WIMiIP, IS, st. II, rok 2	MULTISCALE MODELING	16.12.2019
Wojciech Jarosz	2st application report	

1. Graphic user interface:

Graphic user interface is shown on *Figure 1*. Application window is divided into two parts: on left microstructures are drawn and on the right part main menu can be found. There is also menu bar when export/import functionalities buttons are placed.

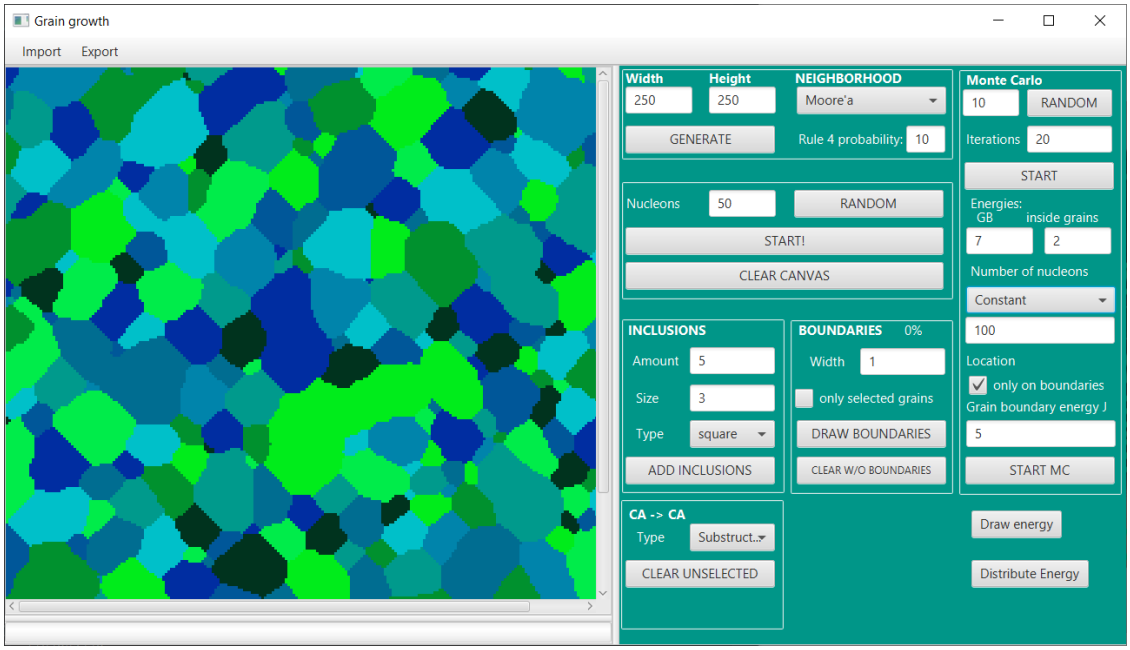

Figure 1. User intarface

2. Functionalities:

Monte Carlo grain growth algorithm

MC algorithms allows to generate microstructure with given from GUI iterations amount. On Figure 2. We are able to see a result after 0, 20 and 40 iterations. Number of nucleons which randomly fill the microstructure at the beginning of algorithm is also taken from user.

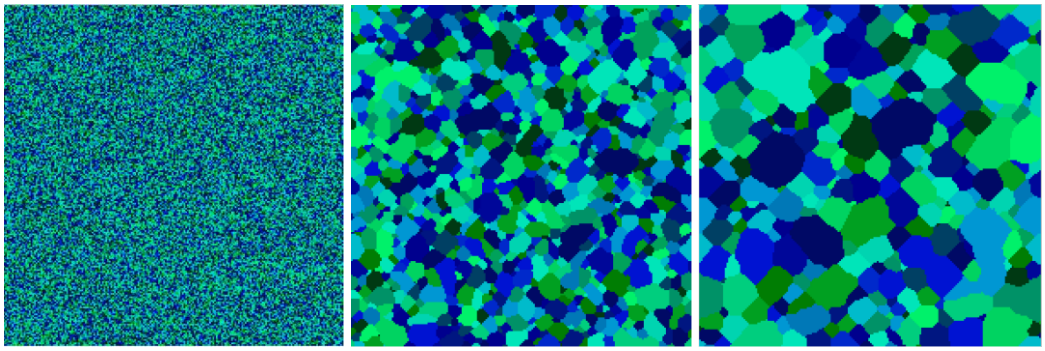

Figure 2. Monte Carlo after 0, 20 and 40 iterations

Main step of MC algorithm is calculating energy with Kronecker delta:

