AGH UNIVERSITY OF SCIENCE AND TECHNOLOGY

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MULTISCALE MODELLING
Report

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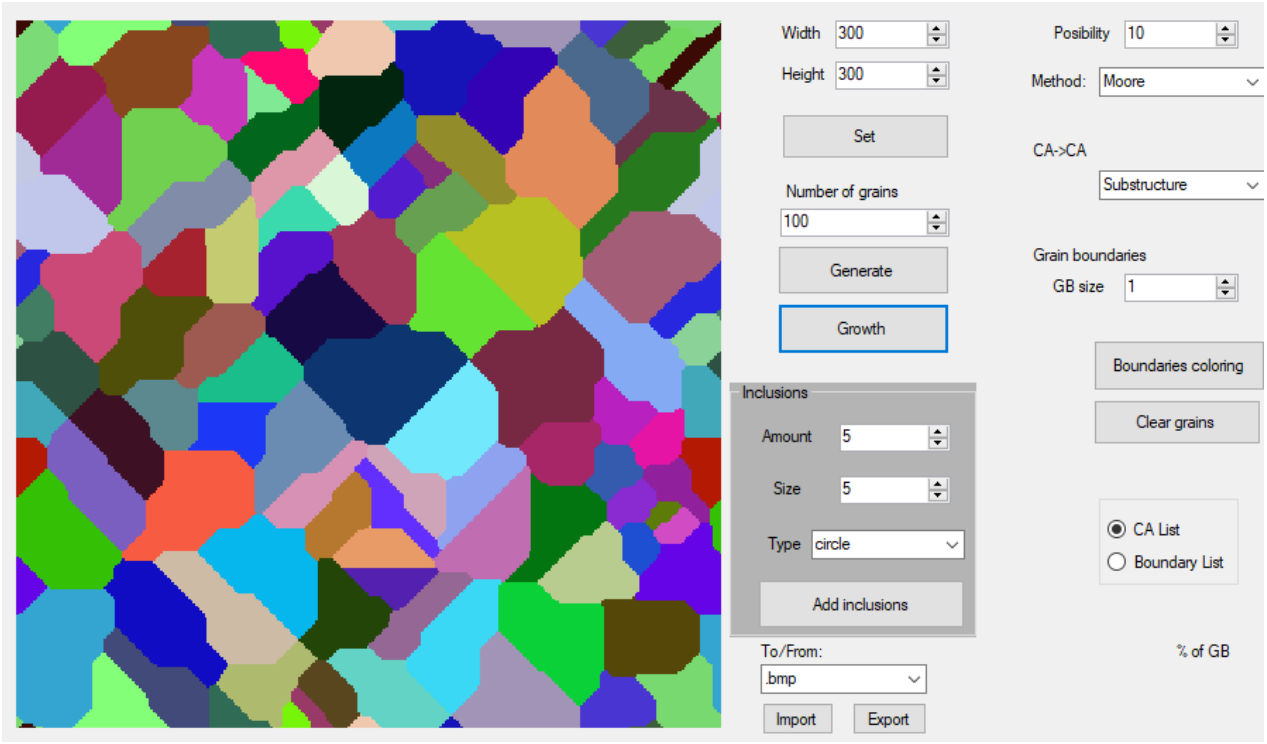
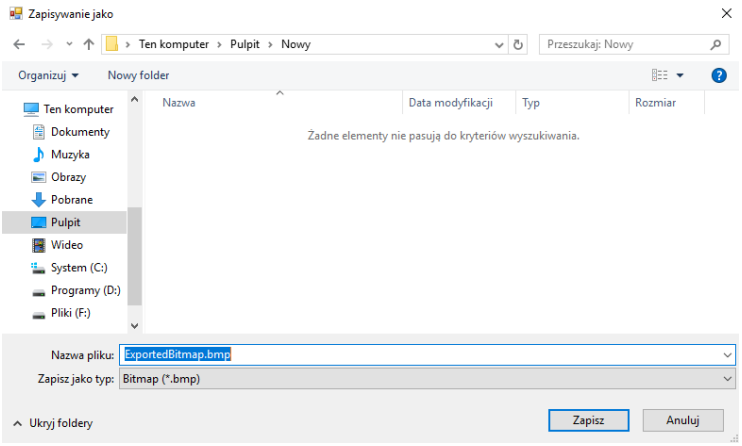
1. Simple grain growth was implemented by using Cellular Automata method. Cells have clearly defined interaction rules between each other. It was used Moore neighborhood and periodic boundary conditions. It is possible to change size of microstructure by using width- and height-UpDown field on the GUI. There is also possibility to set number of grains. All features to set are visible on GUI (Picture 1).

