Multiscale Modelling
Raport z części aplikacji 1-6
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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.

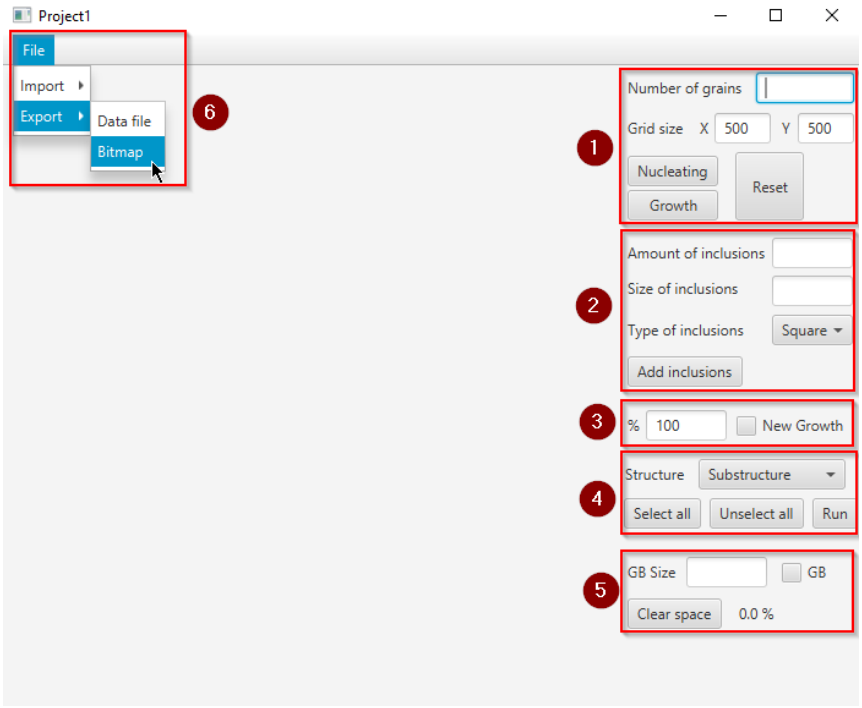

Figure 1 - Presentation of all GUI options

Each area contains controls that allow you to perform other operations:

• Area No. 1 allows: controlling the size of the grid area, adding new seed germs at random locations, seed growth (Moore neighborhood), resetting the entire area to its original state

• Area No. 2 allows: adding inclusions both before and after seed growth, determining the number of inclusions and their size and type

• Area No. 3 allows: enabling a new grain growth option and determining the threshold of probability of completing the last step of this algorithm

• Area No. 4 allows you to: select after growing grains for re-simulation, where specific grains will be treated as Substructure or as Dual Phase. You can choose single grains or all of them. You can also unselect selected grains. The Run button starts the re-growth simulation, where the number of new grains is determined in the first text field from area 1

• Area No. 5 allows: after selecting individual or all grains, outline them with the given thickness. The grain contour is treated as an inclusion. After stroking, all grains are removed and information about the percentage share of the stroked area relative to the area of the entire grid is displayed.

• Area No. 6 enables: exporting and importing the generated structure to a text file and to a graphic file.

Functionality associated with inclusions is presented in Figure 2.

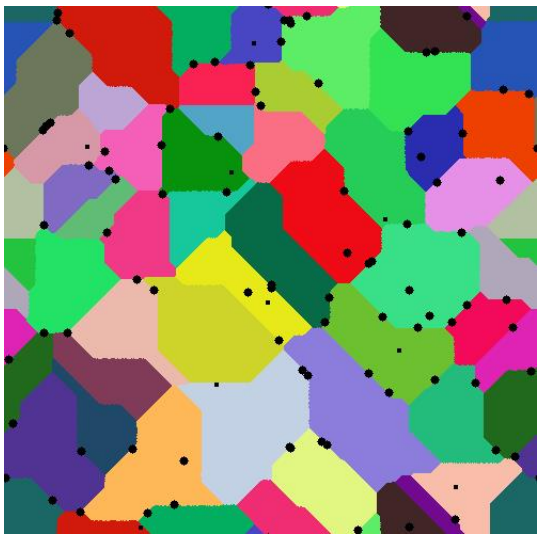

Figure 2 – structure with inclusions

Even before generating the structure, the grid size (500 x 500 px) was defined and several inclusions of various sizes and shapes were added - they can be square or circle. When there are no grains, the inclusions appear in random places. The grid size can be freely adjusted in the range from 1 x 1 px to 500 x 500 px. In the application, some colors are special: inclusions and grain boundaries are black, dual phase grains are red, empty space is white. A structure was generated by adding 50 nucleons and expanding them. The default neighborhood type is Moore neighborhood, while the edge type is periodic. Then further inclusions were added. After generating the structure, inclusions can appear only at the grain boundaries.

