First Report

Multiscale Modeling

User interface

Presented user interface [Fig. 30] contains all updates performed during the whole process of system creation. Basic parameter which user can provide is *number of grains*. User can also select the *neighbourhood type* for the grain growth process. By pressing the *Start simulation* button user can start the process of grains growing. The growth process is carried out in accordance with assumptions of CA method. Resulted structure is displayed on the right side of the panel with options.

Number of grains

This number defines the number of grains that we observe in the resulted structure.

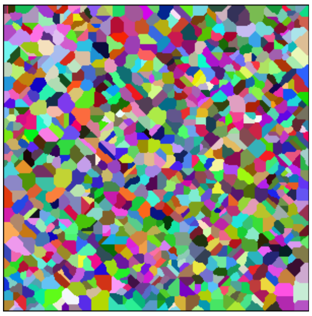
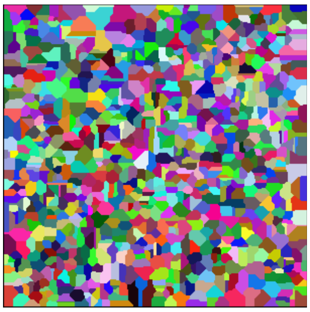
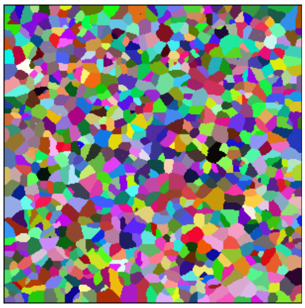
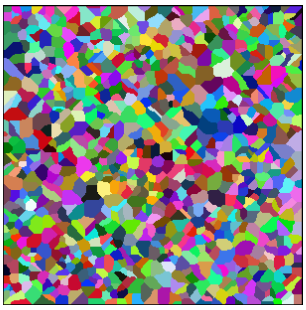
Neighbourhood type

This parameter is a very important one. It is who defines the change in shape of each grain visible in the resulted structure. For more advanced neighbourhood type, which is Extended Moore, special rules were introducd to perform the process of grains gtowth. In one of these rules particular grain can growth with some probability – its value can be also specified by the user.

Save / read structures

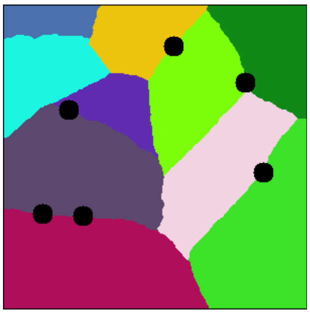
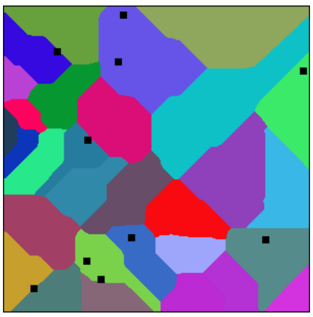
The user have the possibility to save the generated microstructure as a text file or a bitmap image. When have a structure saved in the file containing required content, usercan read it into the interface as the current scope. User can aslo specify file name and location through save / read dialog.

The following illustrations shows resulted structures processed accordingly to the presented parameters configuration [Fig. 1-8].

Number of grains: 10 Neighbourhood type: Moore	Number of grains: 1000 Neighbourhood type: Moore
 Fig. 1	 Fig. 2
Number of grains: 10 Neighbourhood type: Von Neumann	Number of grains: 1000 Neighbourhood type: Von Neumann
 Fig. 3	 Fig. 4
Number of grains: 10 Neighbourhood type: Extended Moore Growth probability: 10%	Number of grains: 1000 Neighbourhood type: Extended Moore Growth probability: 10%
 Fig. 5	 Fig. 6
Number of grains: 10 Neighbourhood type: Extended Moore Growth probability: 90%	Number of grains: 1000 Neighbourhood type: Extended Moore Growth probability: 90%
 Fig. 7	 Fig. 8

Inclusions

After the structure is generated – after grains growth process or reading structure from the file – user can select the *Inclusions* option. By doing this he will be allowed to provide the *number of inclusions*, their *size* and *type* (square, circular), *time of creations* (at the begining of simulation, after simulation – on grain boundaries). When specified all thoses parameters user can press *Add inclusions* button which starts proper method. As a result of this step user can observe the previously generated structure [Fig. 9] with inclusions of selected type added [Fig. 10-13].

