AKADEMIA GÓRNICZO-HUTNICZA IM. STANISŁAWA STASZICA W KRAKOWIE

Wydział Inżynierii Metali i Informatyki Przemysłowej

Tomasz Gmurkowski

PROJECT RAPORT "GRAIN GROWTH"

WIMiIP

Table of Contents

1. PURPOSE OF THE CLASS

During the Multiscale Modelling classes our goal was creating an application which should have the following functions implemented:

- Simple grain growth CA – Von Neumann and Moore types of neighborhood
- GUI of application
- Microstructures export/import to files .txt/ bitmap
- Microstructures export/import from files .txt/bitmap

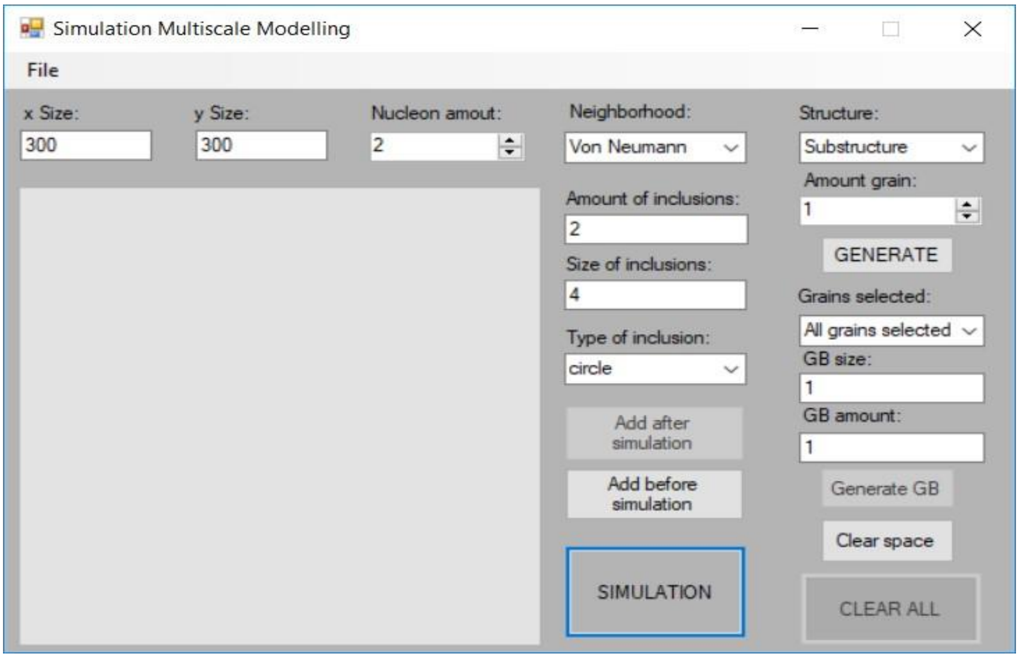
Modification of cellular automata grain growth algorithm which contains inclusions at the beginning or at the end of the simulation.

- Two types of inclusions: square or circular
- Different microstructure types: substructure and dualphase
- Grain boundaries selection

2. GRAPHICAL USER INTERFACE

The application was written in a C ++ programming language. It contains all the required modules. I chose C ++ because I don't work in a programming environment and there were the most manuals and instructions for this language, in addition it was the language I studied in college.

An additional advantage was that many friends also know this language and could help with the implementation of the code. The code was written in Visual Studio. The main program window shown below in the screenshot.



x Size: 300

y Size: 300

Nucleon amout: 2

Neighborhood: Von Neumann

Amount of inclusions: 2

Size of inclusions: 4

Type of inclusion: circle

Structure: Substructure

Amount grain: 1

Grains selected: All grains selected

GB size: 1

GB amount: 1

Figure 1 Main window of program

In the main interface we see fields that can be edited to select the appropriate option that interests us.

The program includes the following options:

