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Year 2, IS WIMIIP

15.11.2017

Multiscale Modelling
Report 1

1. Aim of the project

The goal of the project was to create a program that is able to generate two-dimensional images of statistically representative metallic structures based on the cellular automata discreet model.

The implemented functions include:

- Simple grain growth algorithm (Figure 5.)
- Advanced grain growth algorithm
- Import and export (Figure 6, 7, 8).
- Inclusions
- Microstructure type selection
- Grain boundaries

2. User interface

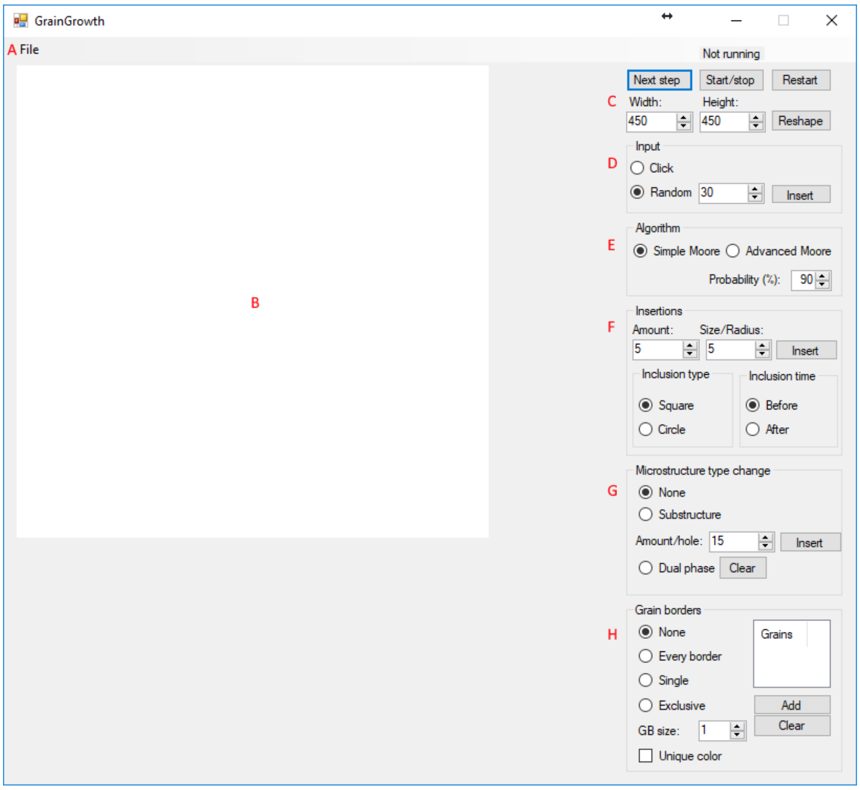


Figure 1. Program's main window.

Main interface elements:

A. Import and export menu
B. Image picture box
C. Growth control and image size panel
D. Nuclei input panel
E. Algorithm selection panel
F. Inclusions panel
G. Microstructure type panel
H. Grain boundaries panel

3. Descriptions of implemented functions

a. Simple growth

This is the program's main feature which we can use to create the most basic structures based on the Moore's neighborhood (Figure 5a., 5b.). The image can be rescaled using the image size panel (Figure 2.).

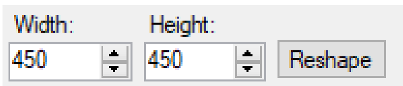


Figure 2. Image size panel.

You can insert the nuclei either manually or you can specify a random number of nuclei to be inserted. (Figure 3.).

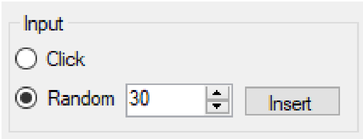


Figure 3. Nuclei input panel.

You can control the grain growth either manually by pressing the Next step button or automatically by pressing the Start/stop button. The growth also can be restarted (Figure 4.).

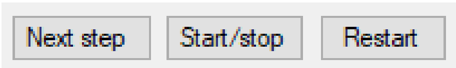


Figure 4. Growth control panel.

