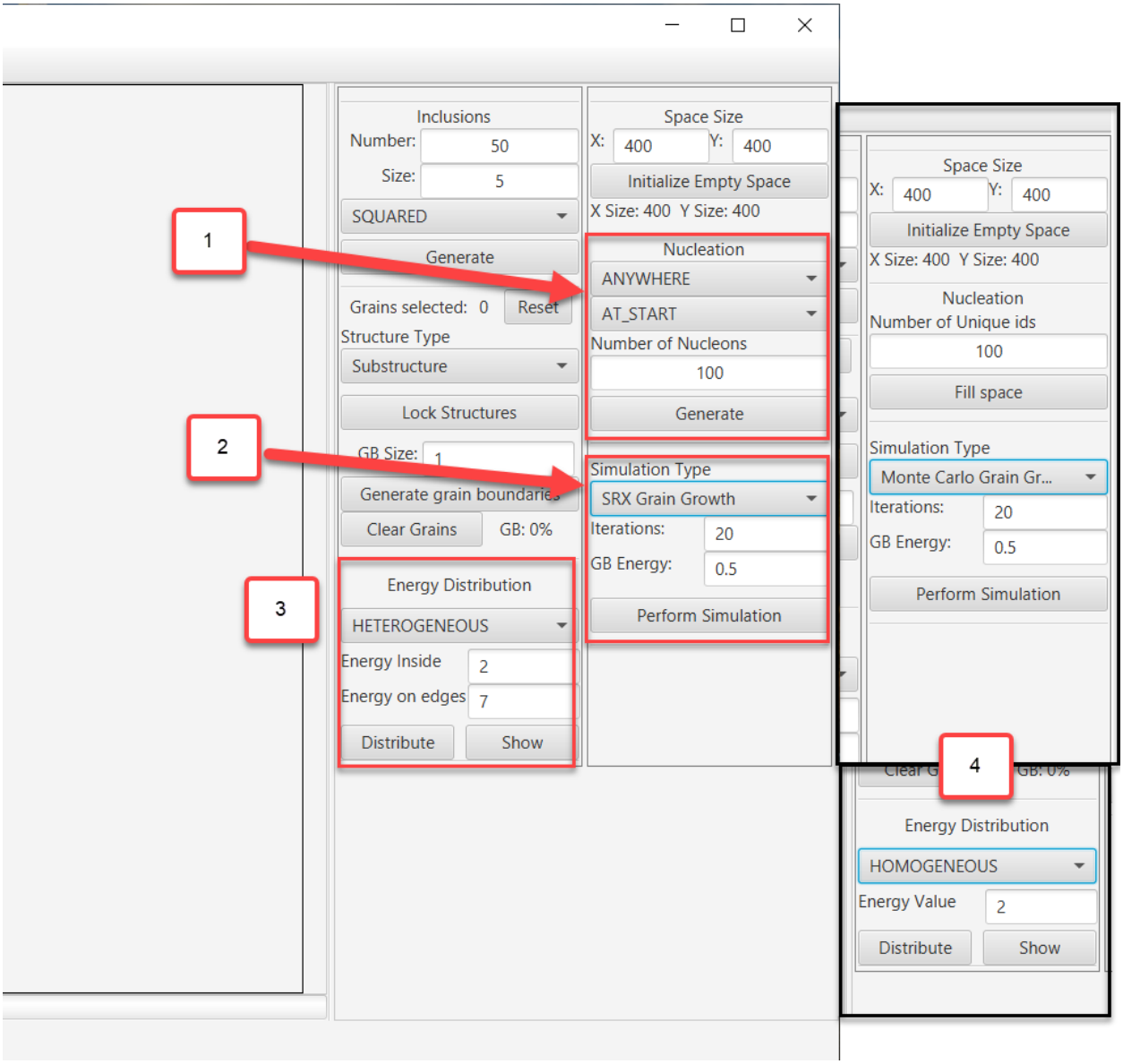

Figure 1. Application main view.

