AGH UNIVERSITY OF SCIENCE AND TECHNOLOGY

Faculty of Metals Engineering and Industrial Computer Science

Multiscale Modelling

Simple grain growth with cellular automata algorithms

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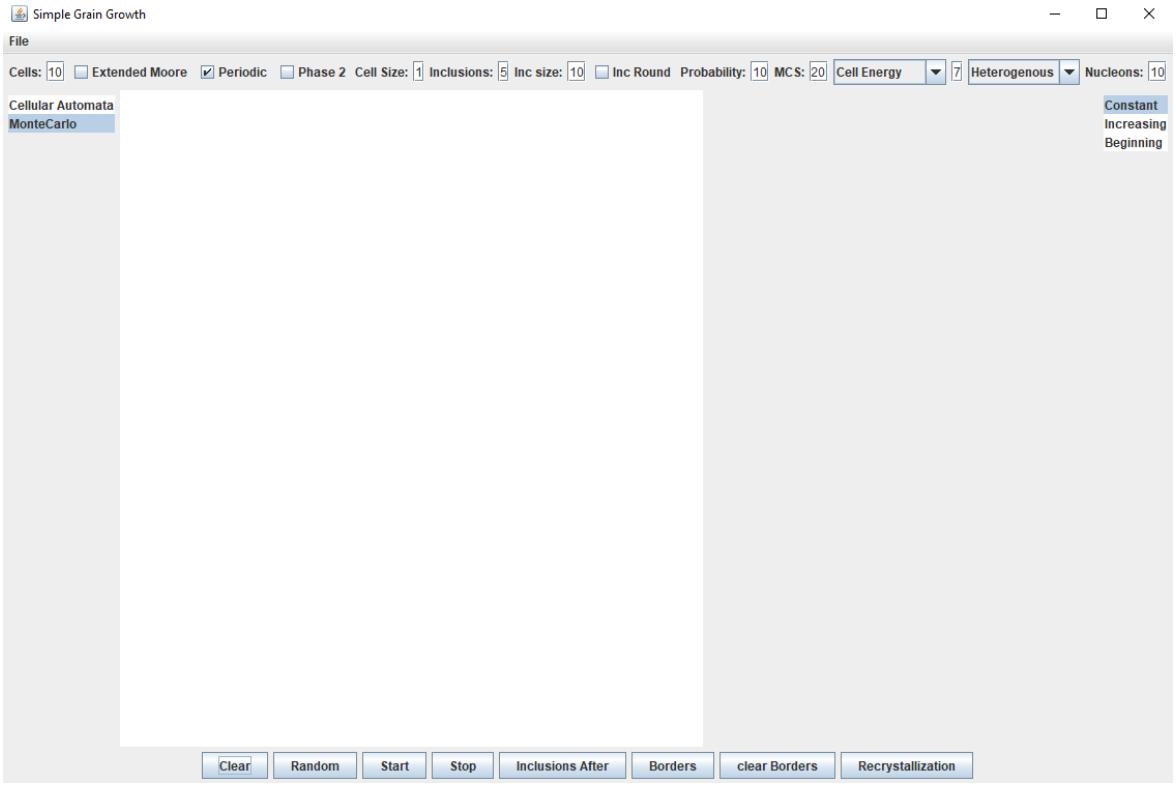
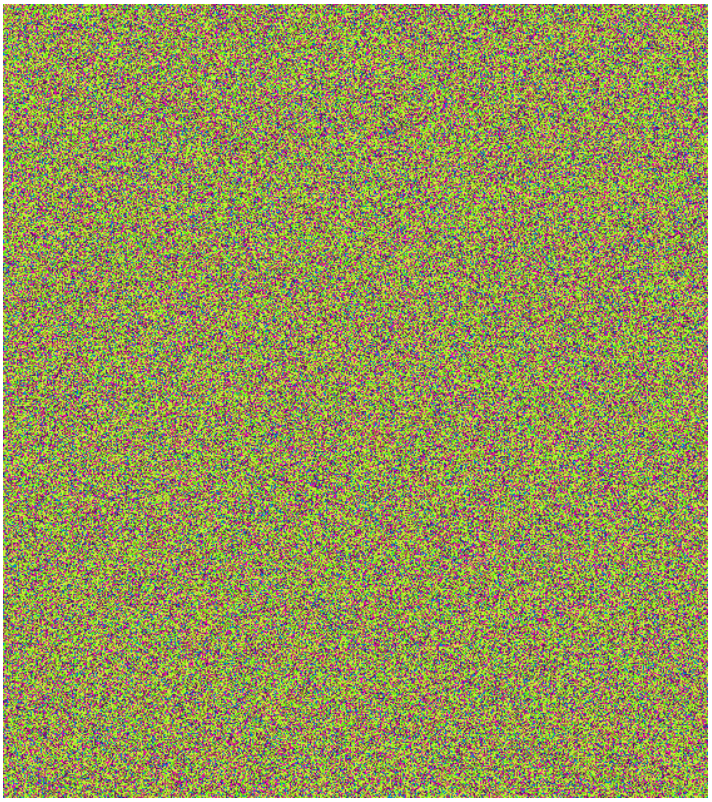
The main assumption of the second part of project was to implement Monte Carlo grain growth algorithm, modification of MC grain growth algorithm (substructures CA, MC) and static recrystallization algorithm with energy distribution, nucleation and growth of recrystalized microstructure.

