Multiscale Modelling
Report on application parts 8-10
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1. Selected technology

It was decided to use Java because this language, apart from being able to run the program regardless of the system platform used, allows easy creation of multi-threaded applications and in the object-oriented programming paradigm. In object-oriented languages, all types of design patterns which are a set of ready-made solutions for many common problems associated with application design can be implemented in an accessible way.

The JavaFX package was used to design the graphical user interface using Scene Builder. It allows to use of a wide range of control elements and gives a simple and quick way to design and modify the entire interface using drag and drop technique.

The application was created using the IDE IntelliJ IDEA. It offers a transparent interface, allows integration with the Git version control system and allows the installation of additional plugins to facilitate the work of the programmer.

2. Application

The created application offers a graphical interface shown in Figure 1. New functionalities have been added that are located in the selected areas.

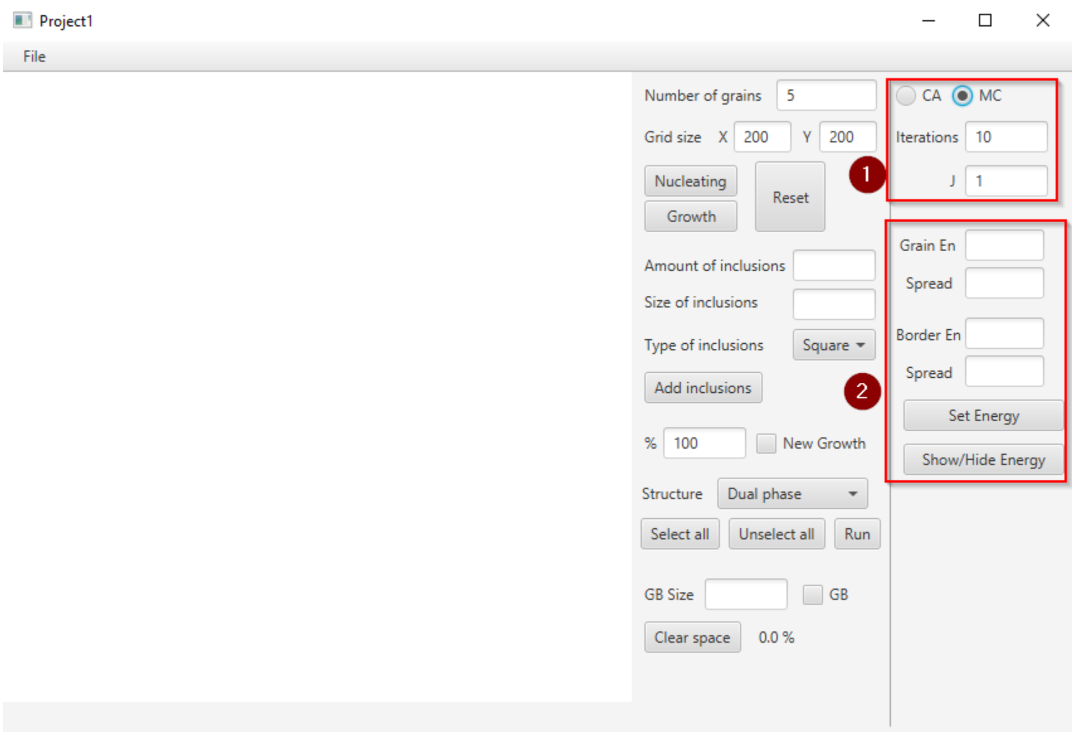

Figure 1 - Presentation of new GUI options

The new areas contain control elements for performing new operations:

- Area No. 1 allows: choose the type of simulation between the previous and new functionality, and choose the parameters of the Monte Carlo simulation.
- Area No. 2 allows: setting energy parameters that will be distributed in grains, starting this process with the Set Energy button, and energy visualization using the Show / Hide Energy button.

The initial state of the structure after using the new Monte Carlo method is presented in Figure 2, the structure after 20 iterations is visible in Figure 3, and after 100 iterations in Figure 4.