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

where J_{gb} – Grain boundary energy <0.1 – 1.0>

If a difference between energy calculated before and after changing the state of cell is non-positive the energy is changed. If not, old state of is restored.

Modifications of MC method – Dual phase:

When grain growth process is finished, user is able to choose to be dual phase or substructure some grains with mouse click. Then, clear the microstructure apart from selected grains. Finally begin new grain growth with both MC and CA algorithms. The process is shown on Figure3.

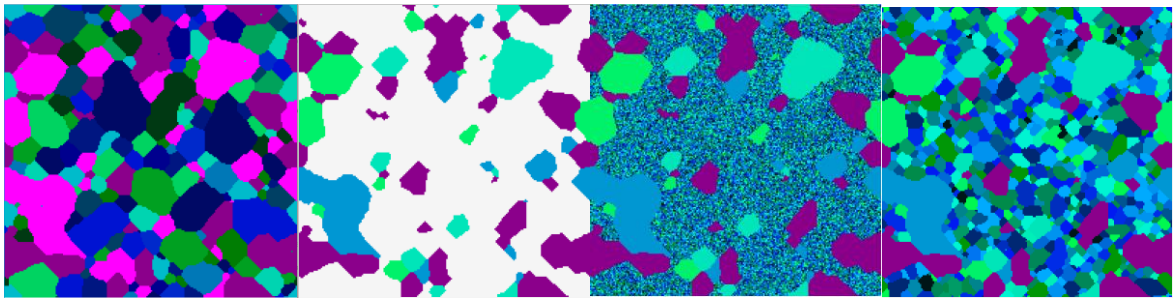

Figure 3. Dual phase and substructure grains in microstructure.

Dual phase grains are selected in pink and substructure in purple.

Monte Carlo static recrystallization

Algorithm allows user to enter energies which will be distributed on inside grains and on their boundaries. By clicking “Draw energy” user can visualize distribution of energies. On Figure 4. It is possible to see the initial distribution before recrystallization.

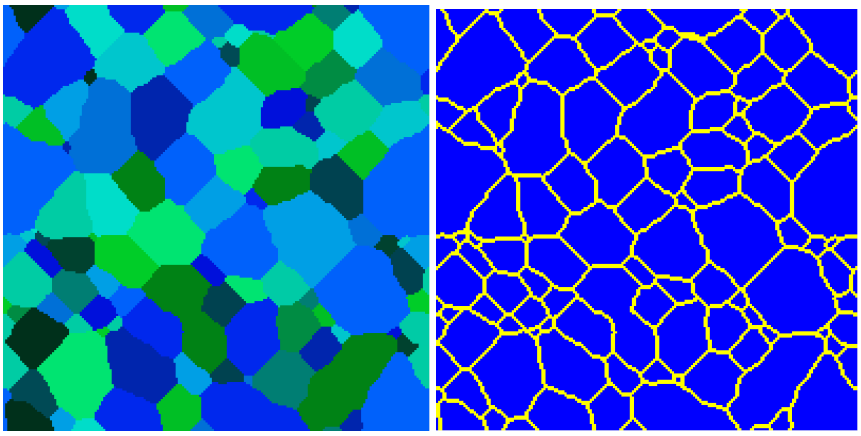

Figure 4. Initial distribution of energies.

Energy which is distributed on microstructure is given by user on GUI.

Figure 5. shows the beginning process of static recrystallization and energy visualization.