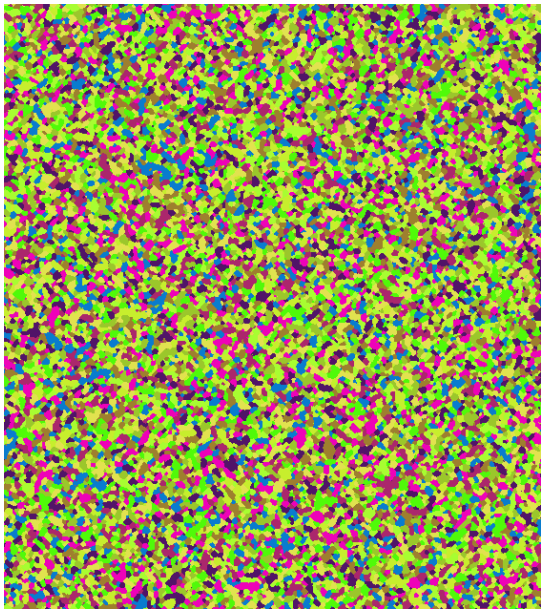
1. MONTE CARLO GRAIN GROWTH ALGORITHM



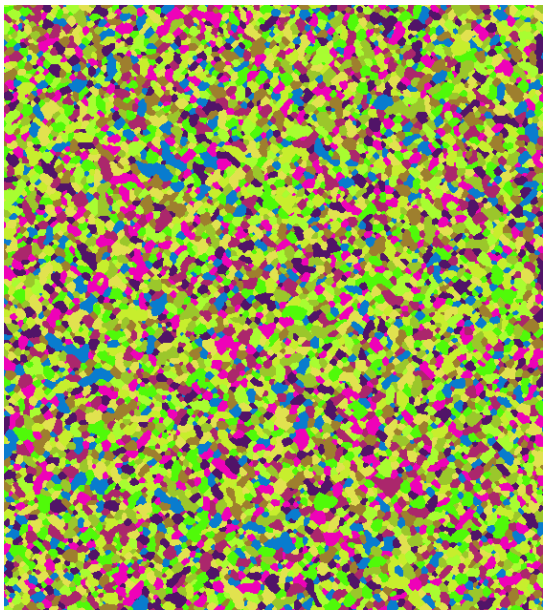
To generate microstructure using MC user need to select Monte Carlo from the list on the left, then press random button to randomly draw seeds, define number of MCS iteration and press start button to start.



