AGH UNIVERSITY OF SCIENCE AND TECHNOLOGY

Faculty of Metals Engineering and Industrial Computer Science

MULTISCALE MODELLING

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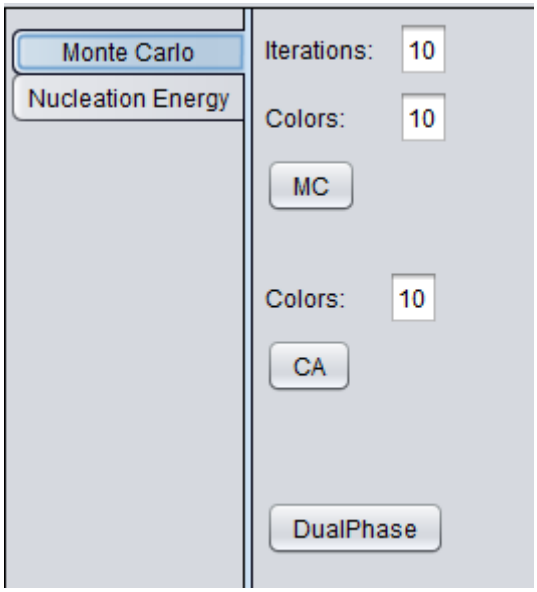
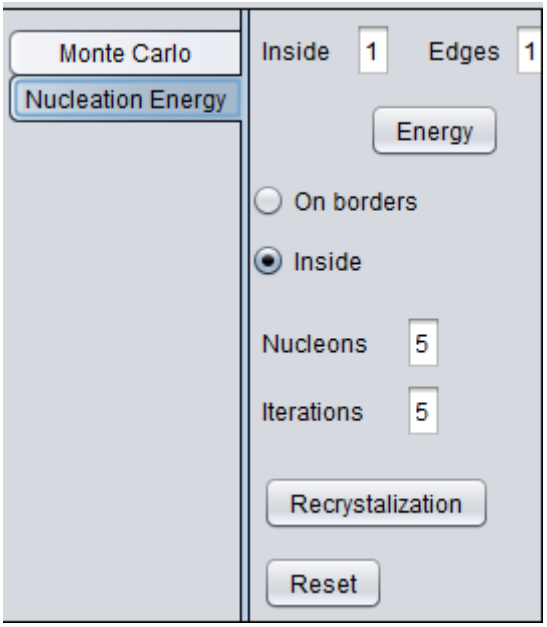
Performance date: 08.01.2019

The aim of the project was to implement Monte Carlo algorithm.
Project was implemented in Java using NetBeans IDE 8.2.
This project is an extension of the previous project. Panel to settings is presented on picture 1 and 2.



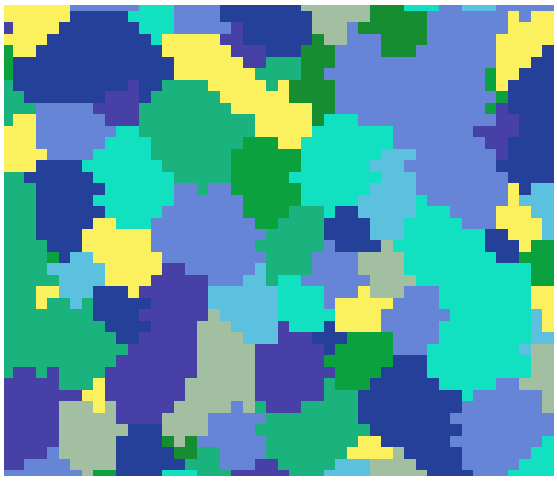
Picture 1: Monte Carlo and DualPhase panel



Picture 2: Grains, Nucleotion Energy and Recrystalization panel

Lab 1: MC grain growth

User can choose parameters to generate structure. User can choose a number of color which be used in Monte carlo algorithm and number of steps. When user add your preferences should choose a MC button.



Picture 3: Completed Monte Carlo grain growth simulation

Picture 3 shows the completed Monte Carlo grains simulations.

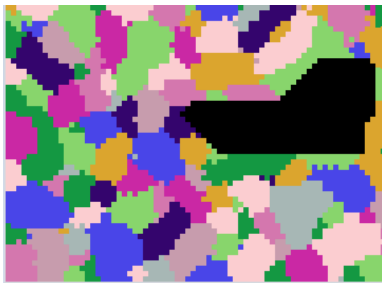
Lab 2: Modification of MC grain growth algorithm - substructures CA, MC

Next part of the project was devoted to generation the substructure and double phase structures. For both of them some grains become solid after the simulation The rest of the structure is removed, a new simulation is running.

