Grzegorz Haczyk
278920

Multiscale Modelling – 2nd report

Introduction

This application was implemented by using MC (Monte Carlo). The main idea of the Monte Carlo technique is to divide a specific part of the material into one-, two-, three- dimensional lattices of cells, where cells have clearly defined rules of interactions between each other leading to minimization of the system energy.

- MC space – finite set of cells, where each cells is described by a set of internal variables describing the state of cell.
- Neighbourhood – describes the closest neighbours of a particular cell. It can be in 1D, 2D, 3D space.
- Energy minimization criterion – E, the energy value of each cell in the lattice is determined by the states of its neighbours and the cell itself.

The MC space in the Pots model as well as types of neighbourhoods are similar to Cellular Automata ones.

Algorithm steps:

Step 1: Randomly select the MC cell with specific orientation.

Step 2: Calculate energy of the MC cell on the basis of neighbouring states. Energy is calculated using following formula:

$$E = J_{gb} \sum_{<i,j>} \left(1 - \delta_{S_i S_j}\right)$$

Step 3: Randomly assign a new state to the MC cell. The orientation is randomly generated from all available orientations.

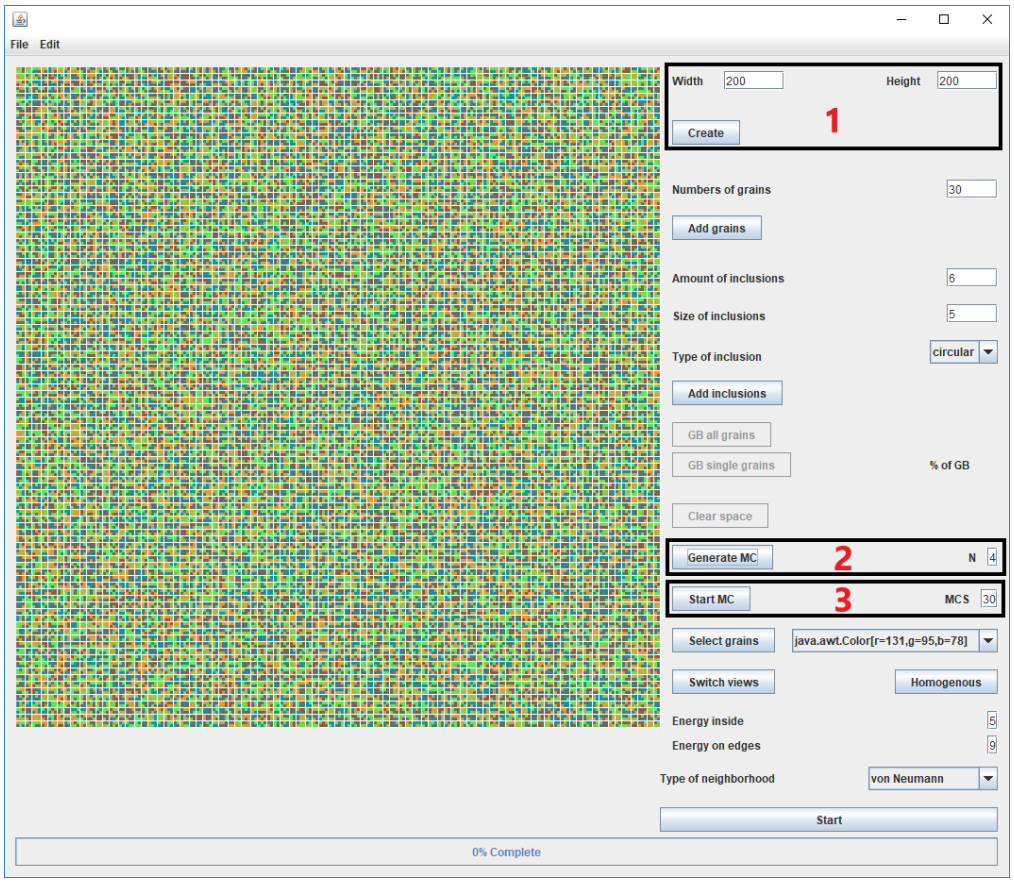
Step 4: Calculate the change in the MC cell energy changes.