- In section no 1. was presented extended nucleation module. The user can specify nucleons location, their type and amount of nucleons to place.
- Section no 2. is a place where the user can choose simulation type. Comparing to previous version of the application there are two new simulation types *MonteCarloGrainGrowth* and *SRXGrainGrowth*, for which user can specify GB energy and iterations number which is duration of simulation.
- In section no 3. the user can perform heterogeneous or homogeneous energy distribution with given values in text fields.
- In section no 4. was presented application's dynamic adjustment to chosen combo boxes values. For example if user picks Monte Carlo simulation, nucleation module changes to fill whole space with number of unique values, while SRX grain growth specific controls are hidden.

All text fields on GUI have validation implemented to forgive user's mistakes.

2. Implemented application functionalities.

Monte Carlo grain growth simulation.

As previously mentioned, two new simulation types were implemented. First of them is Monte Carlo grain growth. Initial number of unique ids to randomly place and duration of simulation is given by user as number of iterations. In figure 2 can be seen space filled with one hundred unique ids and result of ten and fifty iterations of Monte Carlo algorithm.

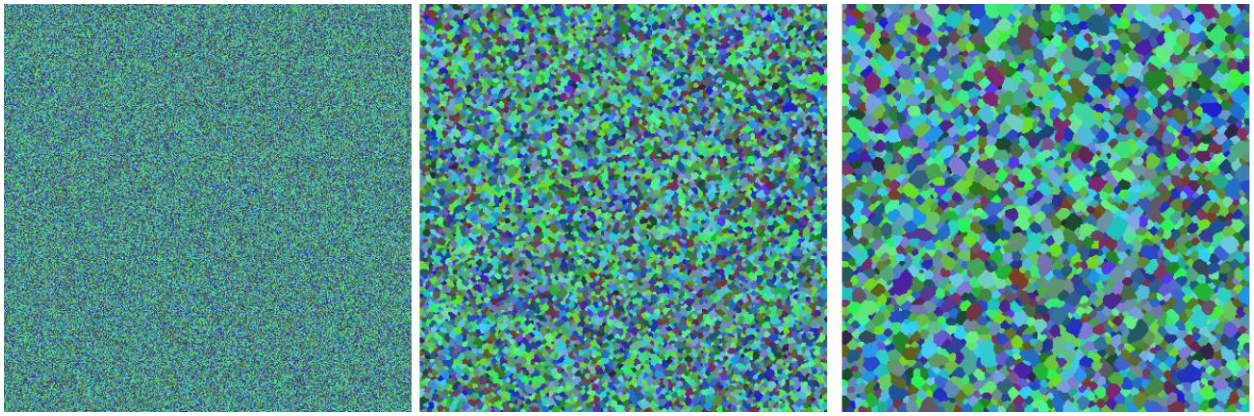

Figure 2. Space filled with 100 unique ids (left) Monte Carlo after 10 (middle) and 50 iterations (right).

Selected grains transformations with MC and CA methods combined

As in previous version of the application described in first report, the user can perform selected grains transformation into three structure types: *Substructures*, *Dual-Phase* or *Grain Boundaries*. That feature is also available with grains obtained from Monte Carlo method. In figure 3 was shown process of growing grains with MC method, turning some grains into dual phase and then performing CA method. Whereas inversed process can be seen in figure 4.