- Ability to change the size of the simulation window

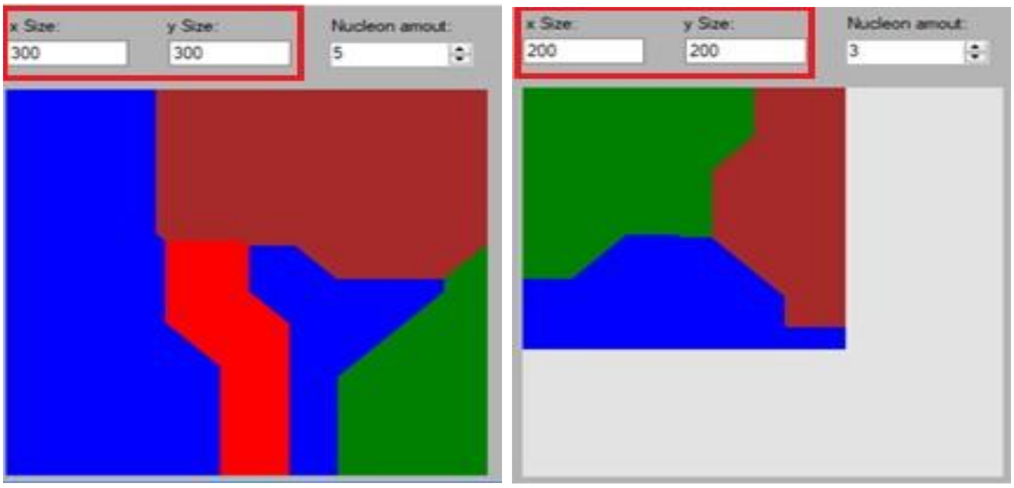
x Size: 300

y Size: 300

Figure 2 Area size selection fields for simulation

In the upper left year we can choose the size of the simulation window, the maximum size is 300 x 300. Minimum size is 100 x 100. As a result, the window of our program is not changed. Only the drawing area is reduced. This is shown in Figure 3

Result:


x Size: 300 y Size: 300 Nucleon amout: 5

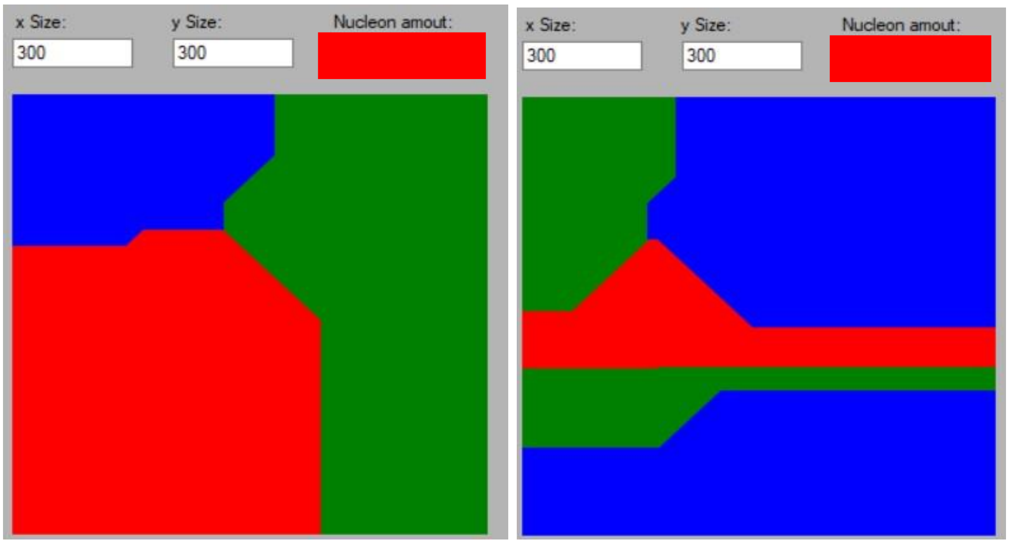
x Size: 200 y Size: 200 Nucleon amout: 3

Figure 3 Simulation result in two variants of size

- **Selection of the number of nucleons**

In this section we can choose the number of grains that we want to simulate. The initial value is 2. The limit is 999, unfortunately with such a large number the program will count for a very long time and the results will not be satisfactory in such a small area.

Result:

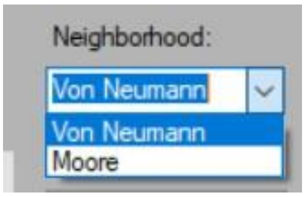

x Size: 300 y Size: 300 Nucleon amout:

x Size: 300 y Size: 300 Nucleon amout:

Figure 4 Simulation result with two variants - 3 and 5 nucleons

- **Choice the type of neighborhood**

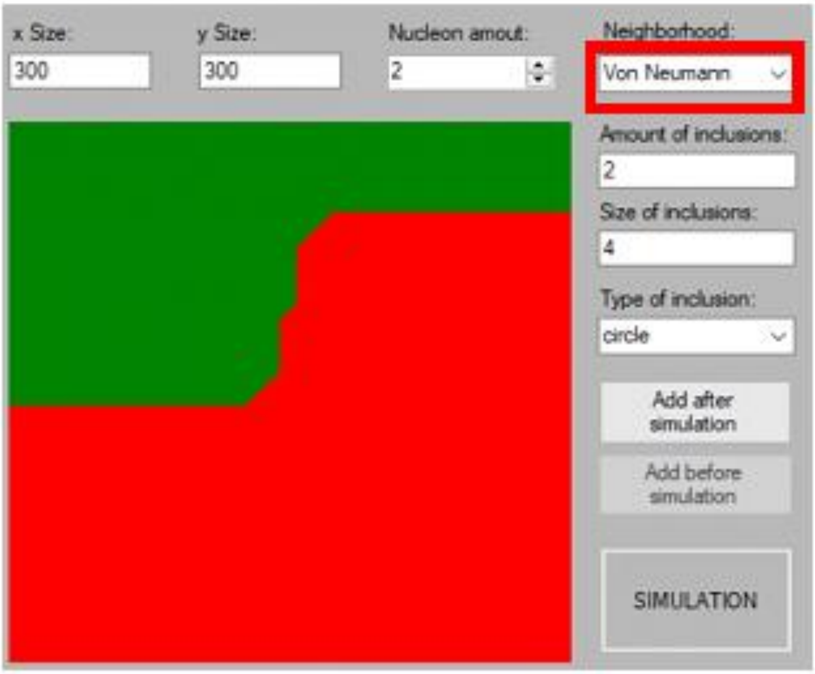
In this section we can choose which neighborhood variant we want, Moore or Von Neumann. We can Control of grain boundary shape: – extension of Moore neighborhood. Moore's neighboring rule was applied with partial fraction and time step control in the current approach to represent the grain growth kinetics more accurately.



Neighborhood: Von Neumann

Figure 5 Neighborhood type selection field

<u>Result:</u>



x Size: 300

y Size: 300

Nucleon amout: 2

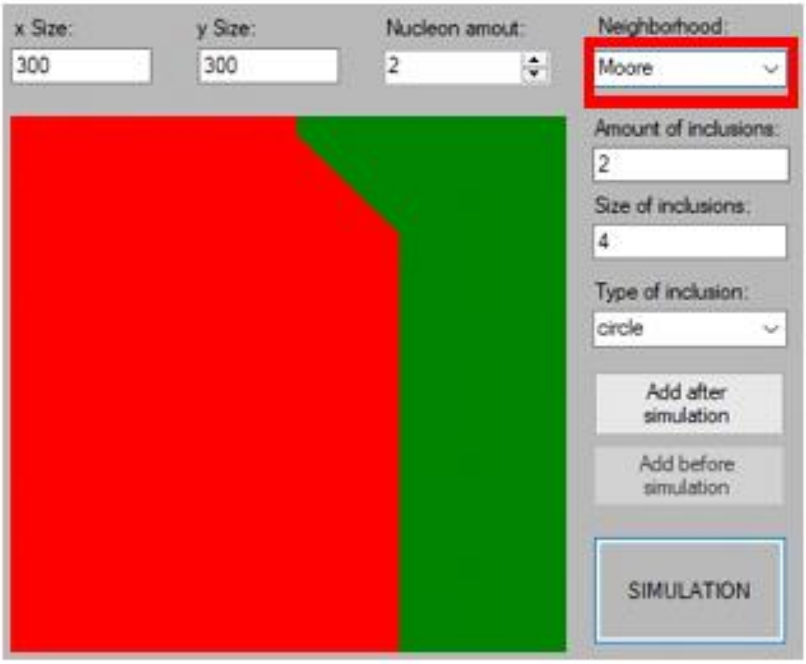
Neighborhood: Von Neumann

Amount of inclusions: 2

Size of inclusions: 4

Type of inclusion: circle

Figure 6 Two examples of growth according to Von Neumann or Moore


x Size: 300

y Size: 300

Nucleon amout: 2

Neighborhood: Moore

Amount of inclusions: 2

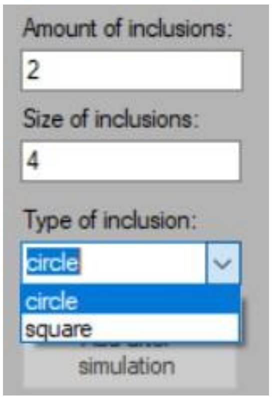
Size of inclusions: 4

Type of inclusion: circle

Figure 6.1 Two examples of growth according to Von Neumann or Moore

- **Possibility to decide about the number of inclusions, their size and shape**

Inclusions are another option in the program. We can turn them on by choosing the number of inclusions, then their size and select the type of inclusions. Will it be circle or square. Inclusions does not growth and could not be covered by other areas.