Step 5: The orientation change is accepted with the probability p:

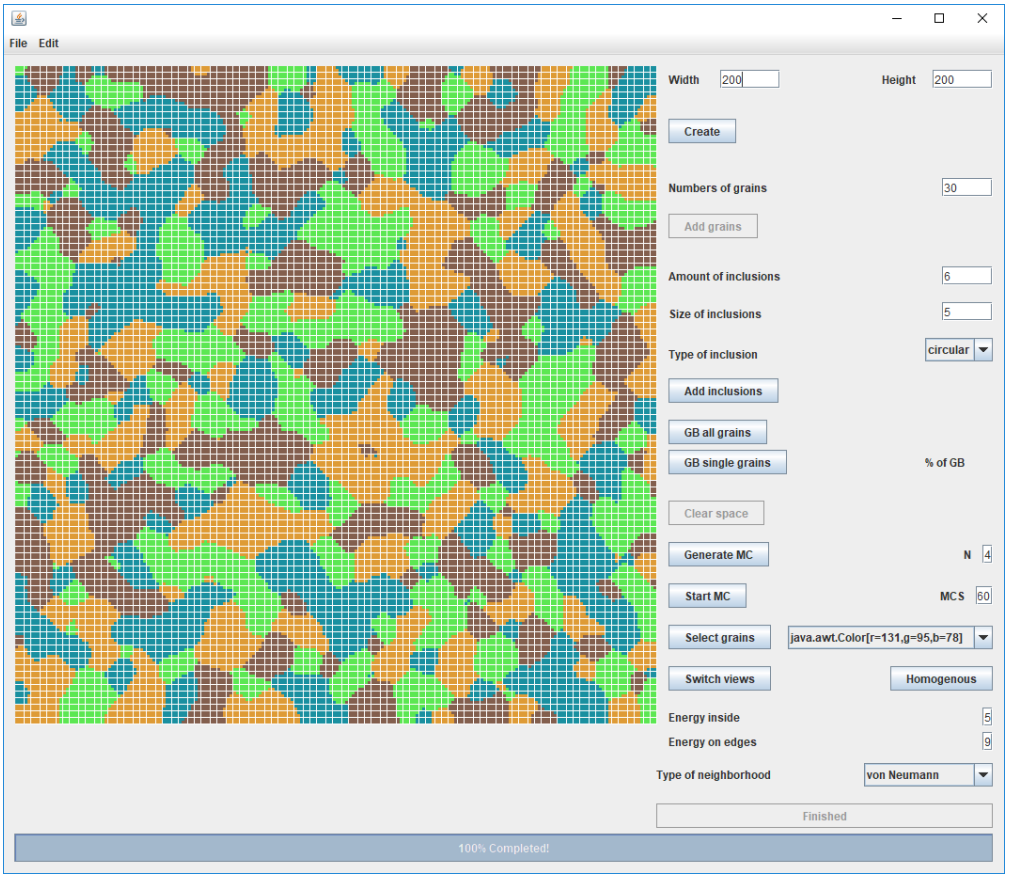
$$p(\Delta E) = \begin{cases} 1 & \Delta E \leq 0 \\ 0 & \Delta E > 0 \end{cases}$$

First functionality – MC grain growth

User can choose parameters to generate structure. User has to set width and height of grid (**1**) which is display on the panel on the left side of the main window. User can generate MC space with the number of colors entered in the text field by pressing button (**2**). In order to run simulation need to click Start MC button, but before it user should enters number of MCSs (Monte Carlo Step)(**4**). It see on the **picture 1**.



Picture 1: Main window, setting up size, generating MC.