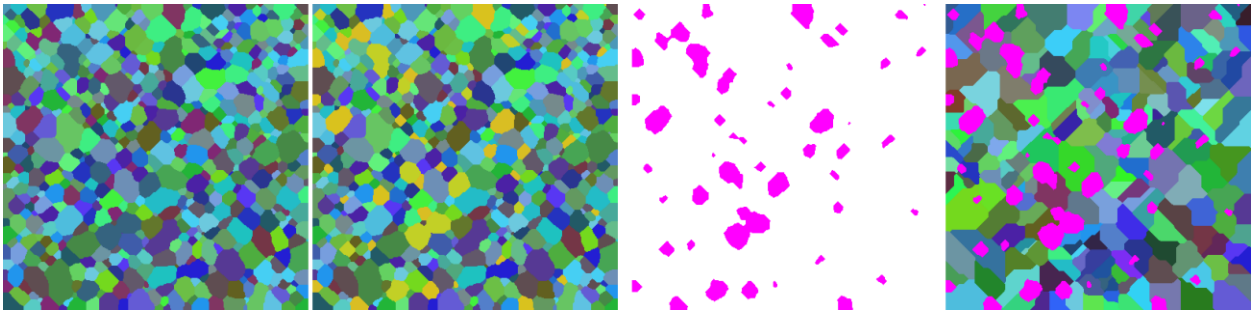

Figure 3. Example of use dual-phase generation combined with performing first MC and then CA method.

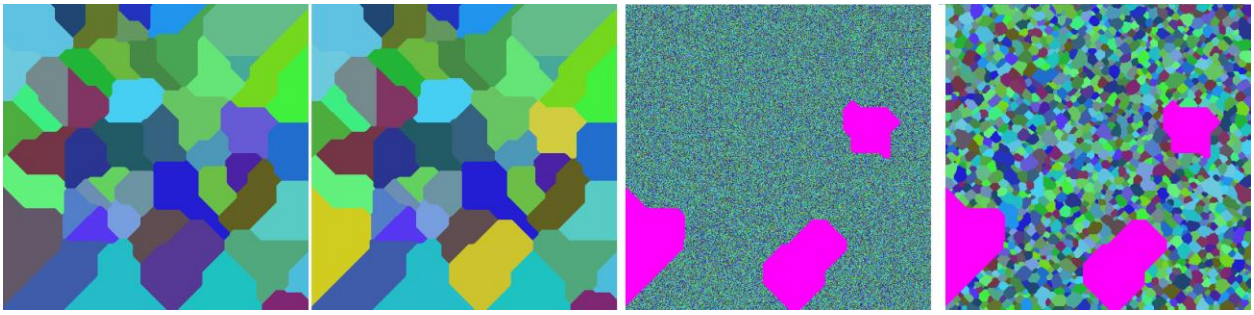

Figure 4. Example of use dual-phase generation combined with performing first CA and then MC method.

Energy distribution

Before user will be able to perform static recrystallization simulation, he must distribute energy in the space. Two distribution types are available: *Homogeneous* or *Heterogeneous*. In every cell energy value given by user is disturbed by ± 10%. The user can see energy distribution in space by clicking *Show* button. In figure 5 result of both distribution types has been shown.