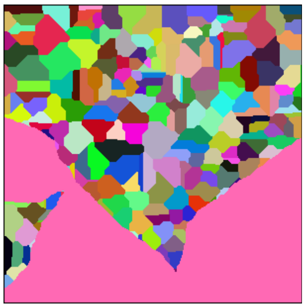
<table>
<tr><td colspan="2">Base structure</td></tr>
<tr><td colspan="2">
Fig. 9</td></tr>
<tr><td>After simulation inclusions
Number of inclusions: 6
Type: Squre
Size (diameter): 10</td><td>After simulation inclusions
Number of inclusions: 6
Type: Circular
Size (radius): 10</td></tr>
<tr><td>
Fig. 10</td><td>
Fig. 11</td></tr>
<tr><td>Begining of simulation
Number of inclusions: 10
Type: Squre
Size (diameter): 10</td><td>Begining of simulation
Number of inclusions: 10
Type: Circular
Size (diameter): 10</td></tr>
<tr><td>
Fig. 12</td><td>
Fig.13</td></tr>
</table>

Other types of microstructure

Other structure change, which can be performed after the grains growth, is creating other types of microstructures. User can choose between *Substructure* and *Dualphase* structure. For both types a number of remaining grains can be provided. After pressing *Generate* button user can observe the structure containing required number of grains from the base structure [Fig. 14, 17] (grains remaining from the base structure) and the rest of a computational scope filled with grains growth accordingly to preferences set by him as simulation paramaters [Fig. 15-16, 18-19].

Base structure

Fig. 14

Microsturcture type: Substructure Number of ramaining grains: 3 Base parameters: Number of grains: 300 Neighbourhood type: Von Neumann	Microsturcture type: Dualphase Number of ramaining grains: 3 Base parameters: Number of grains: 300 Neighbourhood type: Von Neumann
 Fig. 15	 Fig. 16

Base structure

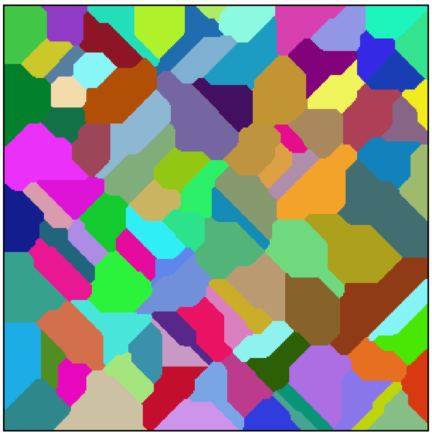
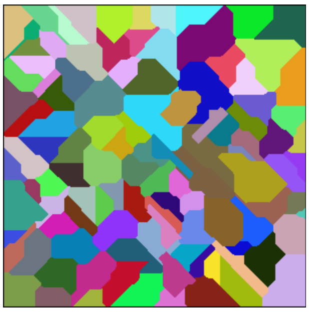
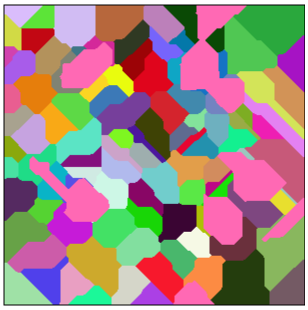


Fig. 17

Microsturcture type: Substructure Number of ramaining grains: 10 Base parameters: Number of grains: 100 Neighbourhood type: Moore	Microsturcture type: Dualphase Number of ramaining grains: 10 Base parameters: Number of grains: 100 Neighbourhood type: Moore
 Fig. 18	 Fig. 19

Grains boundaries

When the structure is generated there is also the possibility to mark / color the grains boundaries. User can choose one of two options: *All grains* (which will mark boundaries of all grains) and *N grains* (which will mark boundaries of N grains). When choosing the second option user can also provide the number of grains (N). For both user can also specify the boundary size. After pressing *Color boundaries* button on the current structure [Fig. 20, 25] user can see black lines of the required size which represents the grains boundaries [Fig. 21-22, 26-27]. When boundaries are generated user can press the *Clear background* button which will resutl with the white board only containing grains boundaries [Fig. 23-24, 28-29].