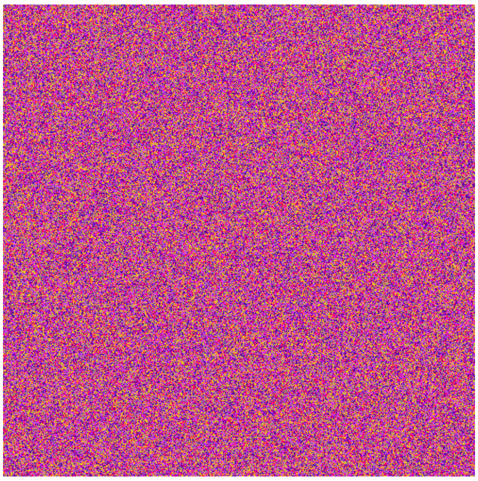

Figure 2 - initial state of the structure

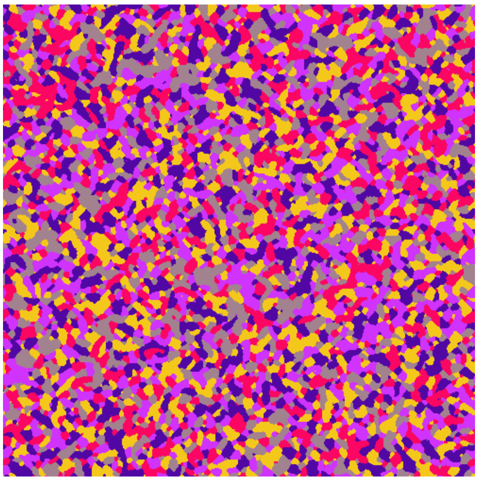

Figure 3 - structure state after 20 iterations

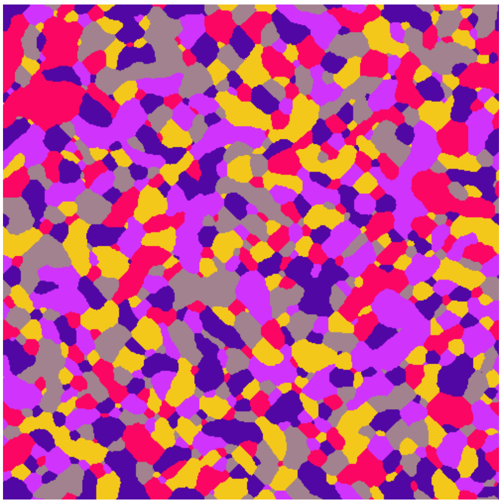

Figure 4 - structure state after 100 iterations

The structure was randomly filled with five different grains. Each grain has its own unique color. This can be seen in Figure 2. The Monte Carlo method in subsequent iterations is shown in Figure 3 and Figure 4.

The Monte Carlo method is able to work together with the re-growth functionality with substructure and dual phase elements from previous classes. It can also be combined with the basic type of grain growth. This is shown in Figure 5 and Figure 6.

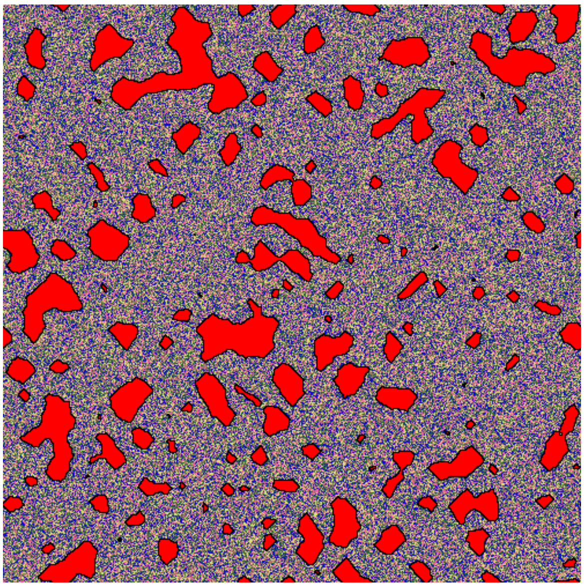

Figure 5 - re-growth with the Monte Carlo method

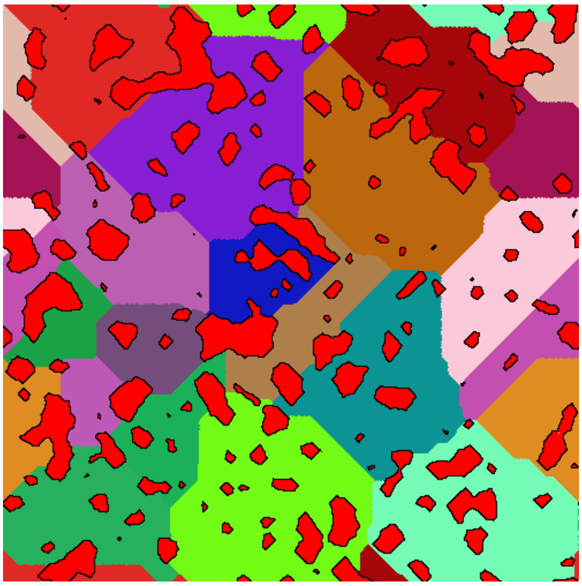

Figure 6 - re-growth with the method from previous classes

The application also offers the possibility of determining energy in grains. This can be seen in Figure 7. The darker the cell color, the more energy it has.

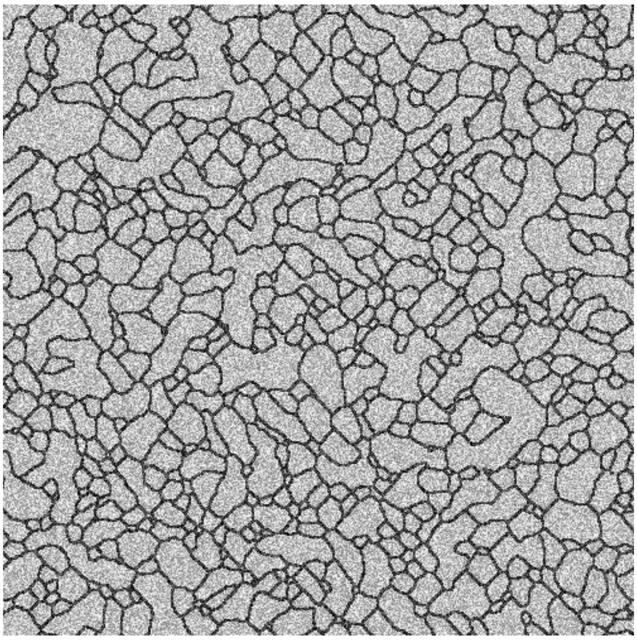

Figure 7 – visualized energy of grains

The energy setting parameters can be controlled using 4 text areas from area No. 2. You can set the energy level in the grains, at the grain boundaries and their noise.