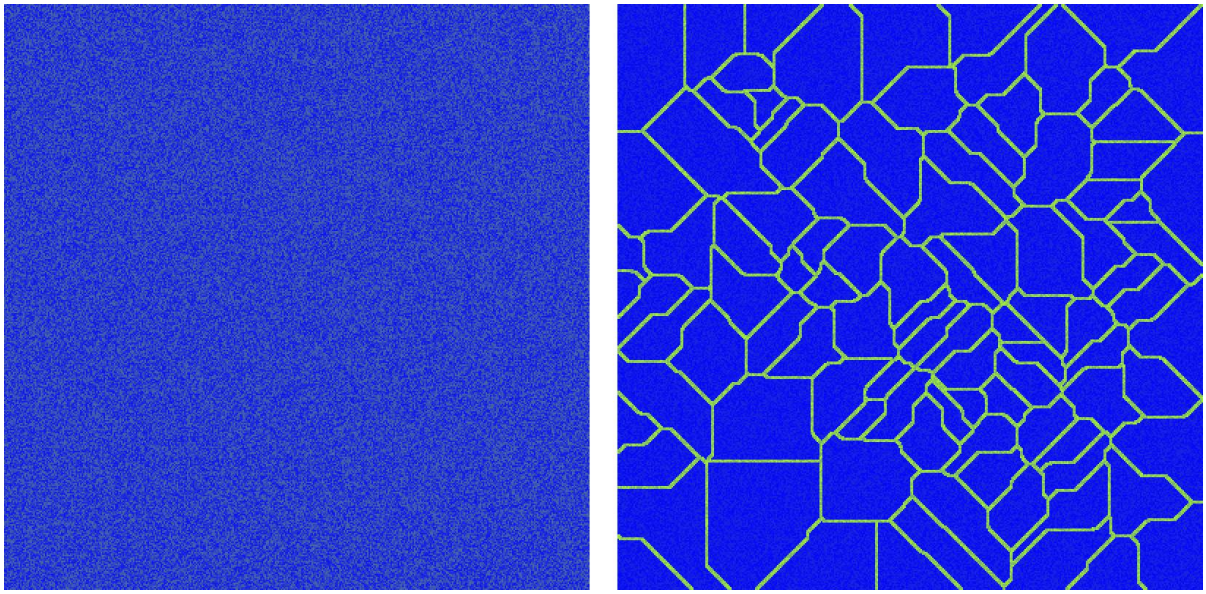

Figure 5. Homogeneous (left) and heterogeneous (right) energy distribution.

SRX nucleation module.

When energy has already been distributed, the user can perform nucleation of recrystallized grains. Nucleons can be placed either anywhere or in grain boundaries only. Moreover, three types of nucleation module are available: *AT_START* – number nucleons are placed only once before simulation, *CONSTANT* – constant number of nucleons is placed every fourth iteration of simulation, *INCREASING* – number of nucleons placed every fourth iteration is constantly increasing during simulation.

SRX grain growth.

After previously described modules (energy distribution and SRX nucleation) were applied, the user can perform static recrystallization simulation. In the application view recrystallized grains are displayed in shades of red. Result of SRX simulation performed on initial space shown in figure 6, with increasing nucleation on grain boundaries was presented in figure 7.

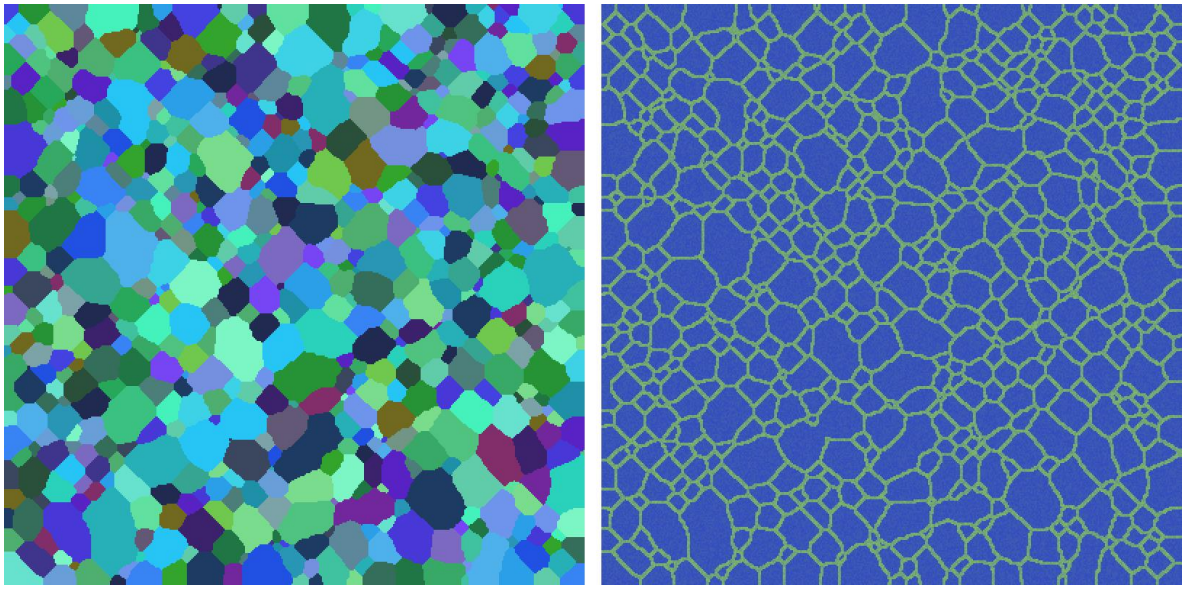

Figure 6. Initial space with energy distribution inside grains value = 1 and on grain boundaries = 2.