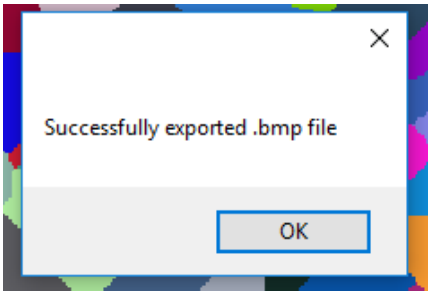


Picture 1 Simple grain growth - genereted strudcture with Moore neigbourhood and periodic condition

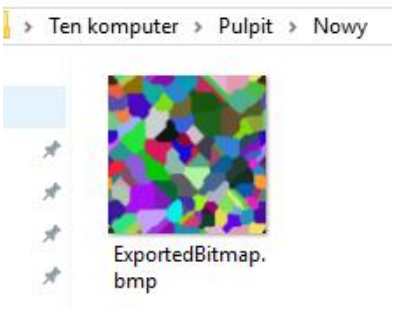
2. Added possibility to import/export structure to bitmap or text file. User have the opportunity (DialogBox) to choose where to save the file or which file import (Picutre 2a, 2b, 2c).



Picture 2a DialogBox to save exported bitmap

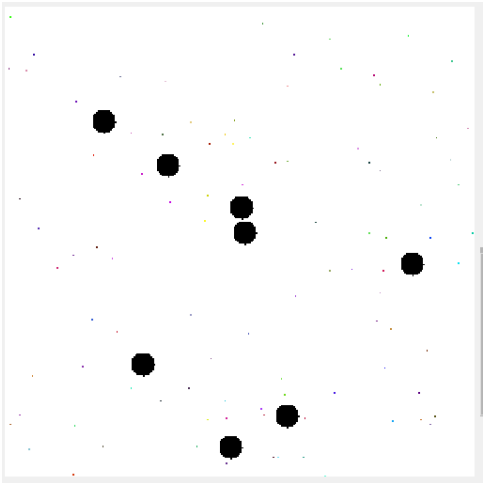


Picture 2b Message Box after exporting bitmap

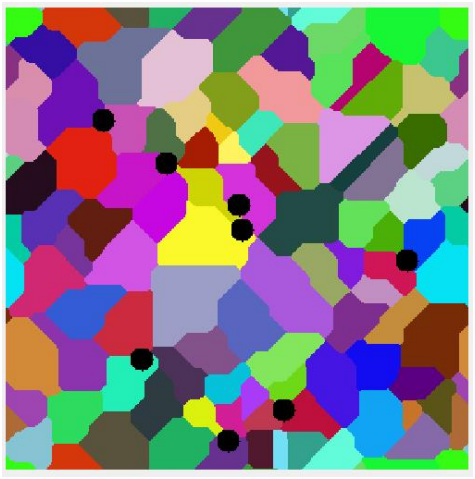


Picture 2c Place where bitmap was saved

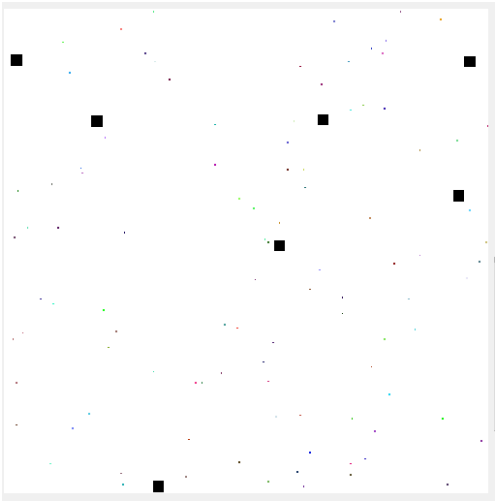
3. Possibility to add inclusions and choose type: circular with radious (set in InclusionsSizeUpDown filed) added on beginning of simulation (Picture 3a, 3b) or square with dimeter (Picture 4a, 4b). It is also possible to add circular (Picture 5a, 5b) or square (Picture 6a, 6b) inclusions after simulation. Inclusions are added on grain boundaries. User has also ability to set amount of inclusions (set in InclusionsUpDown field).