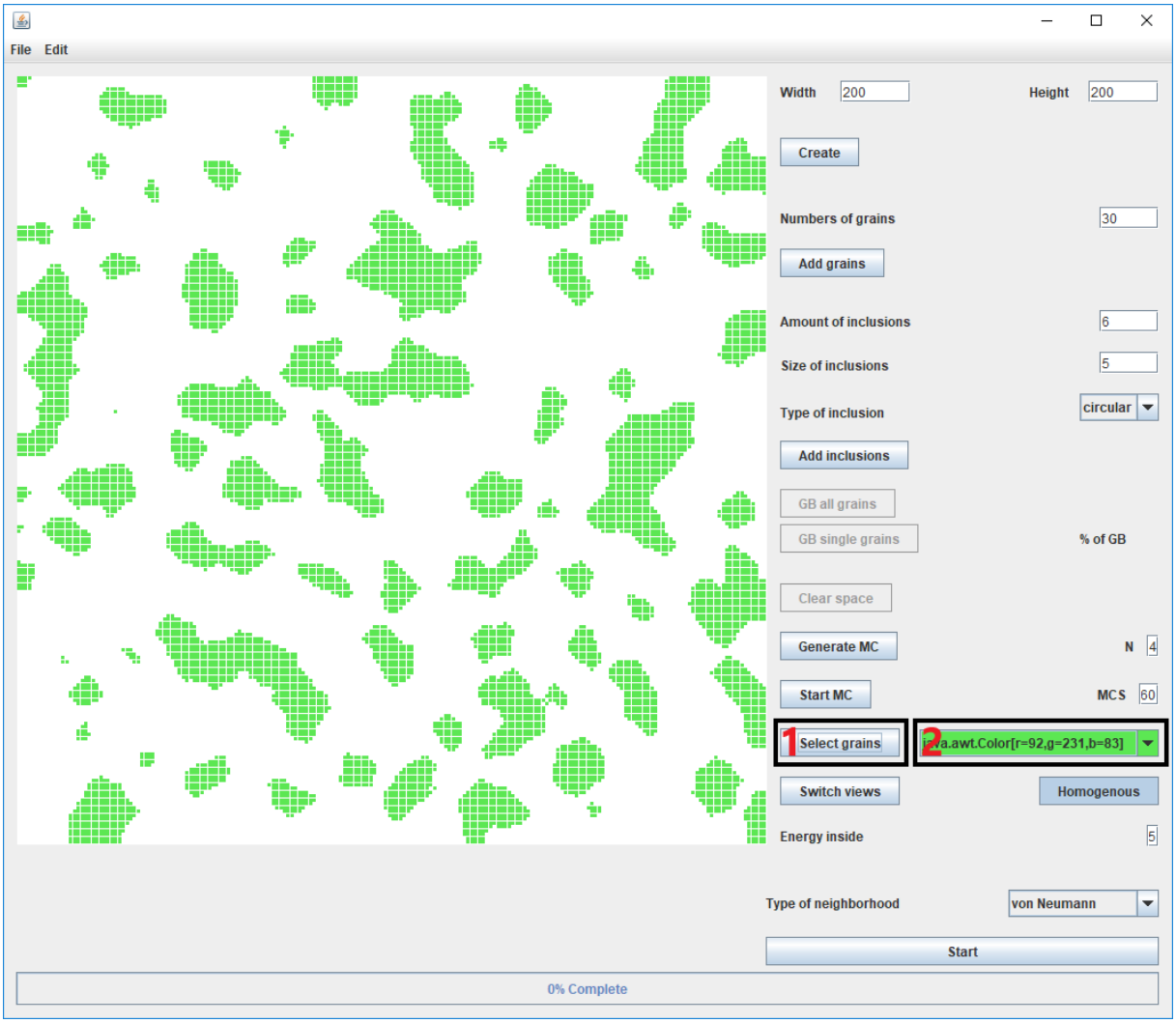


Picture 2: Completed Monte Carlo grain growth simulation.

Picture 2 shows the completed Monte Carlo grain growth simulation for 60 MCS.

Second functionality – dual phase microstructure

Picture 3 shows how user can select grains in order to create dual phase. First of all user should chooses a color from dropdown list (**2**) and then user can press button (**1**). After this user can start simulation.