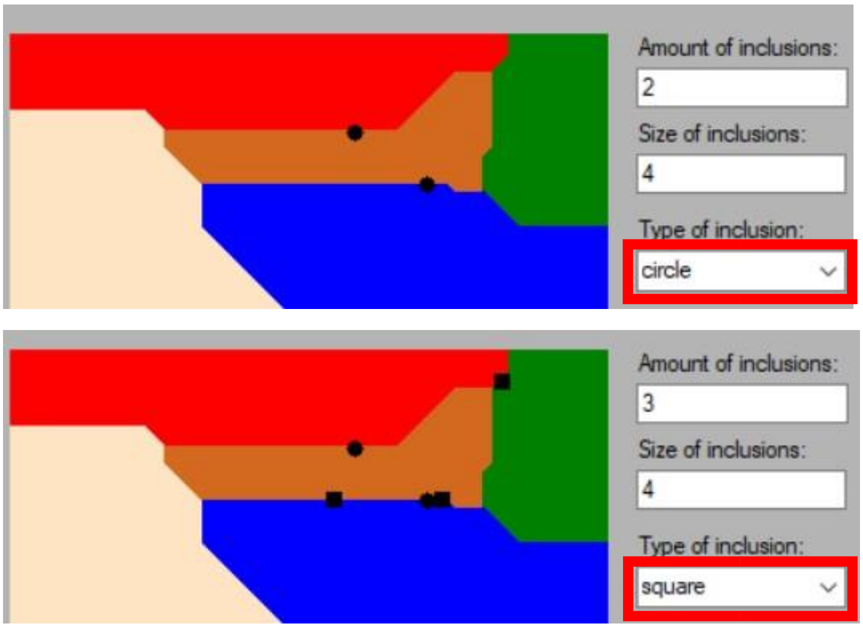

Amount of inclusions: 2

Size of inclusions: 4

Type of inclusion: circle

Figure 7 Check boxes regarding the quantity, size and shape of inclusions

Result:



Amount of inclusions: 2

Size of inclusions: 4

Type of inclusion: circle

Amount of inclusions: 3

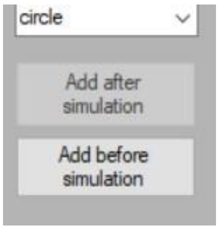
Size of inclusions: 4

Type of inclusion: square

Figure 8 Simulation results for two circle and three square inclusions

- **Buttons for changing the time of adding inclusions – after/before simulation**

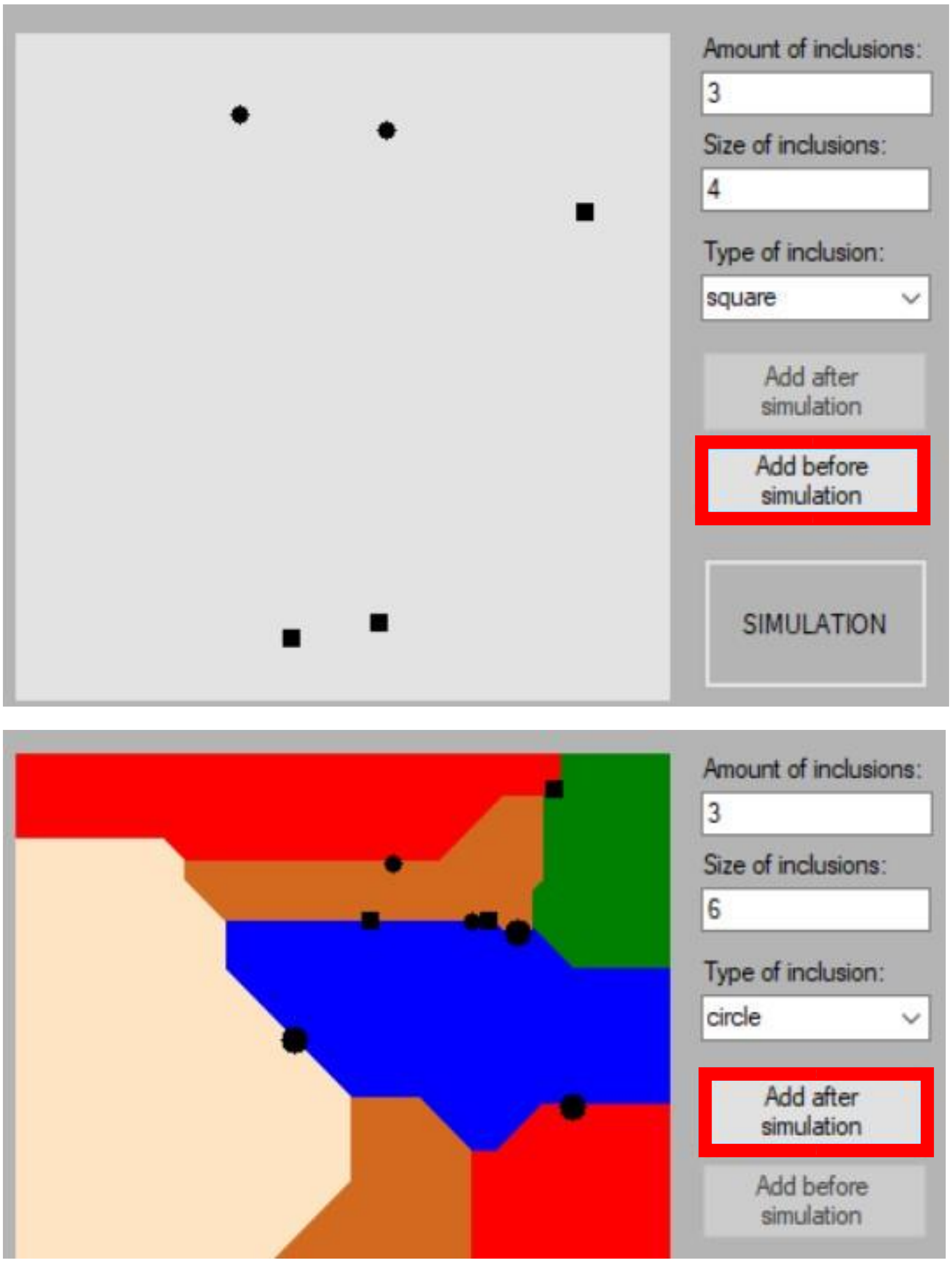
Inclusions can be added before or after the simulation. To do this, we need to click the "Add before simulation" or "Add after simulation" button in Figure 10 shows how the inclusions before and after the simulation work.