Functionality associated with different types of microstructures is shown in Figure 3.

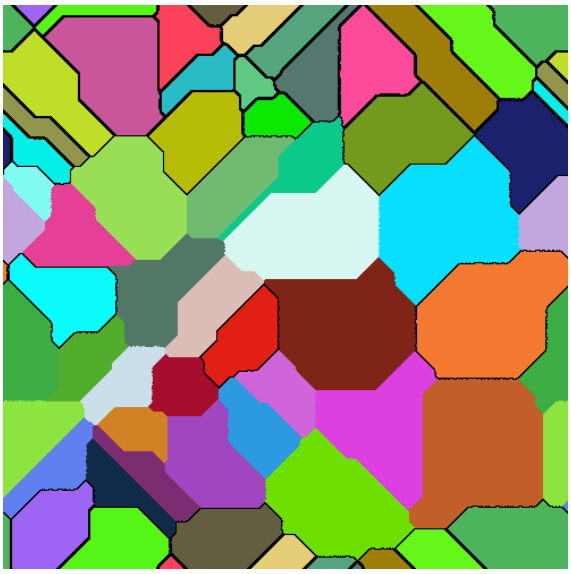

Figure 3 - generated structure with selected grains for substructures

A structure with 50 grains was generated. Some of them were chosen as substructure type and some as dual phase. The interface highlights selected grains by outlining their edges. Grains can be selected and deselected by clicking on them with the mouse or using the buttons. The Run button starts the simulation.

The structure showing the generated structure after re-expansion with substructure and dual phase elements is shown in Figure 4.

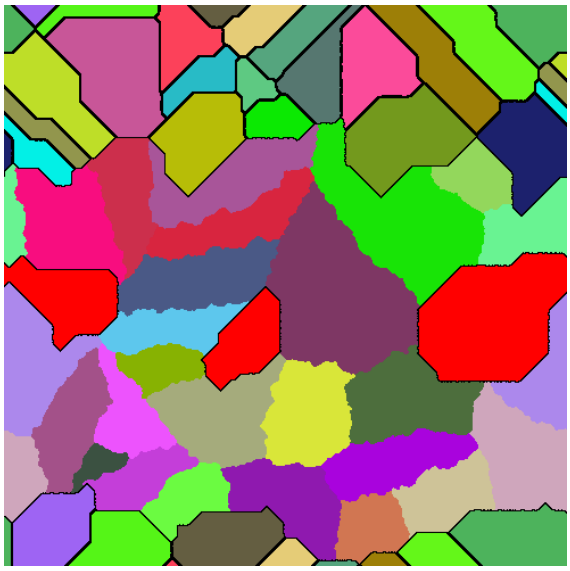

Figure 4 - generated structure after re-expansion with substructure and dual phase elements

Re-growth started this time after selecting New Growth checkbox. This growth was started at the 10% level for the last simulation step. You can distinguish between grains generated by the original and extended method.

The functionality related to grain contouring is visible in Figure 5.

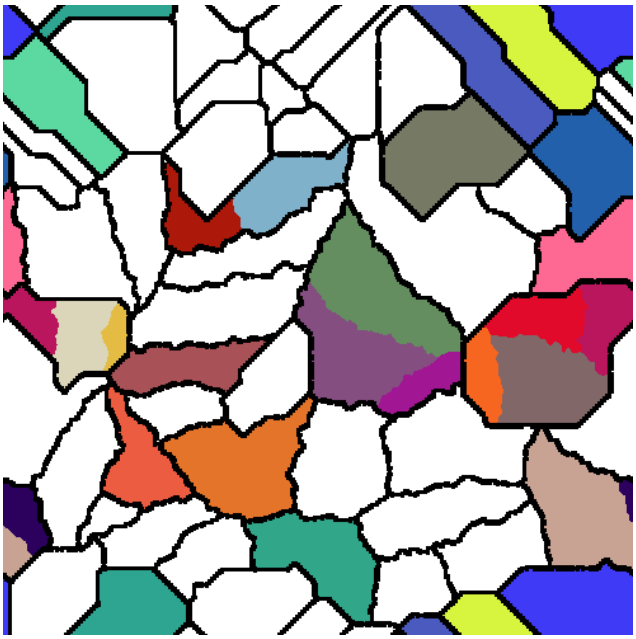

Figure 5 - re-growth after leaving only grain boundaries

The GB option was selected and the edge thickness was set to 3 px. Then the structure was cleared with the clear space button leaving only the grain boundaries. In the structure obtained from the previous step, grain growth was again carried out. The application allows you to trace not only all grains, but any amount.