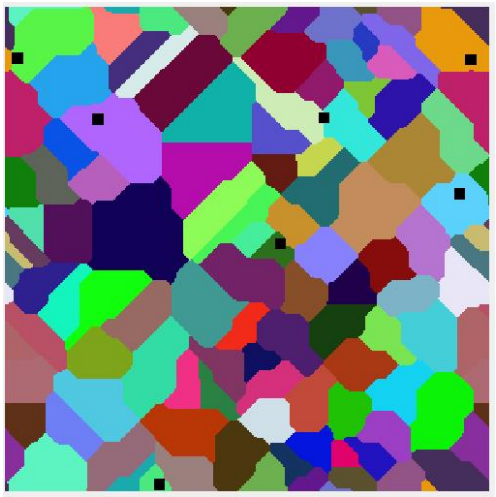
Picture 3a Circular inclusions before simulation



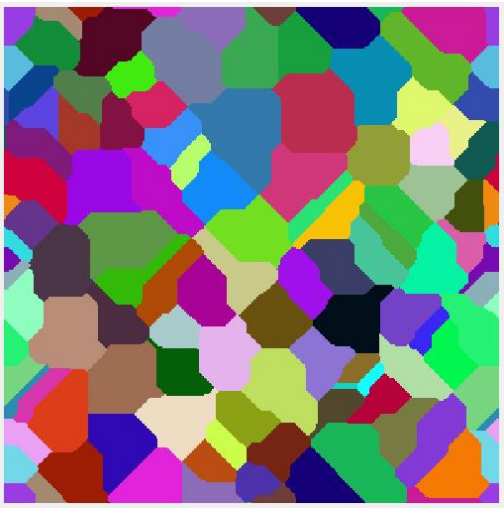
Picture 3b Structure after simulation (with circular inclusions)



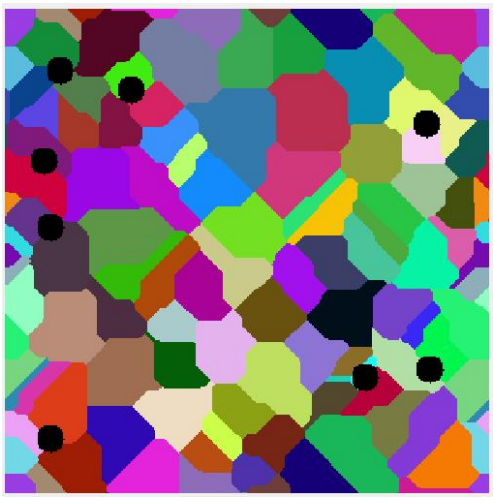
Picture 4a Square inclusions before simulation



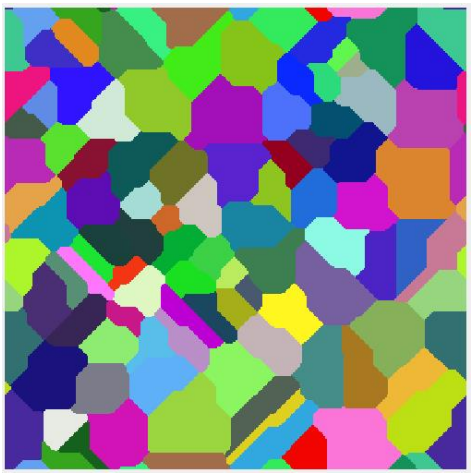
Picture 4b Structure after simulation (with square inclusions)



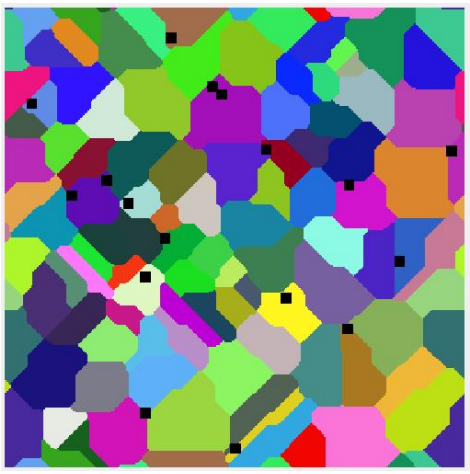
Picture 5a Structure after simulation without inclusions