Picture 1 MC 0 MCS



Picture 2 MC 10 MCS

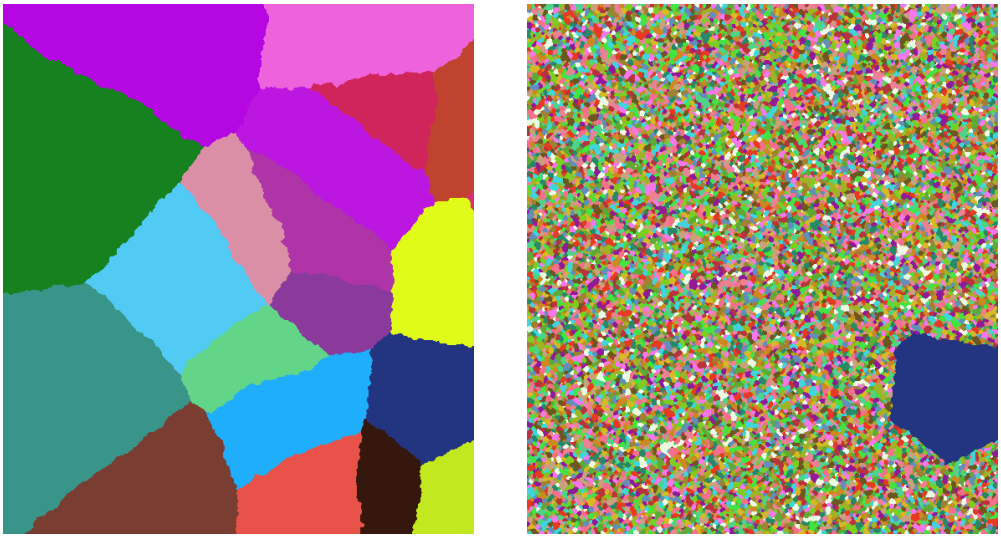


Picture 3 MC 20 MCS

As you can see there is a difference between these three pictures in shape and size of the grains. On the picture 1 was before start of the iterations (0 MCS), on picture 2 was after 10 MCS and on the picture 2 after 20 MCS.

2. MODIFICATION OF MC GRAIN GROWTH ALGORITHM (SUBSTRUCTURES CA, MC)

In this part of project, we used functionality implemented in previous part of project – dual phase. After generating microstructure using CA or MC user is able to leave random grain and start new growth with different type of grain growth