circle

Figure 9 Decision buttons for adding inclusions before or after simulation

Result:



Amount of inclusions:
3
Size of inclusions:
4
Type of inclusion:
square

Amount of inclusions:
3
Size of inclusions:
6
Type of inclusion:
circle

Figure 10 Simulation results - adding inclusions before or after this operation

- **Selection of the type of structure**

Next section is selection Structure, this allows us to choose a simulation area for some parts. We do this to block and tear into substructure or dual-phase. The default is Dual-phase, select substructure, enter amount grain and generate. After it use "material" don't remove this areas, and could random new additional seeds and growth it again. Blocked areas does not growth and cannot be covert by other areas.

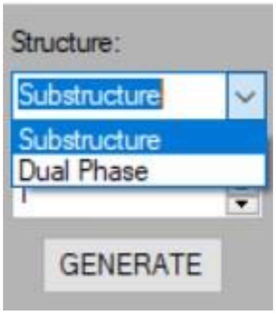
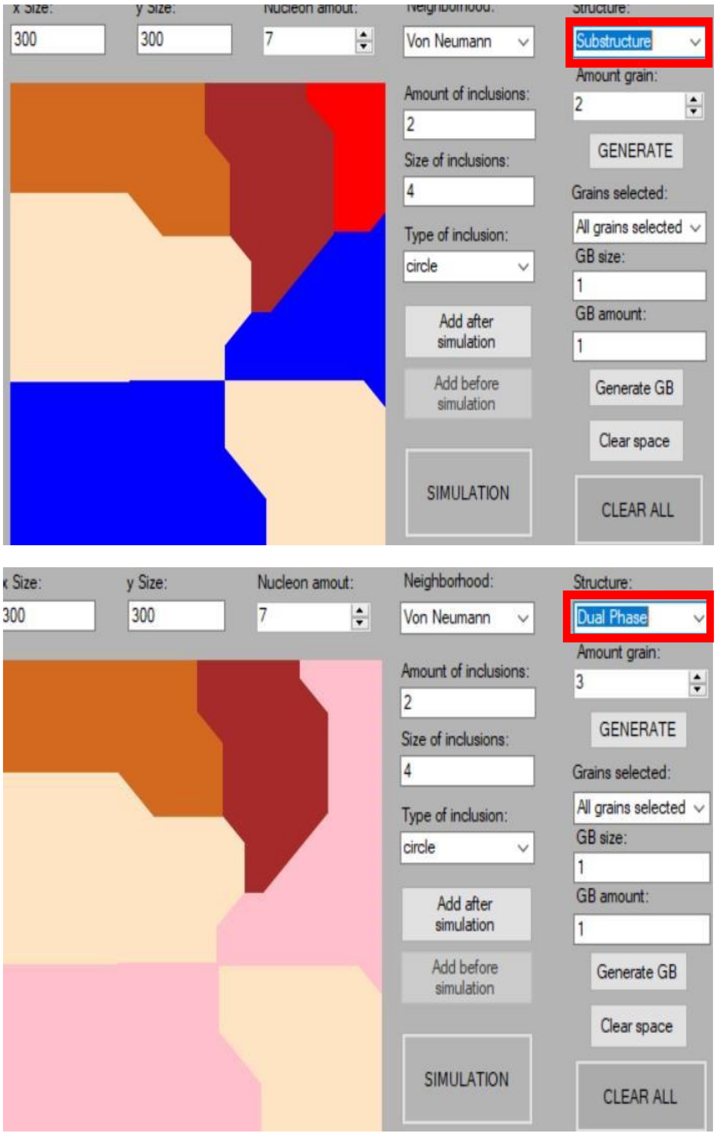