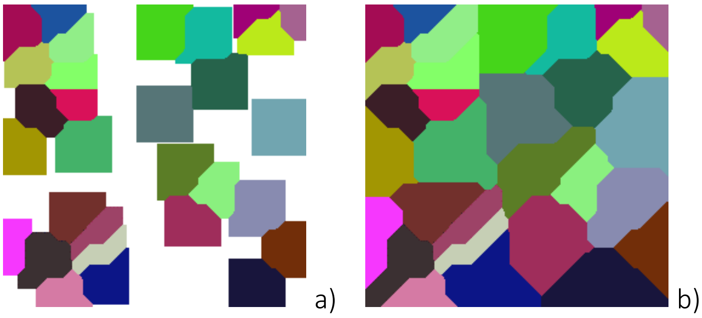


Figure 5. The 250x250 size microstructure with 30 nuclei created by using the simple algorithm a) after a number of steps, b) after it is completed.

b. Import and export

This function can be used to import or export a generated structure from/to a BMP or TXT file. The user can manually select an imported/exported file using the system's default open file dialog (Figure 7.). It is located in the compact menu in the upper left corner of the main window (Figure 6.). After the import, growth can be continued as normal (Figure 3, 4, 5).

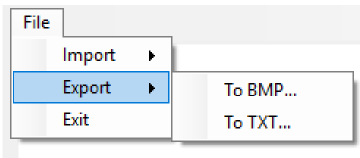


Figure 6. The import/export menu.

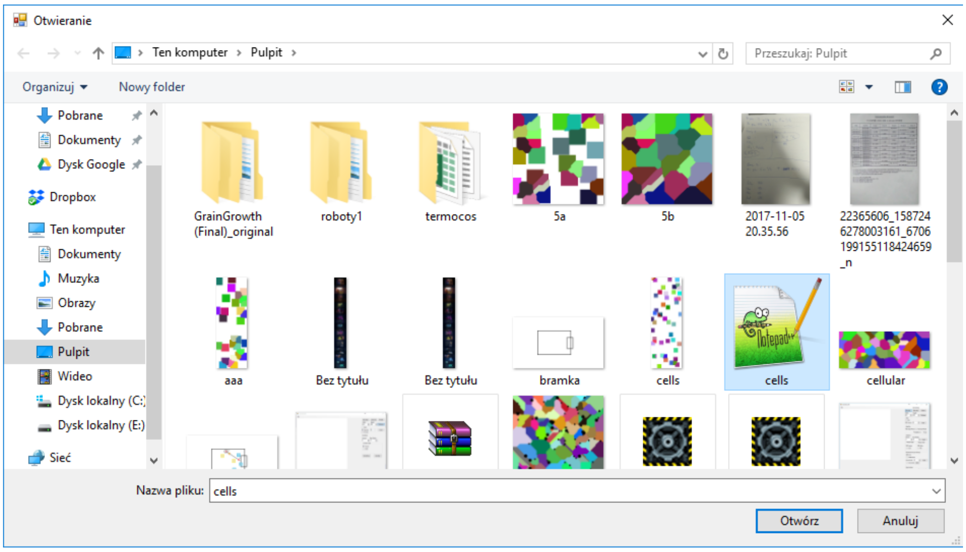


Figure 7. Invoked open file dialog for importing a TXT file.

The imported/exported file is formatted in a following way:

```
Width height
X Y Id
```

Where ID is a hexidecimal number of the color (Figure 8.).


cells — Notatnik

Plik Edycja Format Widok Pomoc

```
450 450
0 0 #FFFFFF
0 1 #FFFFFF
0 2 #FFFFFF
0 3 #FFFFFF
0 4 #FFFFFF
0 5 #FFFFFF
0 6 #FFFFFF
0 7 #FFFFFF
0 8 #FFFFFF
0 9 #FFFFFF
0 10 #FFFFFF
```

Figure 8. The text file format in a cells.txt file.

c. Inclusions

This function can be used to insert inclusions. An inclusion is any material that is trapped inside a mineral during its formation. User can specify their amount, size, type and time of inclusion (Figure 9.).

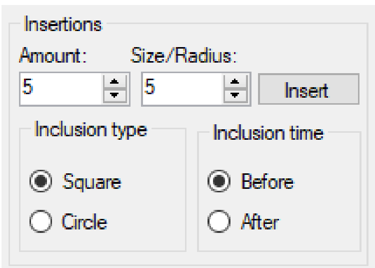


Figure 9. Inclusions panel.

Inclusions can either be added before the growth – anywhere in the space – or after it – on the grain borders (Figure 10a., 10b.).