3. Comparison of the obtained results with the image of the actual microstructure

Using the created application, an attempt was made to generate a structure similar to the real one. The first example of a real microstructure is shown in Figure 8. Next to the original in Figure 9 you can see the structure generated in the application, similar to the structure in Figure 8.

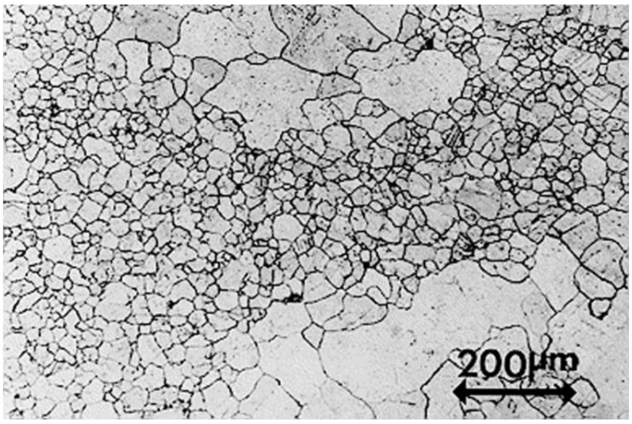

Figure 8 – first example of a real structure [1]

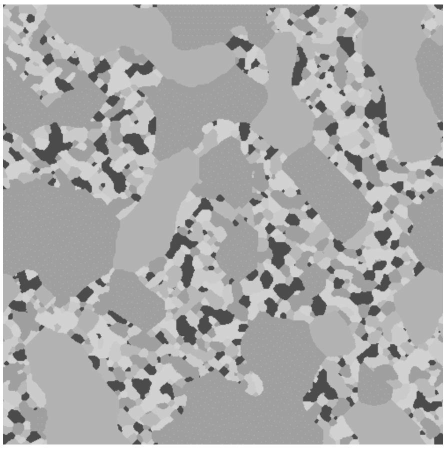

Figure 9 - generated structure in the application based on the actual structure shown in Figure 8

The microstructure shown in Figure 8 is Beryllium Copper heated and mechanically treated. The resulting structure in Figure 9 shows similarity to the original. The shape of larger and smaller grains is similar. Moreover, there are also inclusions both inside the grains and at their borders.

The second example of the actual microstructure is shown in Figure 10. Next to the original in Figure 11, you can see the structure generated in the application, similar to the structure in Figure 10.

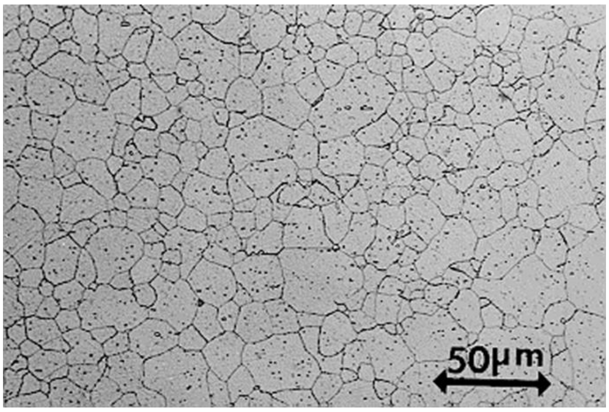

Figure 10 – second example of a real structure [1]

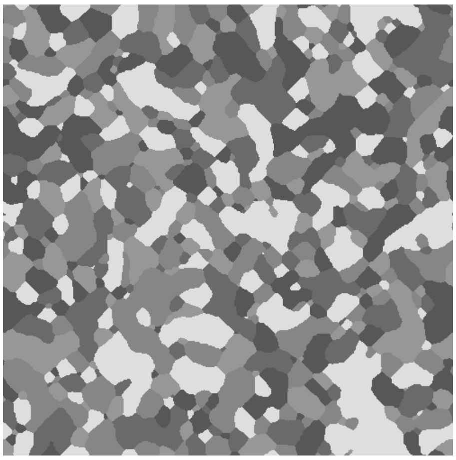

Figure 11 - generated structure in the application based on the actual structure shown in Figure 10

The microstructure shown in Figure 10 is Beryllium Copper heated and mechanically treated, but in a different way than the structure in Figure 8. The resulting structure in Figure 11 shows similarity to the original. The shape of larger and smaller grains is similar. Moreover, there are also inclusions both inside the grains and at their borders.

4. Sources

[1] https://www.copper.org/resources/properties/microstructure/be_cu.html