<table>
<tr><td colspan="2">Base structure</td></tr>
<tr><td colspan="2">
Fig. 20</td></tr>
<tr><td>All grains
Boundary size: 10</td><td>2 grains
Boundary size: 10</td></tr>
<tr><td>
Fig. 21</td><td>
Fig. 22</td></tr>
</table>

Clear background

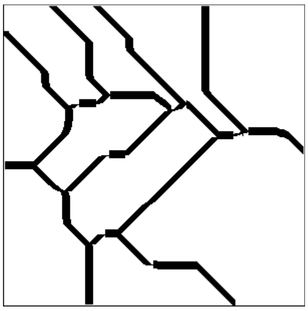


Fig. 23

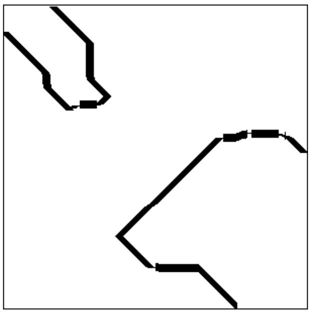


Fig. 24

Base structure

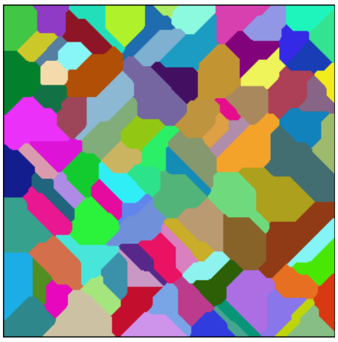


Fig. 25

All grains
Boundary size: 1

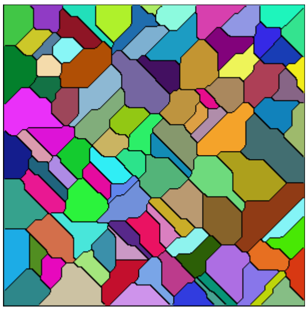


Fig. 26

20 grains
Boundary size: 1

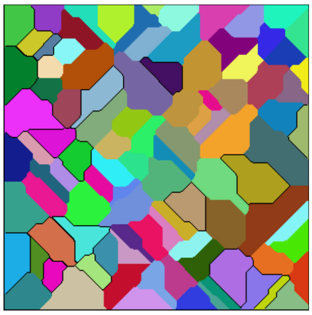