Picture 5b Circular inclusions after simulation

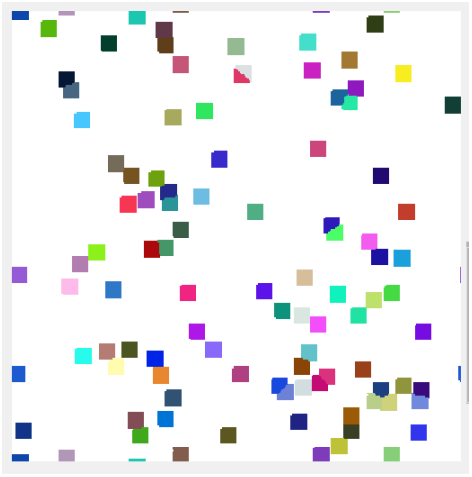


Picture 6a Structure after simulation without inclusions

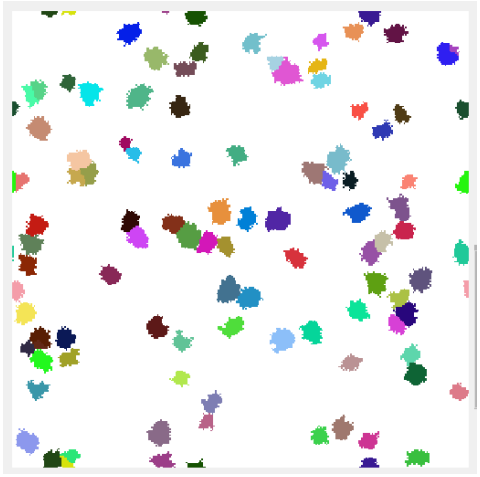


Picture 6b Square inclusions after simulation

4. Modification of CA grain growth algorithm - influence of grain curvature. Added 4 rules – the first for Moore neighbors (if five to eight of the cells neighbors id's is equal to S, then cell transforms to the state S), the second for nearest Moore neighbors (if three of the cells neighbors id's is equal to S, then cell transforms to the state S) and the third for further Moore neigbors (if three of the cells neighbors id's is equal to S, then cell transforms to the state S). The fourth rule determined by global probability of change and it was Moore neighborhoods. Probability influences shape which is more (Picture 7a) or less (Picture 7b) regular.



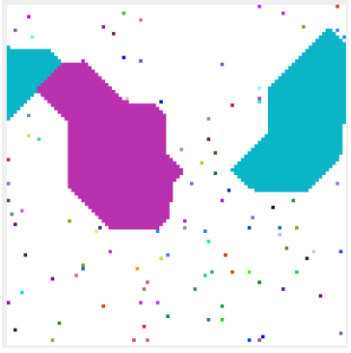
Picture 7a Grain growing with probability 90%



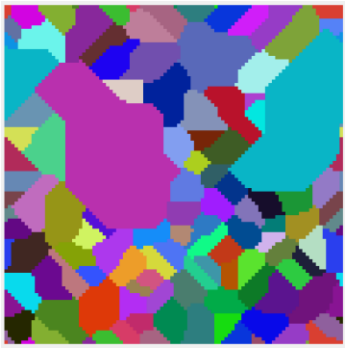
Picture 7b Grain growing with probability 10%

5. Added different microstructure type: substructure (Picture 8a, 8b, 8c) and dual phase (Picture 9a, 9b, 9c). It is possible to select grains (selected grains not growth in second simulations).

Picture 8a First grain growth

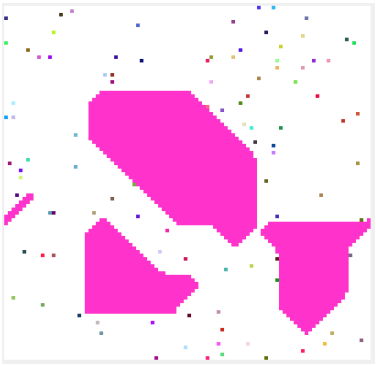


Picture 8b Selected grains (substructure)