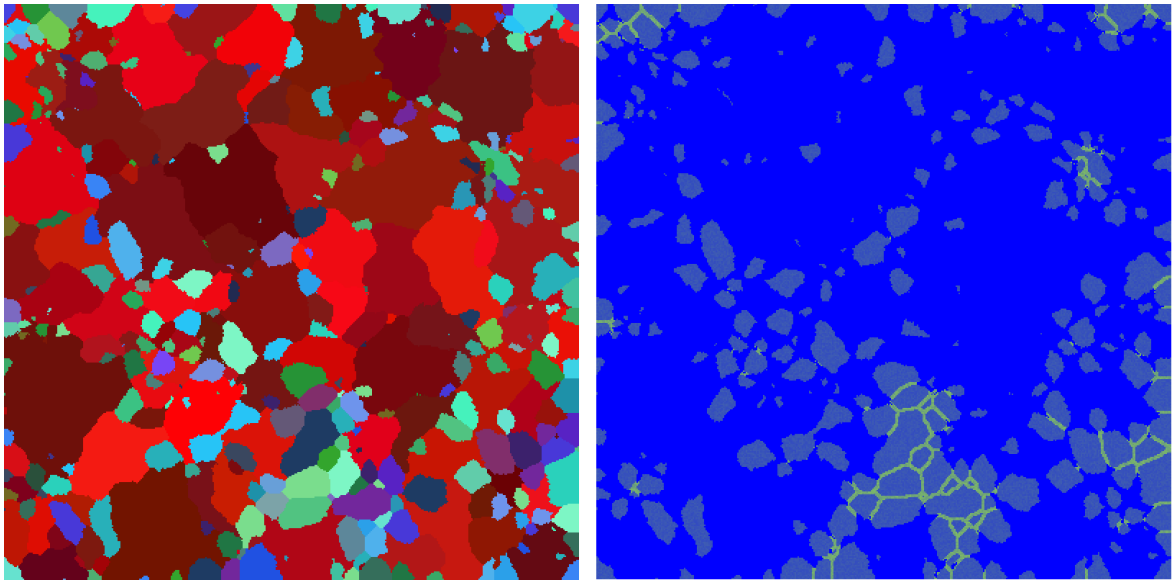

Figure 7. Space after 25 iterations of static recrystallization with 5 nucleons initially placed with increasing rate.

3. Reconstruction of real microstructures

With use of the application an attempt was taken to reconstruct real microstructures. First micrograph is showing well-recrystallized grains of ferrite and austenite [1]. In figure 8 comparison of real micrograph and generated microstructure was presented.