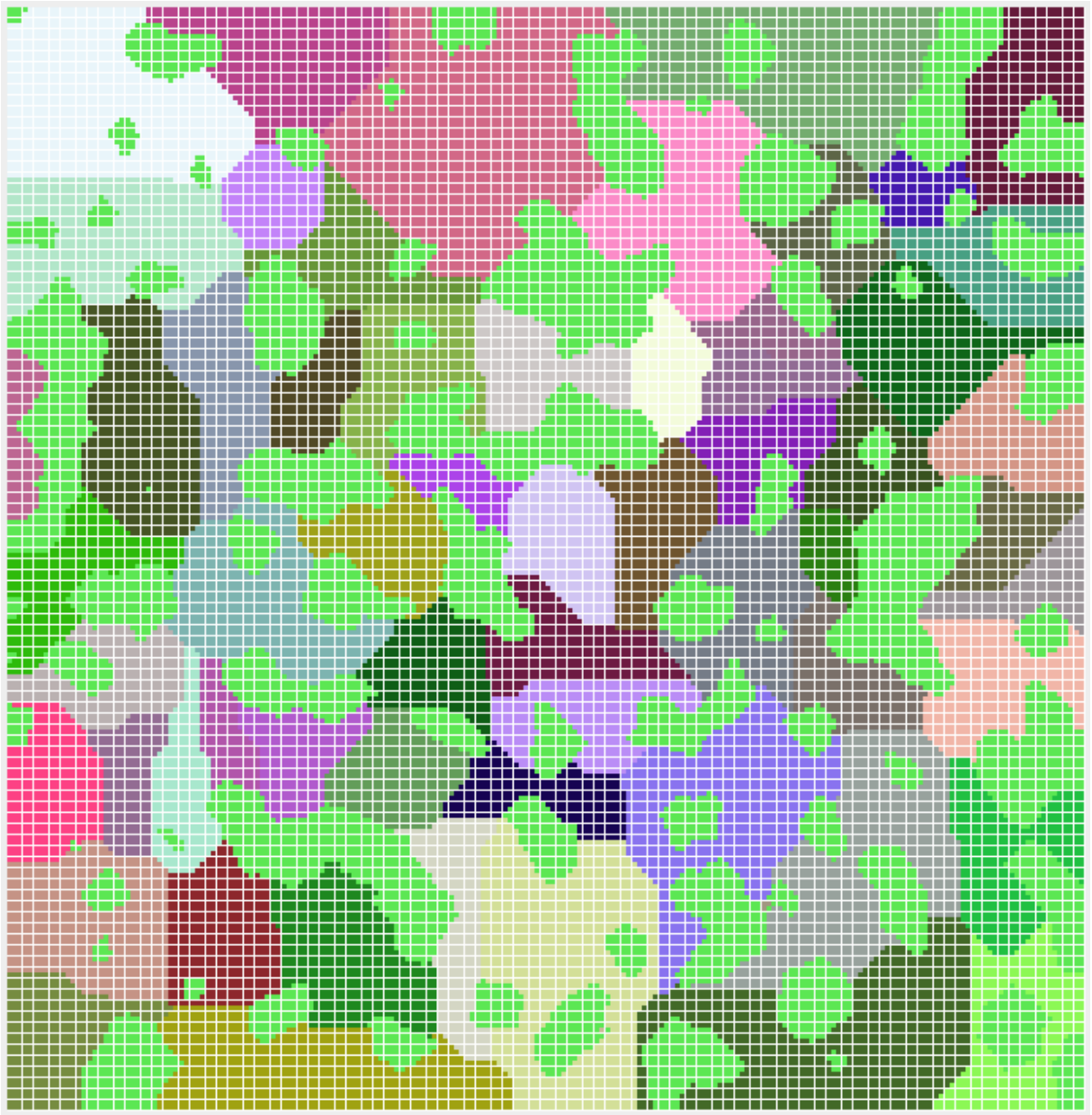


Picture 3: Dual phase microstructure.

User has four ways:

1. From CA to MC.
2. From CA to CA.
3. From MC to MC.
4. From MC to CA.

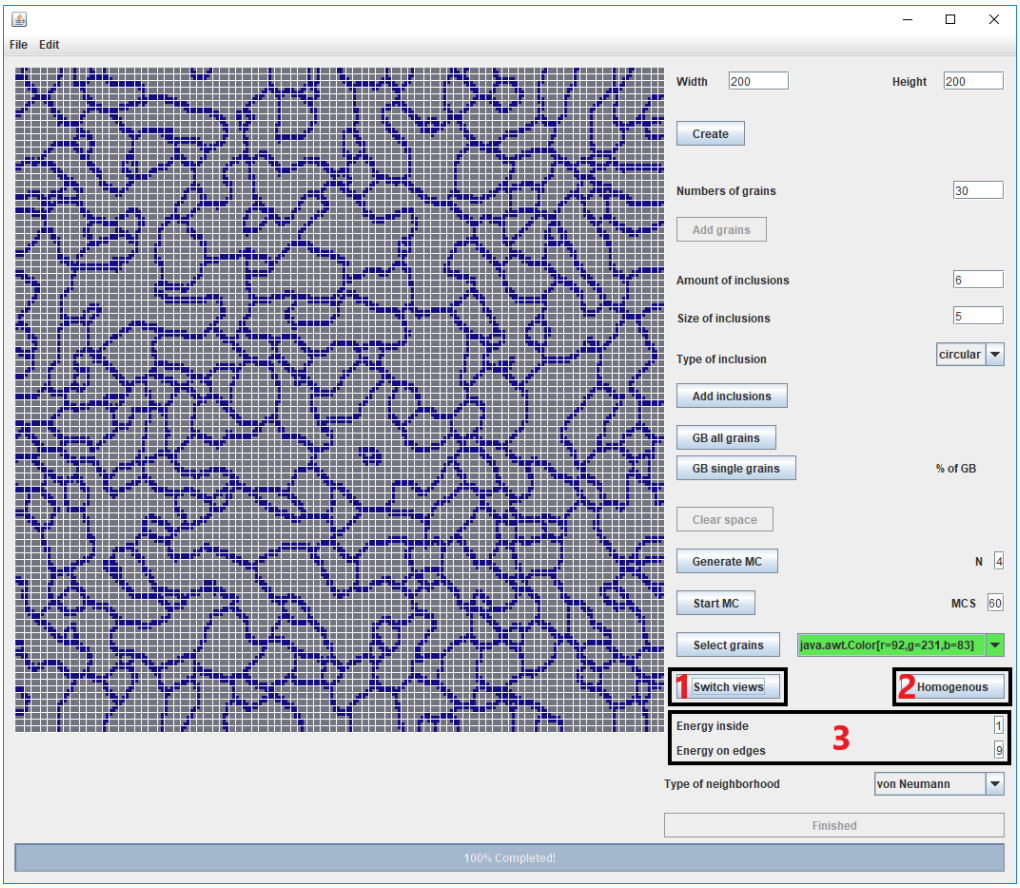
Picture 4 shows what the microstructure looks like after performing the MC simulation, selecting the dual phase and performing the next simulation of the CA.



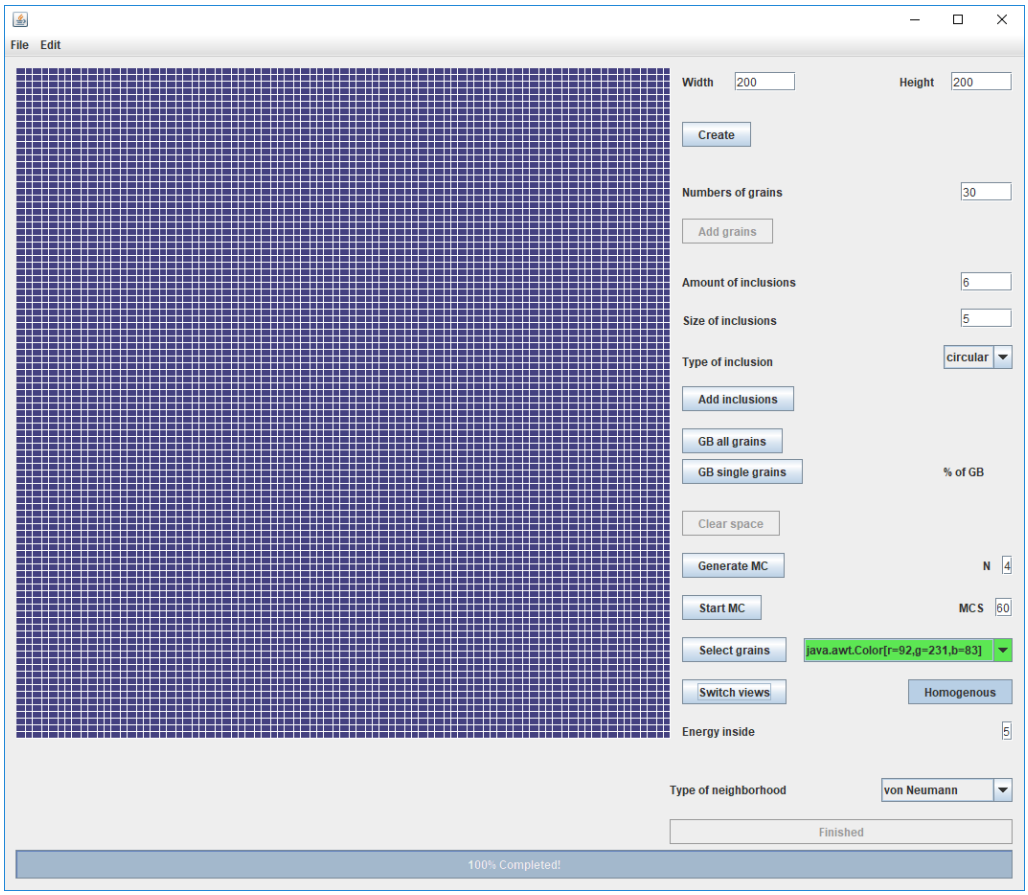
Picture 4: Dual phase microstructure. From MC to CA.

