# Multiscale Modelling – First report

*Tymoteusz Przyłucki*

*Applied Computer Science*

## Introduction

This application has been developed for creating microstructure by using CA methods. The main priority was to develop a complete and easy to use program. It is provided by GUI which allows typing input data to customize simulation. To meet these expectations, the application has been written in C# using Windows Forms as a graphical class library.

This library provides tools to create easy to use and clear GUI. In comparison to Python and Java, creating GUI in C# - Windows Forms requires less amount of code which speeds up the development process of application.

## Interface

In Figure 1, we can see the main view of the interface. On the board, there are text boxes for customizing the process of simulation. Buttons are responsible for the run process and also triggers additional actions.

The size of the simulation board can be adjusted by changing values in text boxes **Height** and **Width**. Next input fields **number of grains** and the **number of inclusions** allows the user to specify the number of those parameters (grains and inclusions) which will take part in the simulation process. Before generating a board, it is required for the user to choose when inclusions will be placed on the board - **before** or **after** grain growth (Show in Figure 2 and 3). For this process, there are two checkboxes. The application allows marking both of them. In this case, inclusion will be added before and after simulation.

The button **Generate**, creates a board of simulations and places grains and inclusions randomly. **Start** runs the process of grain growth.

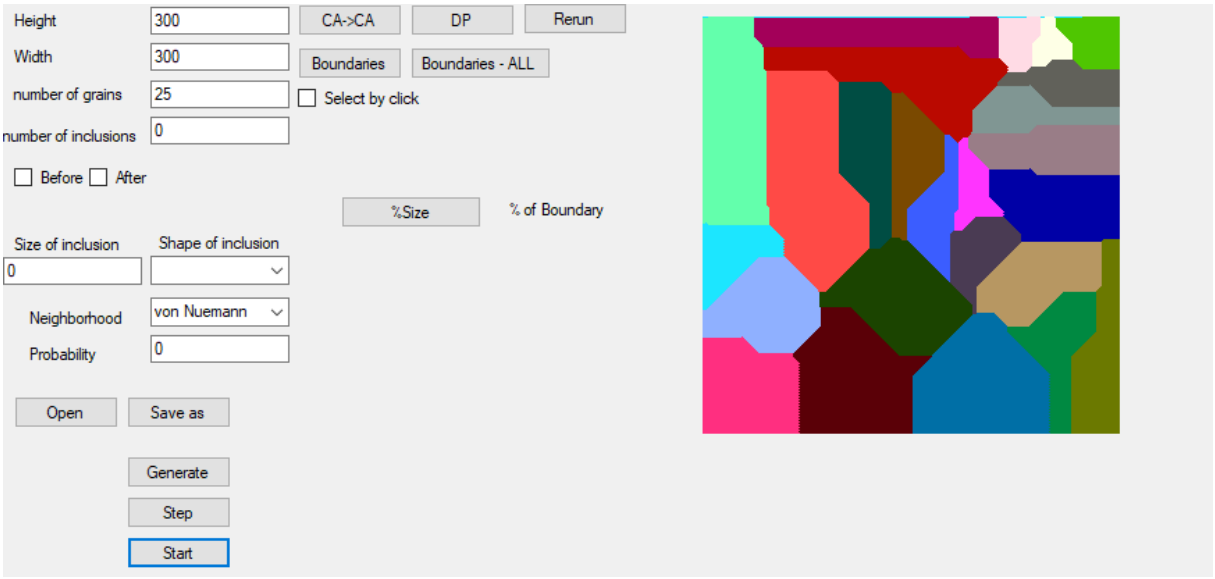


**Figure 1 Example microstructure generated by application**

**Figure 2 Inclusions added before simulation**

**Figure 3 Inclusions added after simulation**

## The application has additional features

1. Grain growth with modified Moore rules and probability of state change. Simulation is strongly related with **probability value** which is set by user. Differences in microstructures simulated with probability 1 and 99 are shown in Figures 4 and 5.

**Figure 4 Simulation with probability 1**

**Figure 5 Simulation with probability 99**

2. Selecting grains which will be moved to the next simulations. Grains which are not selected will be removed from the board. For selected grains we can change state to Dual Phase.