The functionality related to the import and export of the structure is shown in Figure 6.

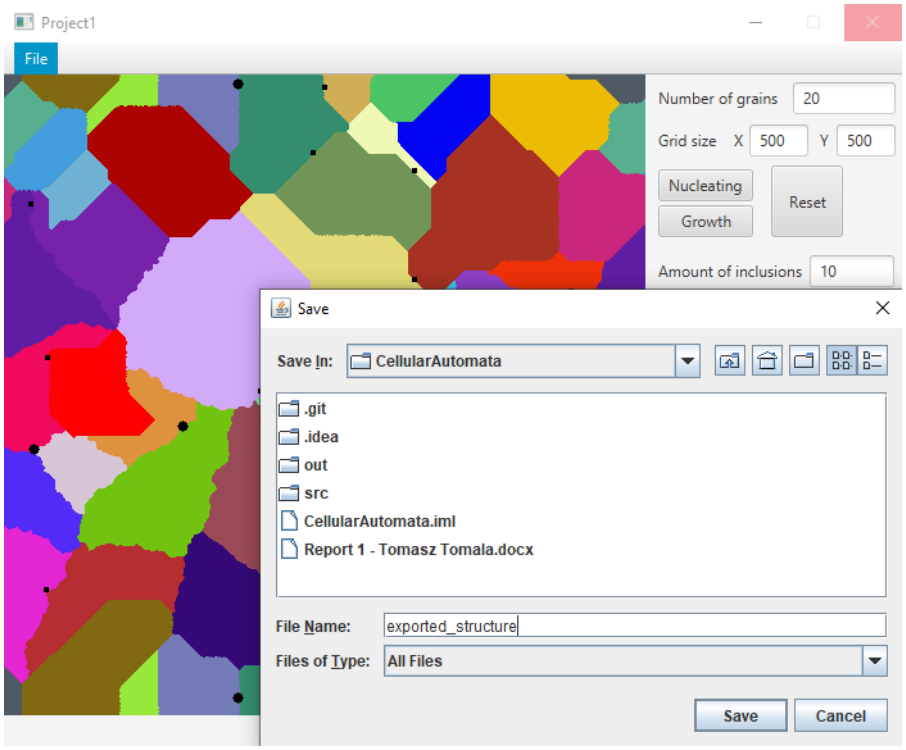

Figure 6 - export of the resulting structure

The structure of the exported text file is shown in Figure 7.

exported_structure.txt

```
500 500
0   0   35  0x4f5b64ff  GRAIN   false
0   1   35  0x4f5b64ff  GRAIN   false
0   2   35  0x4f5b64ff  GRAIN   false
0   3   35  0x4f5b64ff  GRAIN   false
0   4   35  0x4f5b64ff  GRAIN   false
0   5   35  0x4f5b64ff  GRAIN   false
0   6   35  0x4f5b64ff  GRAIN   false
0   7   35  0x4f5b64ff  GRAIN   false
0   8   35  0x4f5b64ff  GRAIN   false
0   9   35  0x4f5b64ff  GRAIN   false
0   10  35  0x4f5b64ff  GRAIN   false
0   11  35  0x4f5b64ff  GRAIN   false
0   12  35  0x4f5b64ff  GRAIN   false
0   13  35  0x4f5b64ff  GRAIN   false
0   14  35  0x4f5b64ff  GRAIN   false
0   15  35  0x4f5b64ff  GRAIN   false
0   16  35  0x4f5b64ff  GRAIN   true
0   17  35  0x4f5b64ff  GRAIN   true
0   18  42  0x57b090ff  GRAIN   true
0   19  42  0x57b090ff  GRAIN   true
0   20  42  0x57b090ff  GRAIN   false
0   21  42  0x57b090ff  GRAIN   false
0   22  42  0x57b090ff  GRAIN   false
0   23  42  0x57b090ff  GRAIN   false
0   24  42  0x57b090ff  GRAIN   false
0   25  42  0x57b090ff  GRAIN   false
0   26  42  0x57b090ff  GRAIN   false
0   27  42  0x57b090ff  GRAIN   false
0   28  42  0x57b090ff  GRAIN   false
0   29  42  0x57b090ff  GRAIN   false
```

Figure 7 - a text file containing the exported structure

The resulting structure can be exported to both a text file and a graphic file. The first line of the file contains information about the size of the grid. In each subsequent line there is information about subsequent cells in the grid. The first two numbers are the location of the cell in the grid, the third number is the grain ID, the fourth column is the color of the grain, the fifth column is the cell type, the sixth column is information whether the cell is on the grain border.