Fig. 27

Clear background

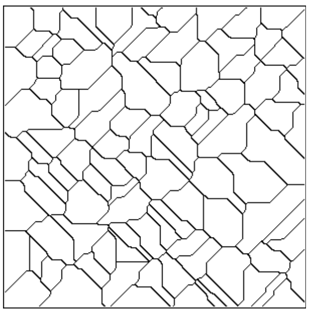


Fig. 28

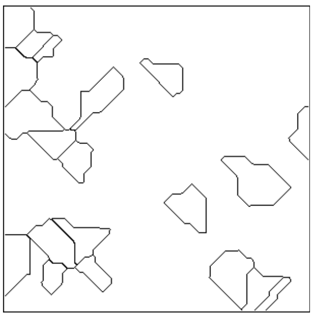


Fig. 29

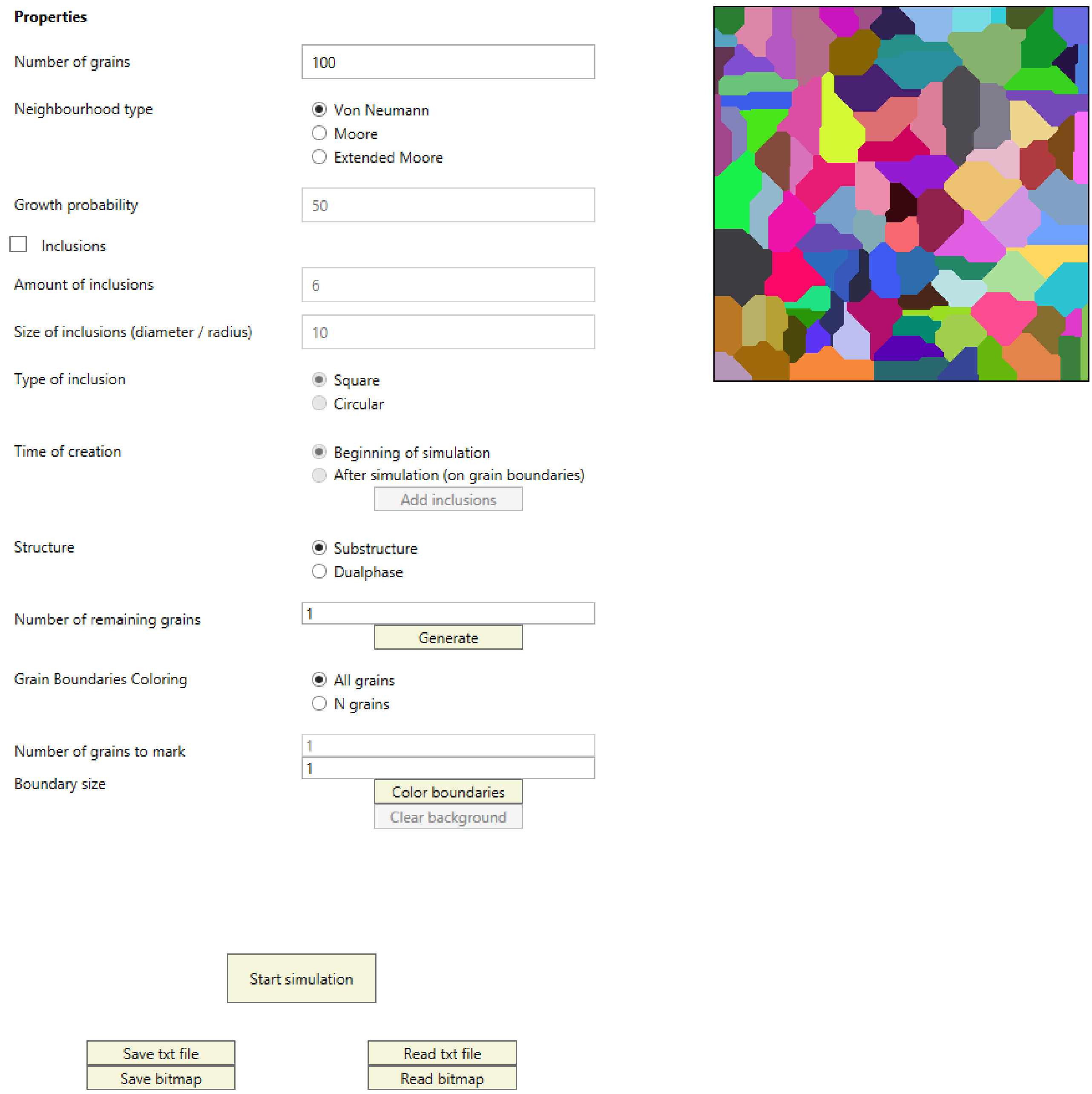


Fig. 30

Technology

For the purpose of building this application the C# programming language (.Net Technology) was used. The user interface was created based on a WPF Form. This technology allows to create fully interactive user interfaces. .Net is also the best known technology for author of this paper and it is absolutely sufficient for this problem solving purposes.