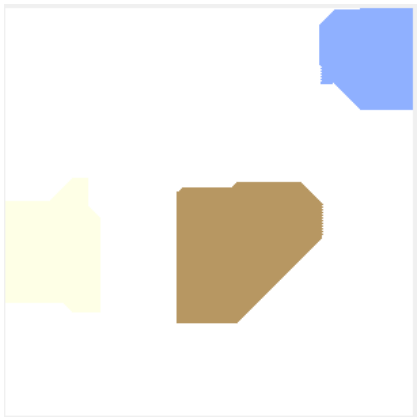

**Figure 6 Selected grains for next simulation**

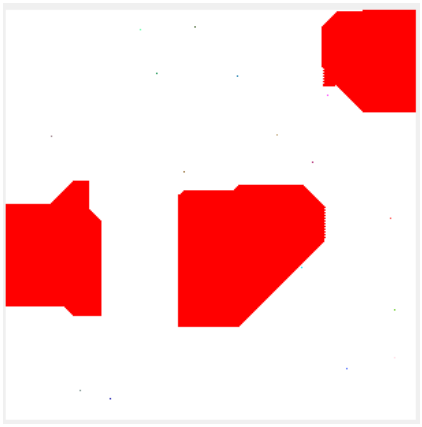

**Figure 7 Selected grains with changed state to Dual Phase**

**Figure 8 Selected grains with second simulation**

3. Mark selected boundaries or all existing on the board (Figures 9 and 10). After mark boundaries, application allows to re-run microstructure simulation. Boundaries are limiting grain growth (Figure 11).

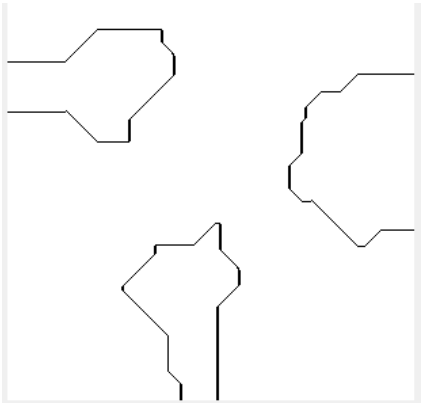

**Figure 9 Marked selected boundaries**

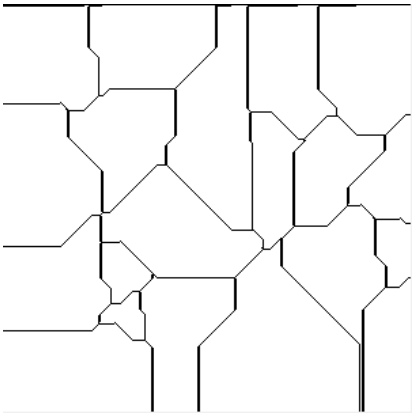

**Figure 10 All existing boundaries has been selected on the board**

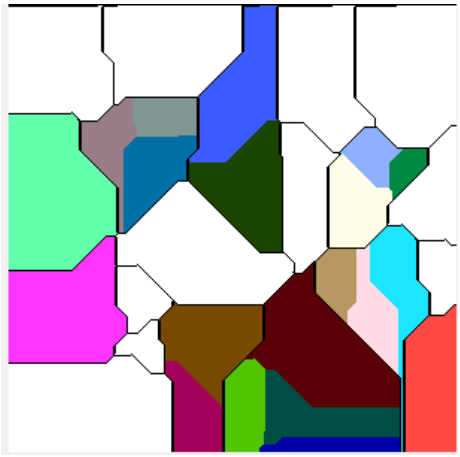

**Figure 11 Simulation with limited space to grow.**

As we can see in Figures 9-11 boundaries are limiting space to growth. Some of spaces are empty (white spaces). This is caused by random appointing grains on the board. The applications can save/load microstructure with two extensions: json and bmp. Json was chosen because of his flexibility in editing (Figure 12).

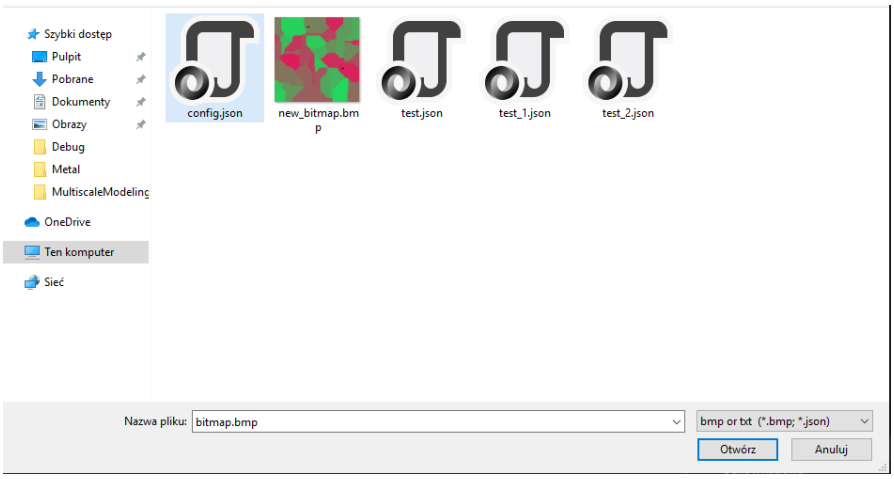


**Figure 11 Open dialog form in application**

# Comparison

In comparison Figures 13-14 and 15-16 we can see that generated microstructure is similar to real. Shapes and sizes of grains are very close to real microstructure. For the analysis, the quality of the generated microstructure should be enough. However, replication is not ideal; the real microstructure has inclusions with different sizes – it should be taken into consideration.