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 7. Next to the original in Figure 8 you can see the structure generated in the application, similar to the structure in Figure 7.

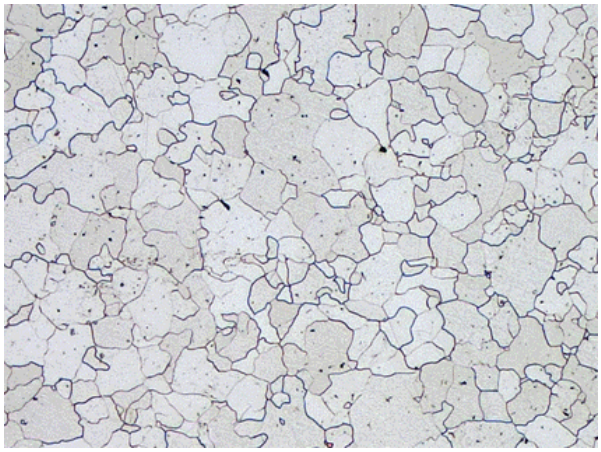

Figure 7 – first example of a real structure [1]

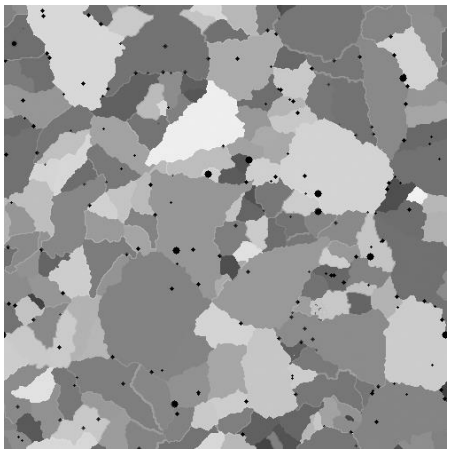

Figure 8 - generated structure in the application based on the actual structure shown in Figure 7

The microstructure shown in Figure 7 is a laser welding of steel used, for example, in ships or offshore platforms. The resulting structure in Figure 8 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 9. Next to the original in Figure 10, you can see the structure generated in the application, similar to the structure in Figure 9.

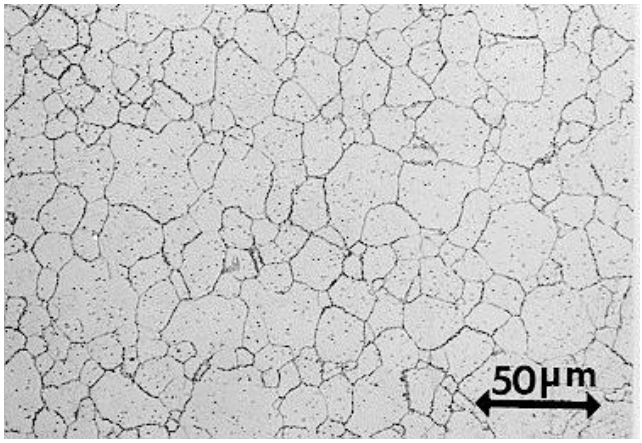

Figure 9 – second example of a real structure [2]

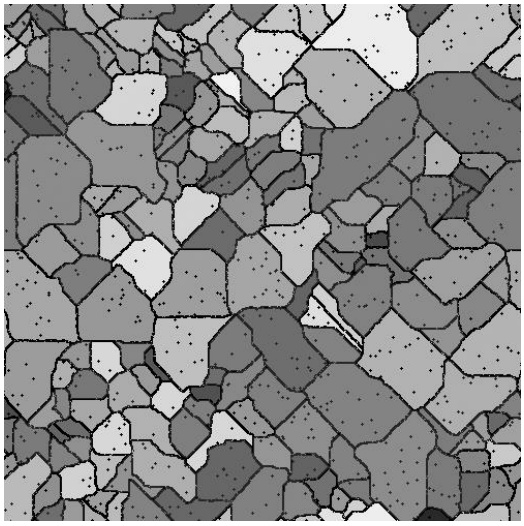

Figure 10 - generated structure in the application based on the actual structure shown in Figure 9

The microstructure shown in Figure 9 is Beryllium Copper heated and mechanically treated. The resulting structure in Figure 10 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://wiki.aalto.fi/display/AMAS/Microstructure+based+prediction+of+continuum+fatigue+properties

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