Real structures

Comparing generated microstructure to the real ones it can be observed that they are just an approximation of real structures [Fig. 31-32]. Random distribution of seed nuleation sites in some cases can cause signifficant differences in the final grains size, this would generate an abnormal grains distributions. Generating inclusions in the material reflects in a relatively good way real formation of inclusions [Fig. 33-34]. Also created substructure has features in common with real one. There can be observed that the distribution of larger grains is irregullar both in generated and real structures [Fig. 35-36]. In case of dualphase structures second phase grains form in little extend corresponds to the real ones [Fig. 37-38], but the whole generated structure can be treated as a very loose approximation of a real structure.

Microstructure

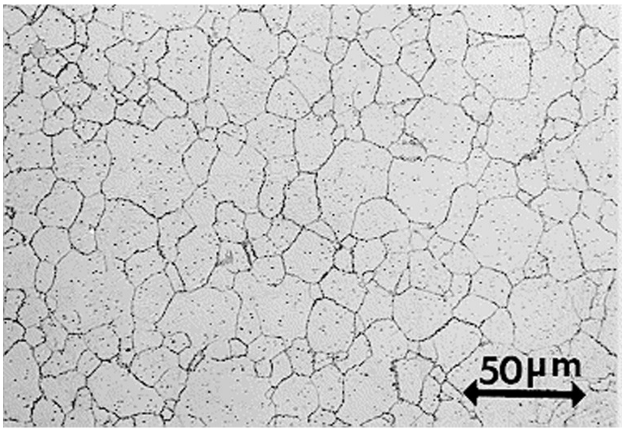


Fig. 31: High Copper Alloys [1]

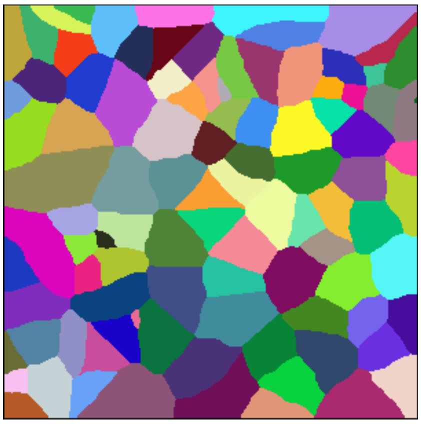


Fig. 32: Generated microsturucture

Microstructure with inclusions

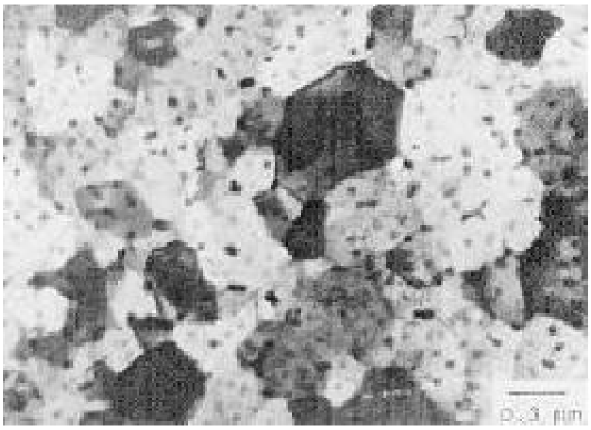


Fig. 33: Real low C steel microstructure with the inclusions [2]

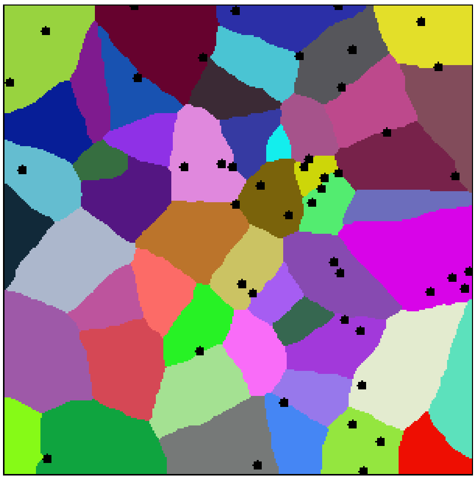


Fig. 34: Generated microsturucture with inclusions added

1 https://www.copper.org/resources/properties/microstructure/be_cu.html, 6.11.18
2 http://nele.studentenweb.org/research/?subject=PFM, 6.11.18