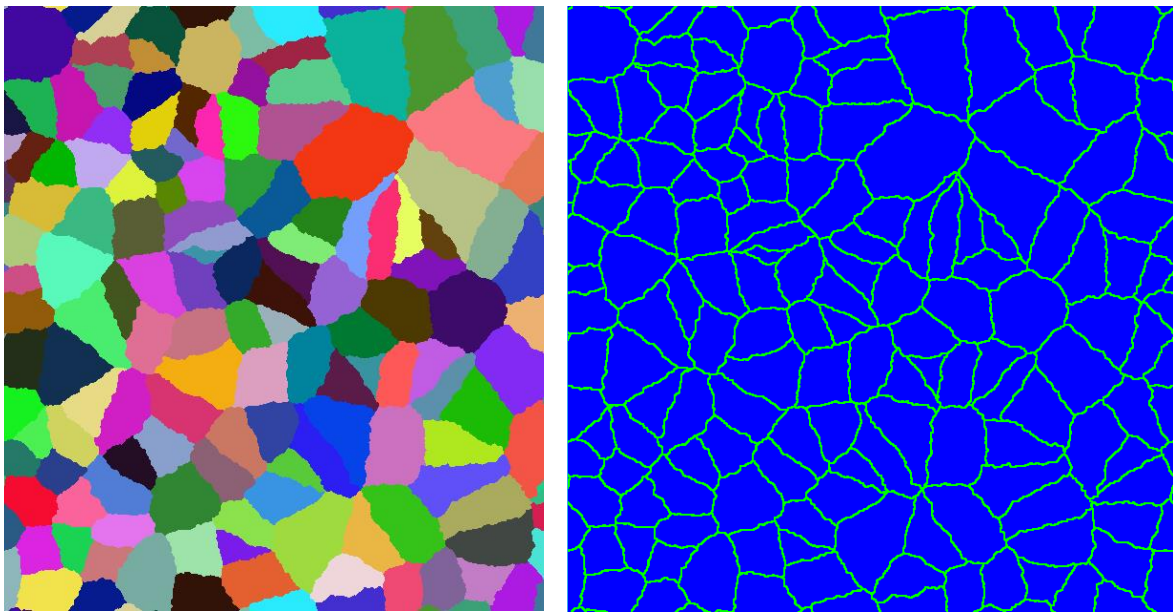


Picture 4 CA -> MC

Unfortunately, for some unknown reason, I was unable to determine why this functionality does not work for the substructure of MC -> CA

3. MONTE CARLO STATIC RECRYSTALLIZATION ALGORITHM (ENERGY DISTRIBUTION)

Recrystallization requires calculation of energy on grains boundary. User can set level of energy distribution and select from dropdown list type of distribution from homogeneous and heterogeneous.

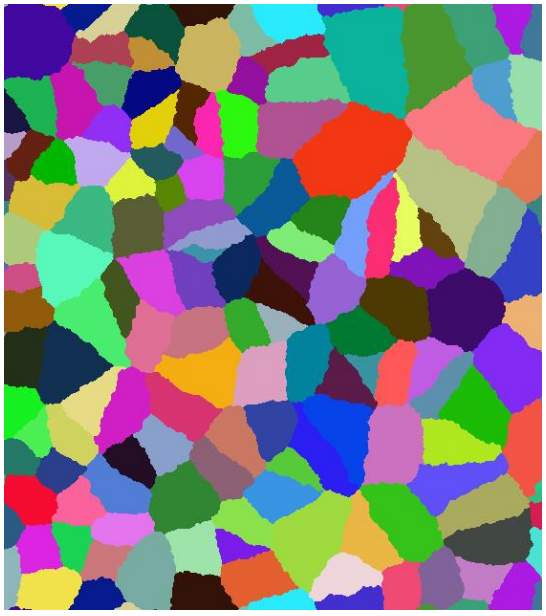


Picture 5 Energy distribution

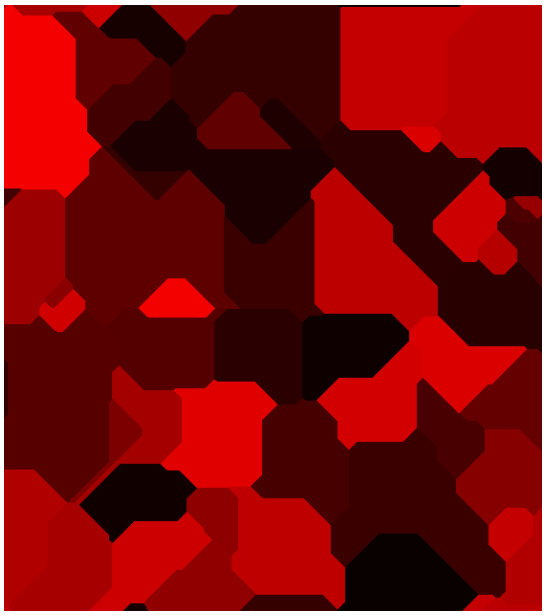
Picture 5 shows energy after distribution. Simulation where done with heterogeneous type of energy distribution. Blue colour symbolized places with minimum amount of energy and green with maximum. Energy was stored near grain boundaries.

4. MONTE CARLO STATIC RECRYSTALLIZATION ALGORITHM (NUCLEATION AND GROWTH)

After the energy is distributed, we can go to recrystallization. We need to define the number of nucleons.



Picture 6 Microstructure before recrystalization



Picture 7 Microstructure after recrystallization

Conclusions

Normal growth of grains and recrystallization by using cellular automata is the best way to simulate how any kind of steel will rise before it will go to the physical process. We can simulate many times as we want without a stress that sample may be destroyed. That is the main reason for implementing algorithms for simulate processes in metallurgy.