Structure: Substructure

Figure 11 Structure selection field

<u>Result:</u>

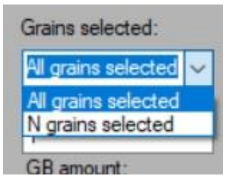

x Size: 300
y Size: 300
Nucleon amout: 7
Neighborhood: Von Neumann
Structure: Substructure
Amount grain: 2
Amount of inclusions: 2
Size of inclusions: 4
Type of inclusion: circle
Grains selected: All grains selected
GB size: 1
GB amount: 1

x Size: 300
y Size: 300
Nucleon amout: 7
Neighborhood: Von Neumann
Structure: Dual Phase
Amount grain: 3
Amount of inclusions: 2
Size of inclusions: 4
Type of inclusion: circle
Grains selected: All grains selected
GB size: 1
GB amount: 1

Figure 12 Simulation result with two variants – Substructure or Dual Phase

- **Grain boundaries selection – all/ n grains**

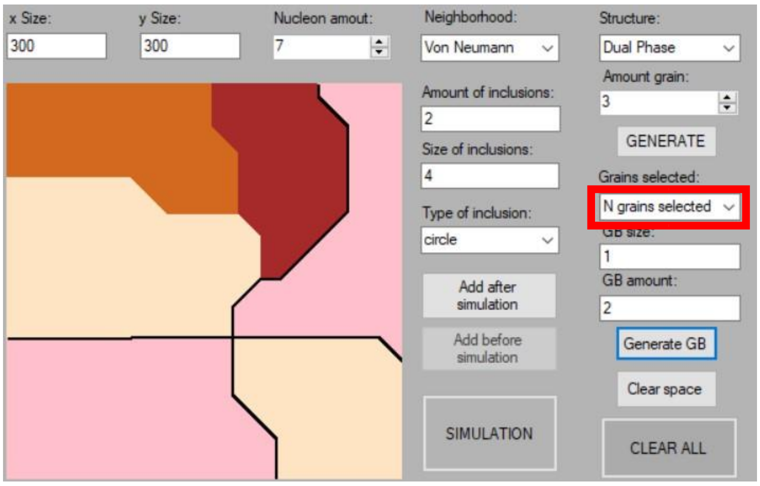
In this section we can choose grain boundaries. We have N grain or All grain to choose from. We can initially select only N grain selected, then select ALL and generate boundaries for all grains



Grains selected: All grains selected

Figure 13 Selection button for grain boundary

Result:



x Size: 300

y Size: 300

Nucleon amout: 7

Neighborhood: Von Neumann

Amount of inclusions: 2

Size of inclusions: 4

Type of inclusion: circle

Structure: Dual Phase

Amount grain: 3

Grains selected: N grains selected

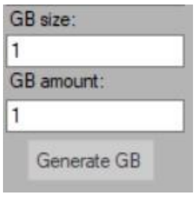
GB size: 1

GB amount: 2

Figure 14 The result of choosing an option "N grains selected"

- **GB size and amount**

In the same section but below we have the option of entering the grain boundary size, this helps when we have large grains and want to accurately define boundaries. After entering the value, to generate boundaries we have to click "Generate GB". In Figure 16 we can see the generated GB with a value of 3. The boundaries are large and clear.