Substructure

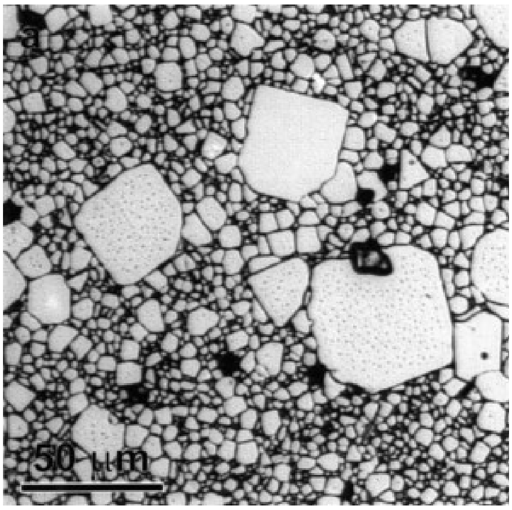


Fig. 35: Exaggerated grain growth in polycrystalline materials [3]

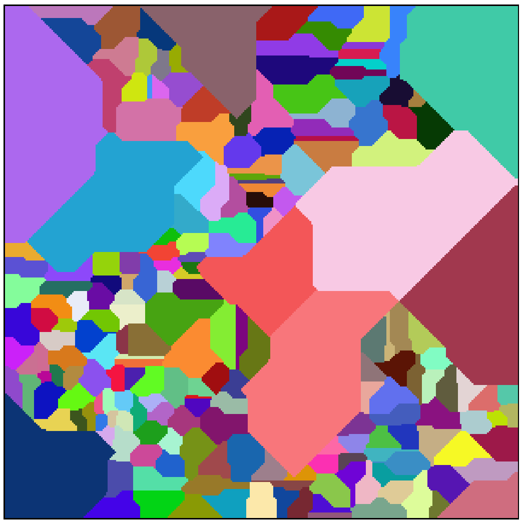


Fig. 36: Generated substructure

Dual-phase

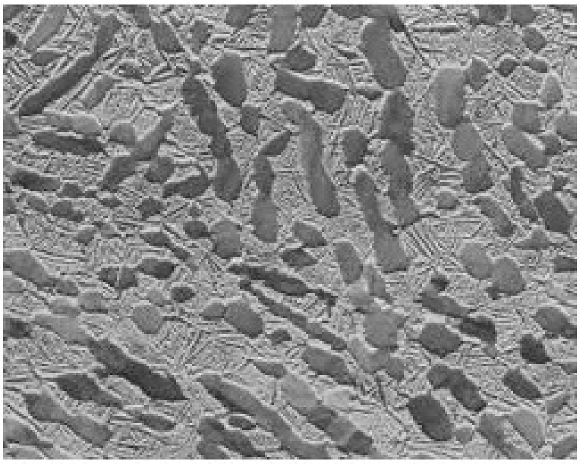


Fig. 37: DP Steel [4]

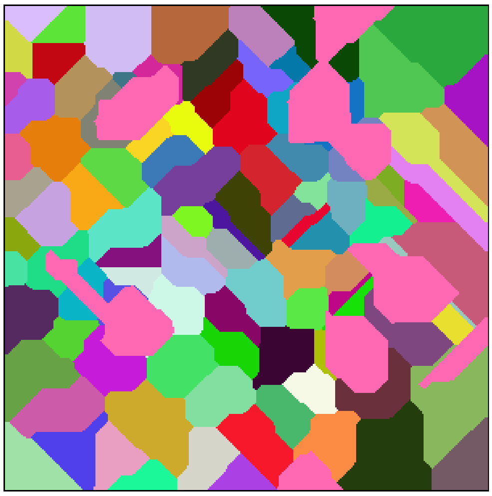


Fig. 38: Generated dualphase microsturucture

3 https://www.sciencedirect.com/science/article/abs/pii/S0955221901001844, 6.11.18
4 https://www.worldautosteel.org/steel-basics/steel-types/dual-phase-dp-steels/, 6.11.18