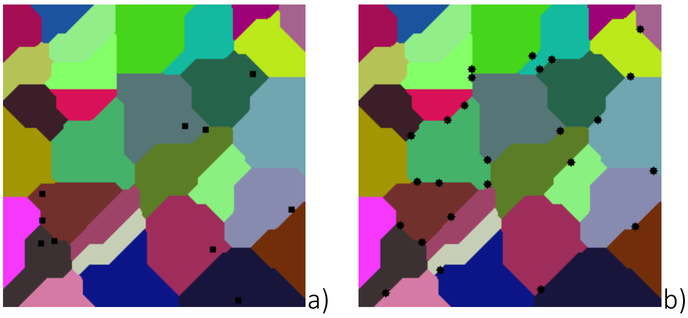


Figure 10. Comparison of a) 10 square inclusions (size 5) added before the growth, b) 25 circle inclusions (size 3) added after the growth.

d. Advanced growth

Advanced growth is the second growth algorithm created according to four rules based on probability and changing neighborhood. The algorithm can be selected and probability can be set from the algorithm selection panel (Figure 11).

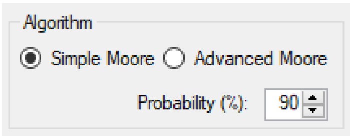


Figure 11. Algorithm selection panel.

After the selection, nuclei input and growth can be proceeded as normal (Figure 3., 4.).

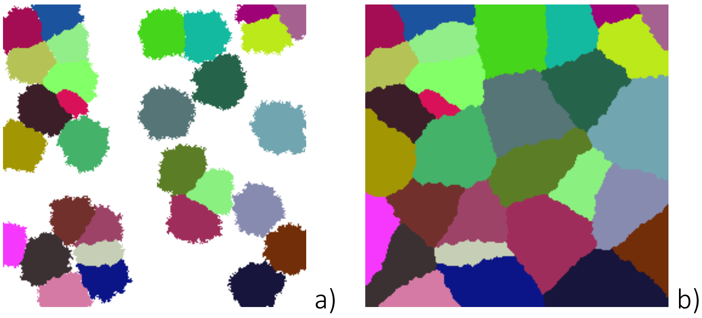


Figure 12. *The microstructure created by using the advanced algorithm with 45% probability a) after a number of steps, b) after it is completed.*

e. Microstructure types

This function can be used to change the desired type of the microstructure. We can select from either a substructure or a dual-phase material. Substructure works by deleting selected (clicked) grains. Dual phase works by deleting selected (clicked) grains and remaining grains turn into the second phase after pressing *Clear*. Remaining grains in both cases do not grow any further (Figure 14a). The user can also insert a specified amont of grains into a hole created after deleting each grain (for substructures only) (Figure 13.).

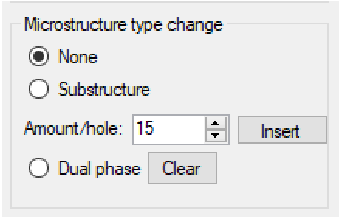


Figure 13. Microstructure type panel.

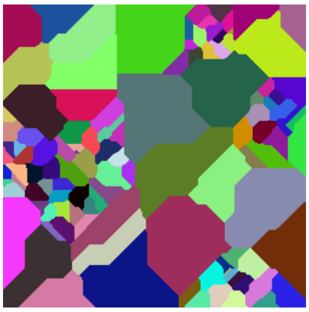
 a)  b)

Figure 14. Comparison of two microstructure types based on the structure generated in Figure 5b.: a) Substructure with 15 new grains in each deleted grain in the initial growth, b) Dual phase with 30 new grains after leaving the same grains intact.

f. Grain boundaries

This function can be used to select and mark grain boundaries. The grain boundaries panel can be used to specify their width (Figure 15.). User can select from one of three types of boundaries and there's also an option to assign an unique color to the selected boundaries. *Add* button adds the boundaries to the picture box, while *Clear* button erases everything but the boundaries and inclusions.

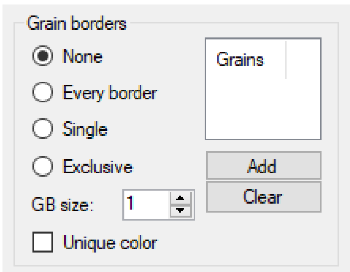


Figure 15. Grain boundaries panel.

Every border type selects the boundaries of all grains (Figure 16.).