Figure 14: Generated microstructure for: 200 grains, 100 inclusions with size 3, board size = 300x300 pixels.

Figure 16: Generated microstructure for: 50 grains, 20 inclusions with size 3, board size = 300x300 pixels. Some grains have been modified by DP function.

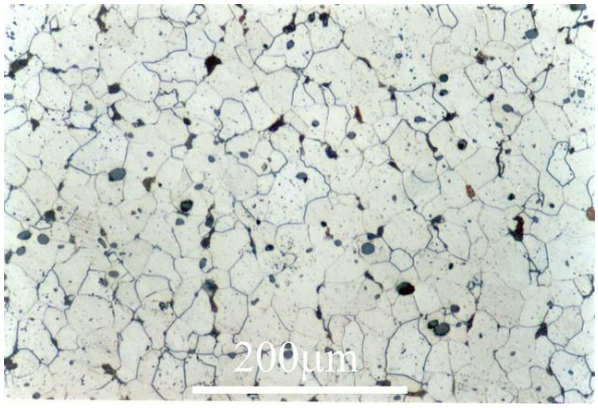


**Figure 13 Normalized low carbon manganese steel** [1]

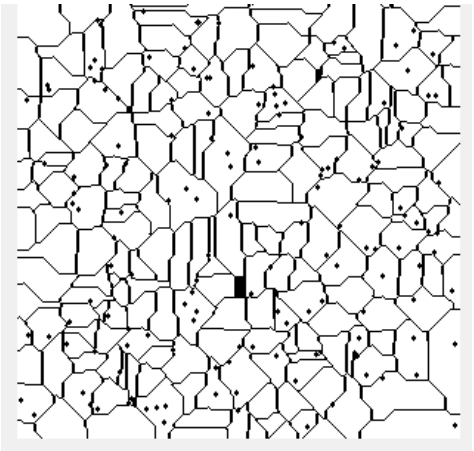

**Figure 14 Generated microstructure with inclusions**

[1] (https://www.doitpoms.ac.uk/miclib/full_record.php?id=206)

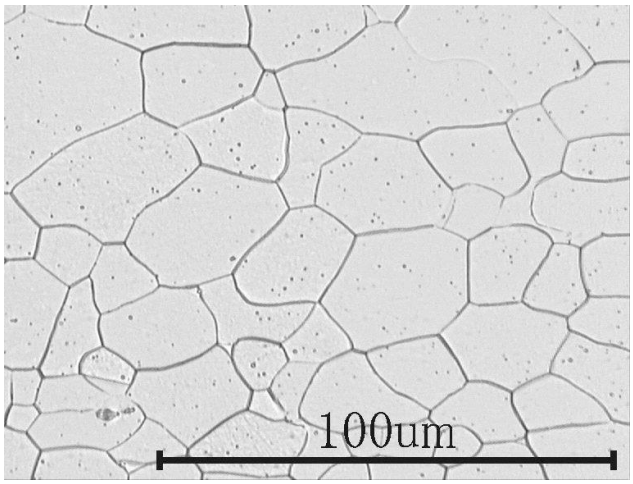


**Figure 15 Microstructure of IF steel sheet material** [2]

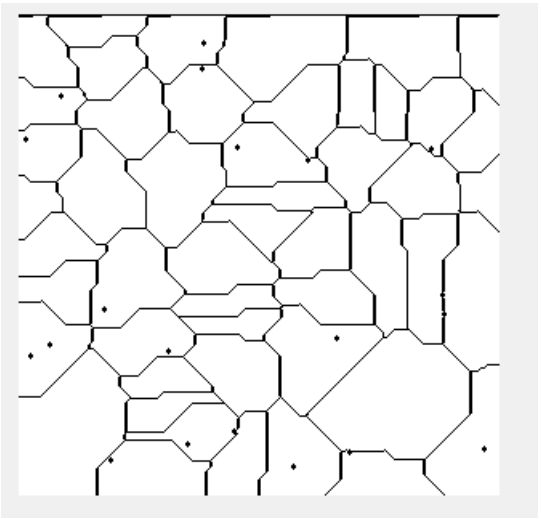

**Figure 16 Generated microstructure with inclusions**

# Conclusion

This application meets all the requirements assumed at the beginning of the project. The main advantage of this application is easy to use for inexperienced users. Another benefit is that, it allows to create a prototype of microstructure with conditions i.e. boundaries, inclusions, Dual Phase. From the perspective of users this application is sufficient to get simple simulation or replication. However, it needs to be added that this program has also limitations such as one size of grain. Application allows only changing size of inclusion. The second thing worth to note is low performance, i.e. for bigger size of board, simulation takes a lot of time and resources. C# and Windows Forms were very useful to create this application. C# provides ready-made solutions. Thanks to them, the development of this application was easier and quicker.

[2] (https://www.researchgate.net/figure/Microstructure-of-IF-steel-sheet-material_fig1_245058525)