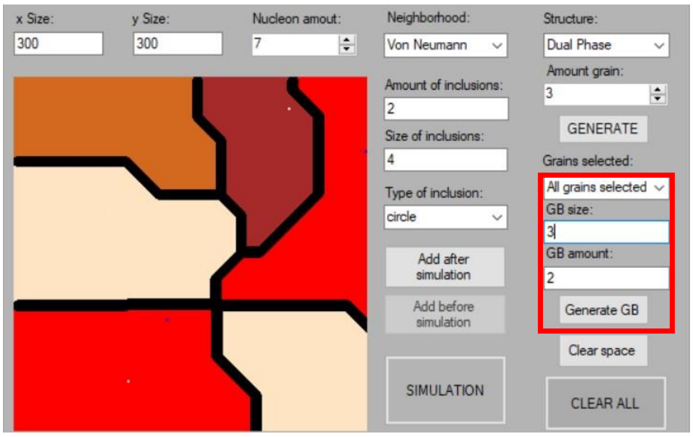


GB size: 1

GB amount: 1

Figure 15 Selection button for size and amount grain boundary

Result:



x Size: 300

y Size: 300

Nucleon amout: 7

Neighborhood: Von Neumann

Structure: Dual Phase

Amount grain: 3

Amount of inclusions: 2

Size of inclusions: 4

Type of inclusion: circle

Grains selected: All grains selected

GB size: 3

GB amount: 2

Figure 16 Simulation result for GB size no 3 and all grains selected

- **Clearing simulation space without grain boundaries**

If we have grains generated and we have drawn borders. For greater clarity, we can clean the area, then we can generate new grains.

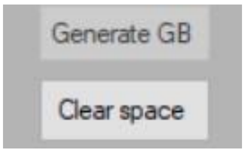
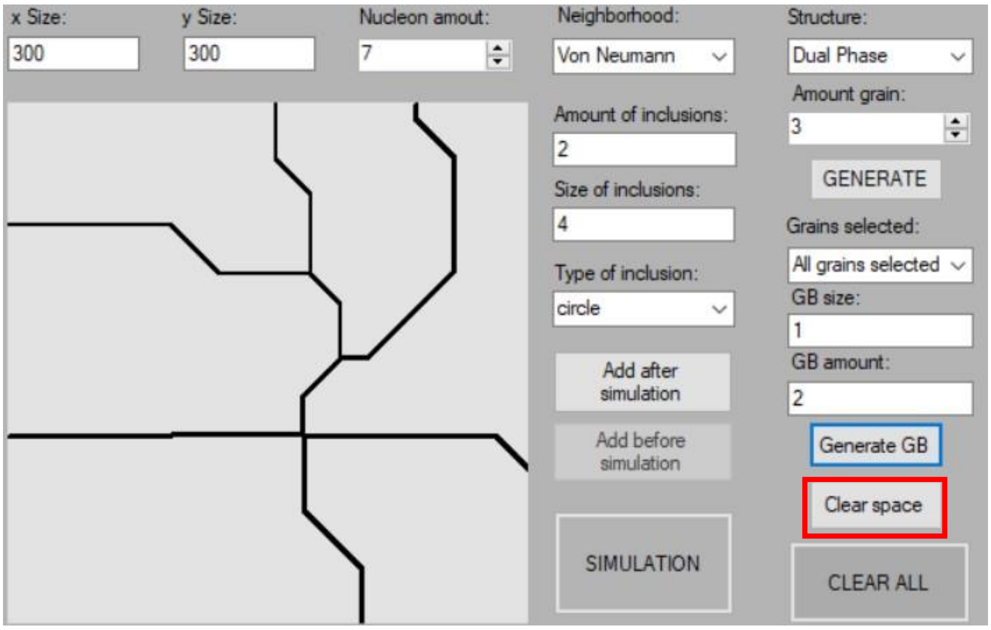


Figure 17 A button used to clear the simulation window, excluding the boundaries

<u>Result:</u>



x Size: 300

y Size: 300

Nucleon amout: 7

Neighborhood: Von Neumann

Amount of inclusions: 2

Size of inclusions: 4

Type of inclusion: circle

Structure: Dual Phase

Amount grain: 3

Grains selected: All grains selected

GB size: 1

GB amount: 2

Figure 18 Simulation window with only grain boundaries

- **Import/export file .txt or bitmap**

The last option is import and export. After generating the grains, we can export the image for saving. We can export to TXT file and to BMP. There is also an Import option that allows us to import the finished structure. We can also import from TXT and BMP