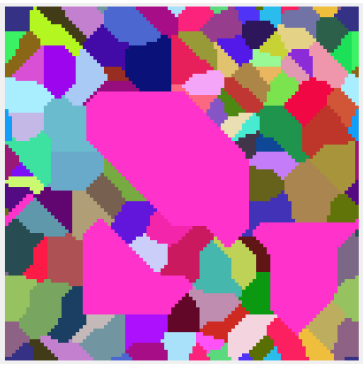


8c Second grain growth

Picture 9a First grain growth

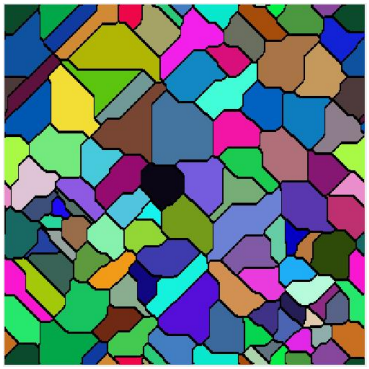


Picture 9b Selected grains (dual phase)

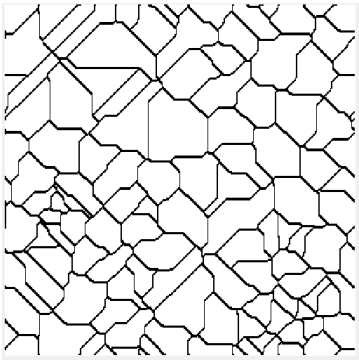


9c Second grain growth

6. Added grain boundary selection (Picture 10a, 10b, 10d, 10e) . It is possible to set size of GB and add boundary to selected grains. Moreover, the percentage of GB is calculated (Picture 10c, 10f).

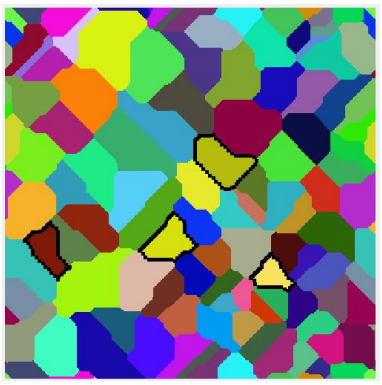


Picture 10a Boundaries (size=1) colored after grain growth

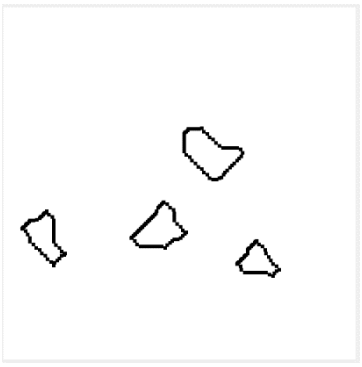


Picture 10b Boundaries after clearing space

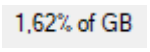
Picture 10c Percentage of GB



Picture 10d Boundaries of selected grains (size=3) colored after grain growth



Picture 10e Boundaries after clearing space

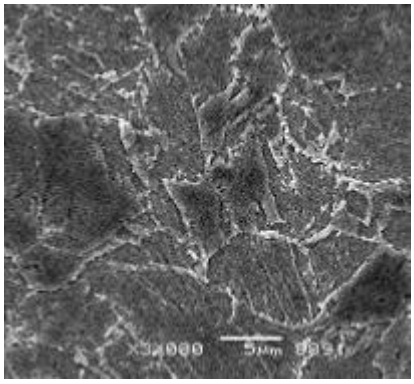


Picture 10f Percentage of GB

Conclusions:

A cellular automata is a collection of colored cells on a grid. It come in a variety of shapes and varieties depend of rules based on the states of neighboring cells. Those rules are applied iteratively for as many time steps as desired to fill the whole grid. It is possible to achieve different simulations and results by using various rules.

Thanks to CA simulation results are much more understandable as it is well visually represented. It is easier to understand grain growth, when it is possible to see simulation of it. There is the possibility to modeling microstructure of the materials by using CA simulation. It allows calculate properties of selected materials.



Picture 11a Microstructure of steel HSLA

Picture 11b Microstructure recived using Moore neigbourhood and grain boundary

Presented program can be used to simulate various grain growth in the microstructure. For example steel HSLA - high strength low alloy steel (Picture 11a) can be recived using Moore neighbourhood and grain boundary (Picture 11b). Both microstructures have sharp grain with clear boundaries of these grains.