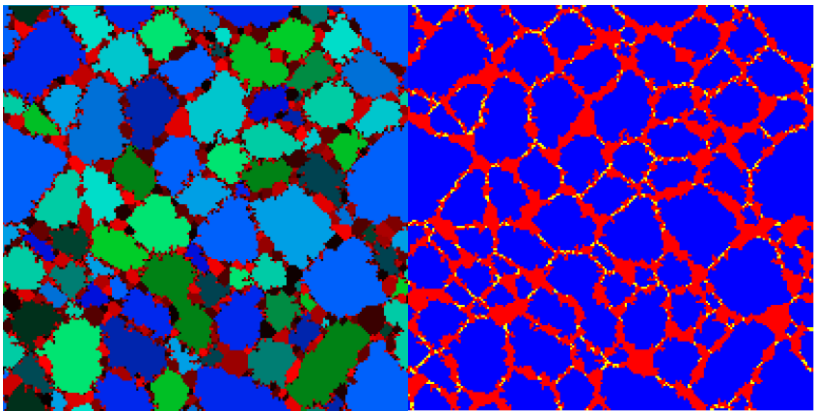

Figure 5. Static recrystallization and energy visualization.

New recrystallized nucleons can be added in three ways:

- Constant – in each iteration the same value of nucleons is added,
- Increasing – in each iteration value of added nucleons increase,
- At the beginning of simulation – nucleons are added only once at the beginning.

3. Technology

   Following technologies was used in project:

   - Java

     Java was chosen because it is object-oriented language, which allows you to create modular programs and reusable code.

     Java is platform-independent, so its ability to move easily from one computer system to another is one of the main advantages.

   - JavaFX

     The biggest advantage of this solution is the ability to create GUI in the MVC Model-View-Controller model. This ensures the purity of the code and the ability to divide the work into creating the view and the controller in which the action is created by associating it with the controls using annotations. Another important advantage of JavaFX is the ability to use CSS files to create a view. There is also a convenient SceneBuilder *drag and drop* tool for generating XML.

4. Microstructures comparison

Figure 6. shows a microstructure during recrystallization process. It is possible to see layouts of bigger and smaller grains on boundaries. Recrystallization started on boundaries. Boundaries are the places with more energy is stored because of more dislocations.

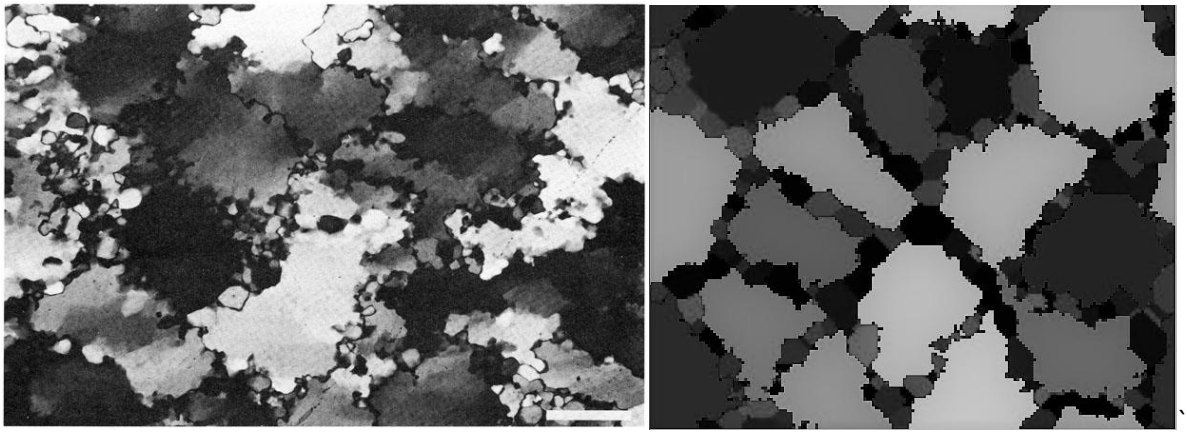

Figure 6. Real and generated microstructures with recrystallization process.

On both picture we can see unrecrystallized bigger grains and small grains which started growing after nucleation of recrystallized grains in bigger energy areas (boundaries).

Sources:

1. http://www.ged.rwth-aachen.de/Ww/projects/rexx/Urai+86Recrystallization/Urai+86Recrystallization5.htm