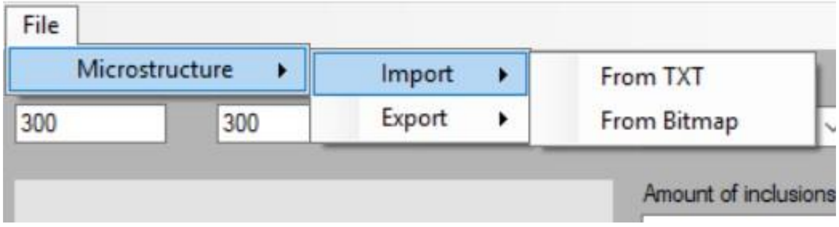


Figure 19 The file import / export selection list

<u>Result:</u>

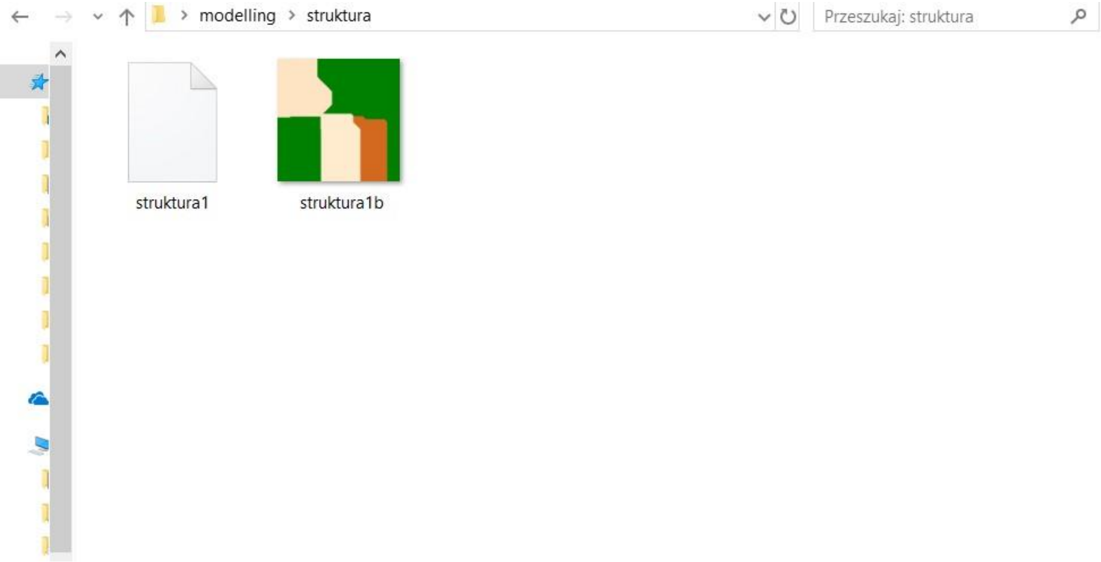


Figure 20 View of exported .txt and bitmap files

3. PROGRAM CODE

The program code has been added in the attachment (pdf file), and VisualStudio files on GitHub website.

4. CONCLUSIONS

A Cellular Automaton (CA) is an infinite, regular lattice of simple finite state machines that change their states synchronously, according to a local update rule that specifies the new state of each cell based on the old states of its neighbors.

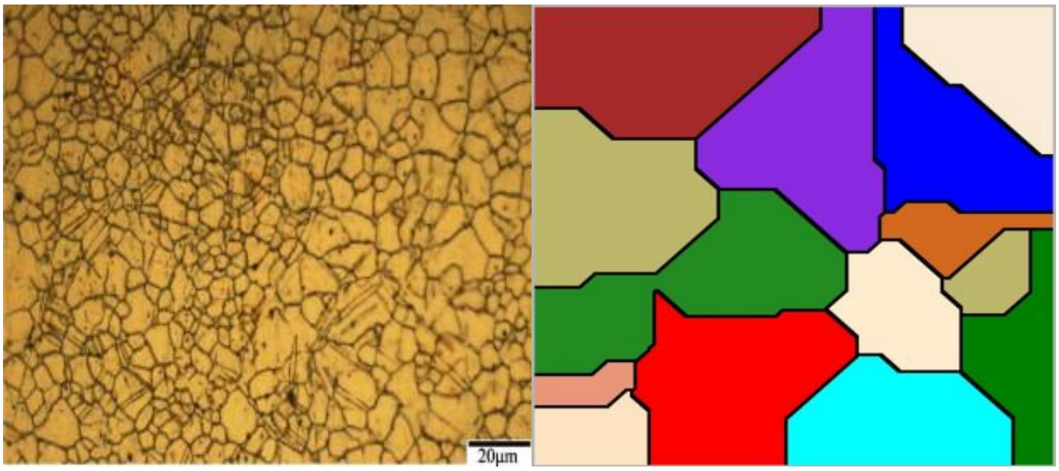


Figure 21 Real microstructure of duplex steel and simulation in the program

The written program gives many possibilities. It allows easy simulation of the microstructure and the grain growth process. Neighborhood can be defined in different ways. The program uses two types of neighborhood - Neumann and Moore. The program that was written, can not assess exactly how the real structure would behave. The generated microstructure is significantly different from the real one observed under the microscope.