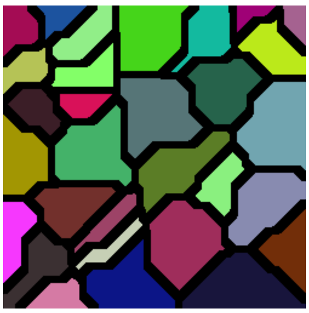
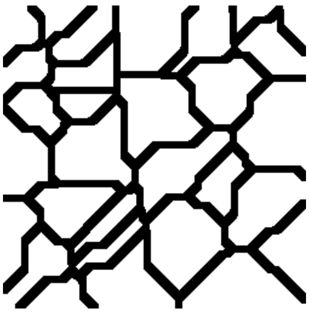
 a)  b)

Figure 16. Microstructure based on the structure generated in Figure 5b.: a) after adding the borders for every grain (size 3), b) after deleting the grains.

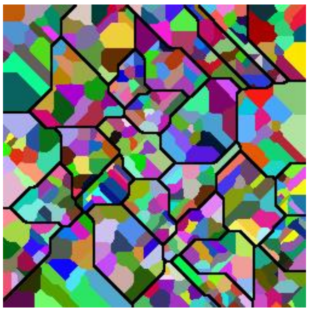


Figure 17. A microstructure with its borders applied, old grains cleared and new grains grown.

Single type can be used to select individual grains (Figure 19.), which will appear on the list to the left of the grain boundaries panel (Figure 18.).

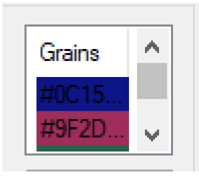


Figure 18. The grain list with three selected grains.

Boundaries will appear only for the selected grains.

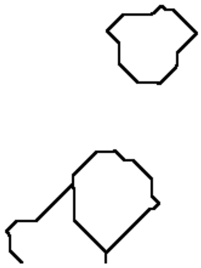
 a)  b)

Figure 19. Microstructure based on the structure generated in Figure 5b.: a) after adding the borders for selected grains (size 1), b) after deleting the grains.

Exclusive type can be used to select individual grains (Figure 20.), which will appear on the list to the left of the grain boundaries panel (Figure 18.).

Boundaries will appear only on the connection points of previously selected neighboring grains.

 a)  b)

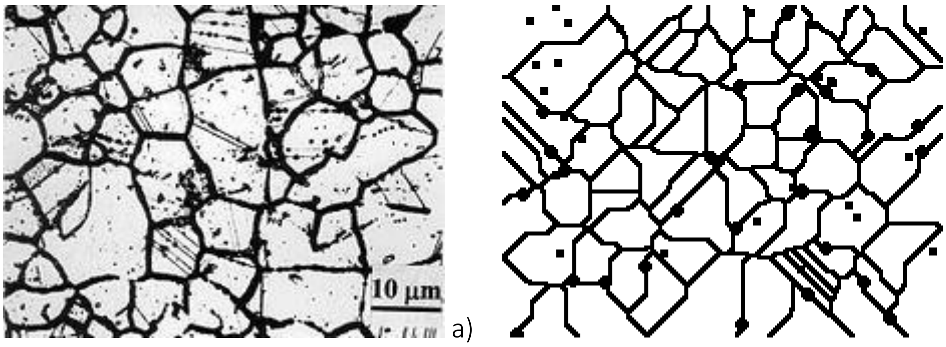
Figure 20. Microstructure based on the structure generated in Figure 5b: a) after adding the borders for selected grains exclusively (size 1), b) after deleting the grains.

The *Unique color* checkbox applies an unique color to the selected grains (Figure 21.).

Figure 21. Microstructure based on the structure generated in Figure 5b. after adding the borders for selected grains with unique colors and various types and sizes.

4. Real structure comparison and conclusion

The generated image (Figure 22b.) closely represents the structure visible on the Figure 22a., which has been generated from a real sample. Users can manipulate the parameters provided by the software to achieve a similar result that is statistically representative to the real sample (e.g. average grain size, number of grains per unit etc.). This is a much cheaper and quicker method of generating valid structure images which can be used in further research with similarly effective results. Cellular automata prove to be superior to optic and microscopic imaging.



a) b)

Figure 22. Comparison of a) heavily sensitized microstructure of type 304 stainless steel (Webcorr, 2017), b) similar microstructure generated in the created program.

Bibliography

Webcorr. (2017). *Corrosion*. Downloaded from Wikipedia: https://en.wikipedia.org/wiki/Corrosion#/media/File:Sensitized_structure_of_304_stainless_steel.jpg