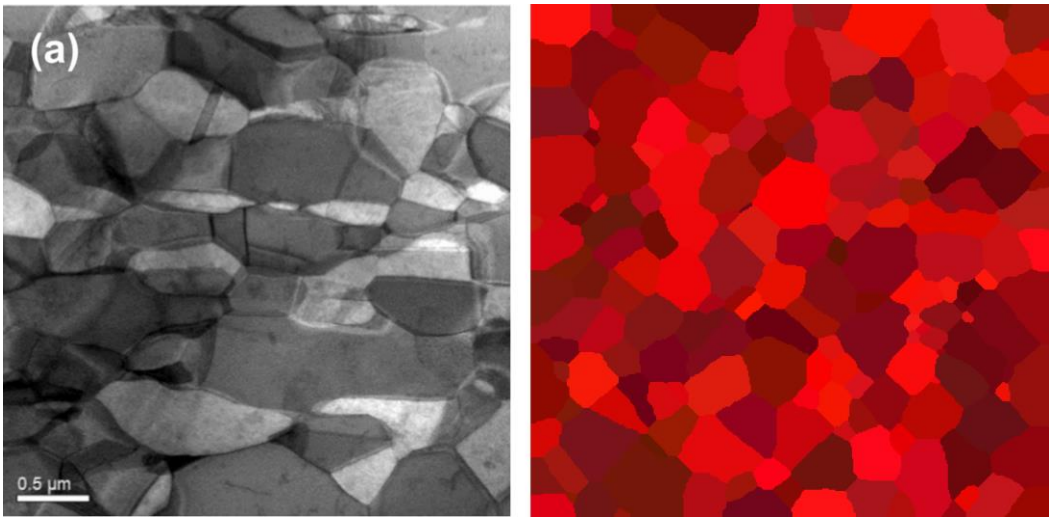

Figure 8. Comparison real (left) to generated (right) microstructure with well-recrystallized grains.

The second microstructure taken to reconstruction is AN12 annealed 4 seconds in temperature of 350 °C [2]. The result obtained is shown in figure 9.

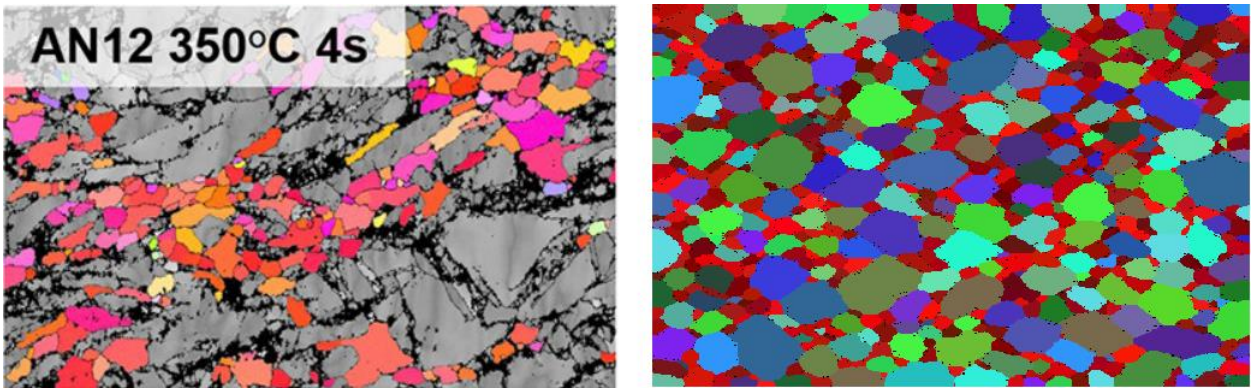

Figure 9. Comparison real (left) to generated (right) AN12 microstructure.

In the presented comparisons, it can be noticed that real and generated microstructures are very similar. Fully recrystallized microstructure was quite easy to obtain, nevertheless result gained is very accurate. Simulation of AN12 recrystallization also seems to be successful. Taking this all into consideration it can be surely said that the developed application can be used for generating microstructures with promising accuracy.

4. Bibliography

[1] Jin-Kyung Kim, Ji Hoon Kim, Dong-Woo Suh, Partially-recrystallized ferrite grains and multiple plasticity enhancing mechanisms in a medium Mn steel, Materials Characterization, Volume 155, 2019, 109812, ISSN 1044-5803.

(http://www.sciencedirect.com/science/article/pii/S1044580319311799)

[2] Xun Zeng, Peter Minárik, Patrik Dobroň, Dietmar Letzig, Karl Ulrich Kainer, Sangbong Yi, Role of deformation mechanisms and grain growth in microstructure evolution during recrystallization of Mg-Nd based alloys, Scripta Materialia, Volume 166, 2019, Pages 53-57, ISSN 1359-6462.

(http://www.sciencedirect.com/science/article/pii/S1359646219301319)