Four cases were considered when implementing this functionality:

- Simple grain growth using Cellular Automata -> Grain Selection -> Grain growth Cellular Automata
- Simple grain growth using Cellular Automata -> Grain Selection -> Grain growth Monte Carlo
- Simple grain growth using Monte Carlo -> Grain Selection -> Grain growth Cellular Automata
- Simple grain growth using Monte Carlo -> Grain Selection -> Grain growth Monte Carlo

Picture 4

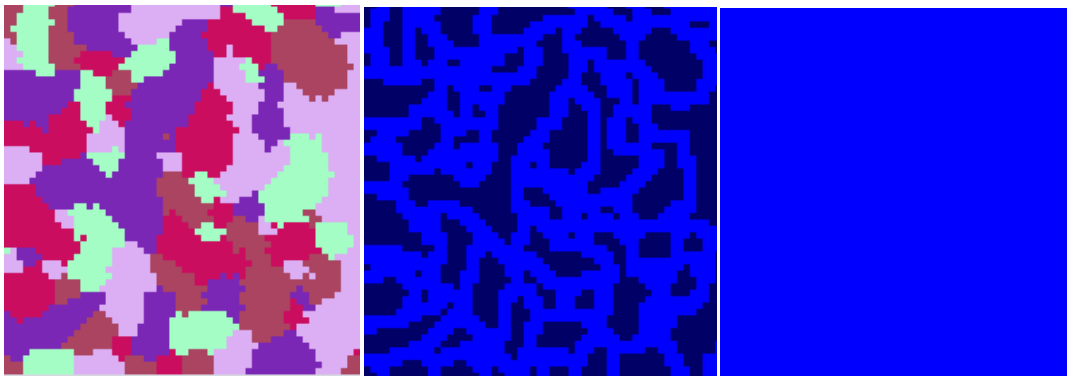


Picture 5

Picture 4 show simple grain growth using Cellular Automata. Next step on this simulation was selection grain and next grain growth simulation. In this simulation was Monte Carlo grain growth (Picture 5).

Lab 3 MC static recrystallization algorithm - energy distribution

The first step on this simulation was the random selection grain and start simulation selected algorithm (Cellular Automata or Monte Carlo). The next step was distribution of energy homogeneous and heterogeneous.

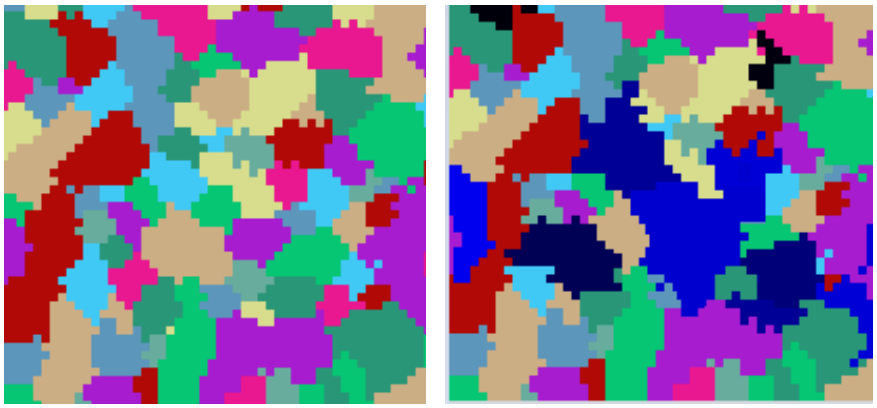


Picture 6 **Picture 7** **Picture 8**

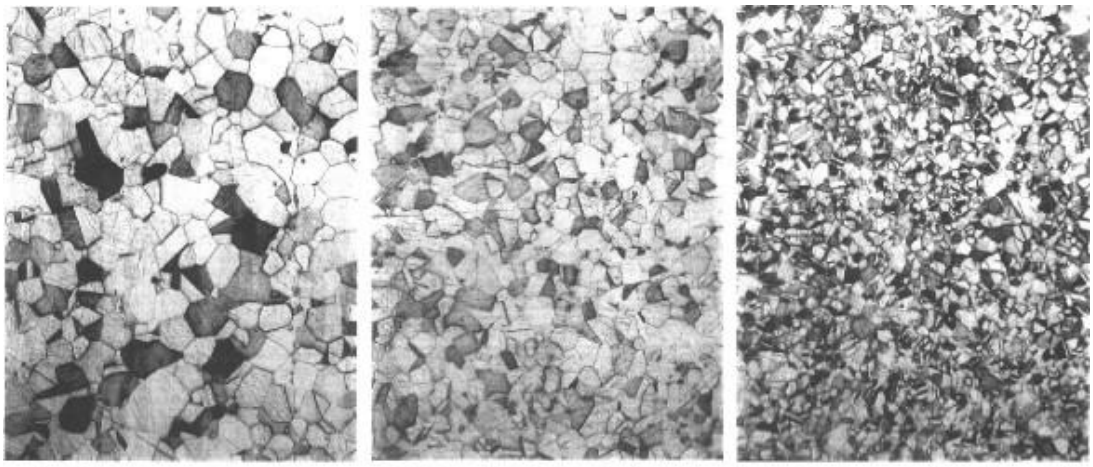
Picture 6 shows the first step, which is necessary to distribute energy. Picture 7 show energy distribution before recrystallization, where parameters in sight = 2 and on borders = 5. Picture 8 shown the homogenous energy distribution (parameters in sight and on borders equals 5).

Lab 4,5 MC static recrystallization algorithm – nucleation and growth

User can select the number of nucleons on the start. User can choose at the beginning nucleation after Monte Carlo Simulation.



Picture 9, 10: At the beginning recrystallization



Picture 6: An example of metal recrystallization
(taken from: https://www.imetllc.com/training-article/recrystallization-anneal/)

Conclusion

The disadvantage of the Monte Carlo algorithm is the very long calculation time. This is related to the probalistic nature of the model. Most of the proposed reorientation of elements leads to an increase in the energy of the network, so the change is not accepted and we do not have to deal with grain growth.

Code: https://github.com/agnieszkabielak/MultiscaleModelling2