Third functionality – MC static recrystallization algorithm – energy distribution

As you can see from the **picture 5** and **picture 6** below, in order to see energy distribution view user can click Switch views button (**1**), but before it user should select distribution type: homogenous or heterogenous by toggle button (**2**). If it is homogenous user sets only one value of energy, but if it is heterogenous user should sets value of energy inside and value of energy on edges (**3**). And then click Switch views button.



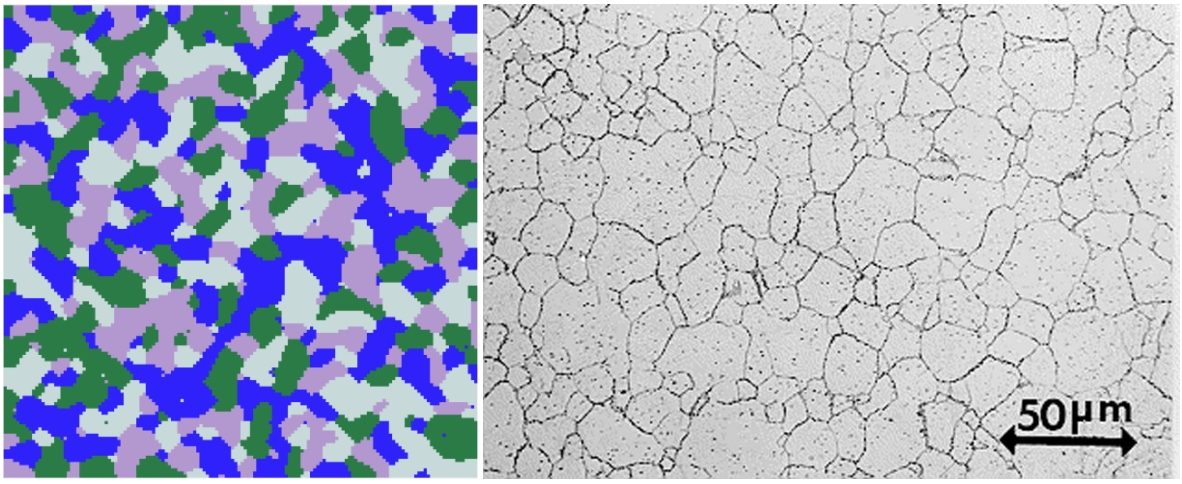
Picture 5: Heterogeneous energy distribution.



Picture 6: Homogeneous energy distribution.

Comparison

The following **picture 7** presents a comparison of the microstructure created in the program and the microstructure of a beryllium copper. The growth in the created application is not as accurate as the real one. The microstructure created in the program has a lot of grains in different colors and identifiers. It does look more realistic in comparison to the simple CA grain growth.



Picture 7: Comparison of the real microstructure with the microstructure from the program. (Source: https://www.copper.org/resources/properties/microstructure/images/505h.JPG)

Conclusions

In this report have presented software designed to implement simulation of the grain growth. The program is based on the Monte Carlo method. There is no single Monte Carlo method – the term describes a large and widely-used class of approaches characterized by common assumptions. Monte Carlo is algorithm that can implemented in many ways. It can be used in many of different areas such as computer science, mathematics, physics, biology, microstructure modelling.

The software has a lot of functionality such as MC grain growth simulation, dual phase microstructure and it can be used in four different ways, possibility of change size, sight of distribution energy, choosing distribution type.