Multiscale Modelling – Report no. 2

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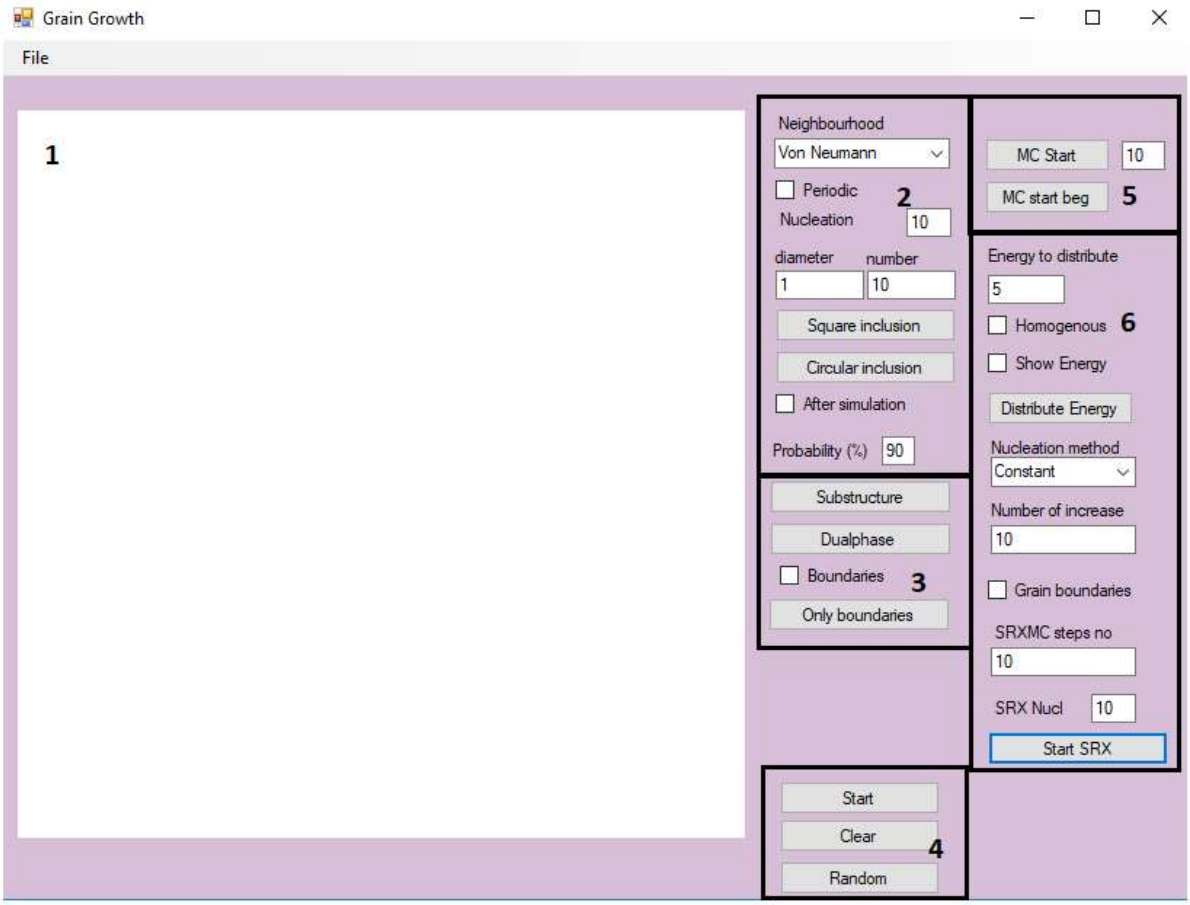
Second part of the semester was about further developing application using .NET Framework to simulate metallurgy processes running in the microstructures. It was written with C# language, UI was built with Windows Forms, and it contains standard Windows controls in order to provide intuitive usage. Work from first part of course ended with program which can present grain growth based on cellular automata algorithm. Second functionality added to application was Monte Carlo algorithm and recrystallization algorithm. I will try to present you briefly user interface and functionality of my program on screens and example results of grain growth.



Picture 1 – Main window of application

You can divide main window (Picture 1) of application to sections. Description of every section is below.

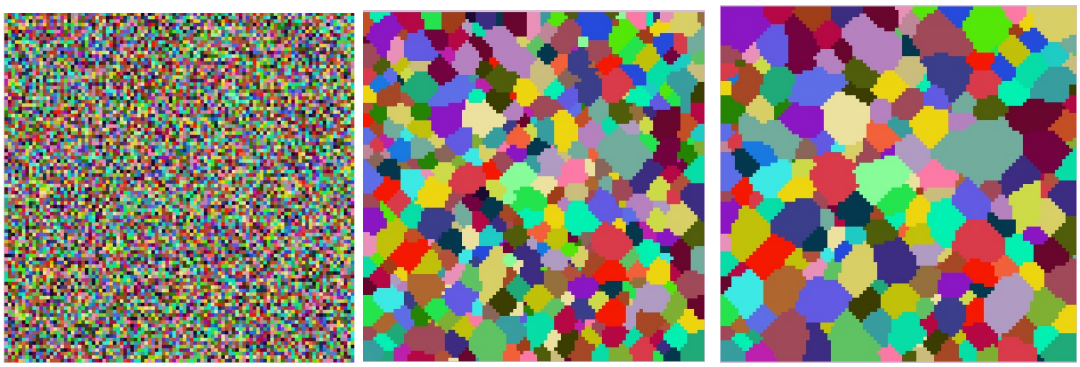
1. PictureBox which will be showing result of grain growth.
2. Part when you can adjust parameters of simulation. You can choose neighbourhood, type of boundary condition (periodic), nucleation, inclusion (and types of inclusions).
3. After every simulation you can choose between Substructure or Dualphase and Buttons to operate grains boundaries.
4. Buttons to start simulation, clear window and prepare seeds to grow.

5. Buttons to operate simulation using Monte Carlo method
6. Functionality connected with recrystallization

Examples are the best to show the functionality of application. In next part of this report, you can see screens of ended simulations.

First of all I will present Monte Carlo method. All simulations done before was based on cellular automata. There are examples of using Monte Carlo step by step, and combine with DP then cellular automata.

1) Monte Carlo algorithm with 50 ID, Moore neighbourhood



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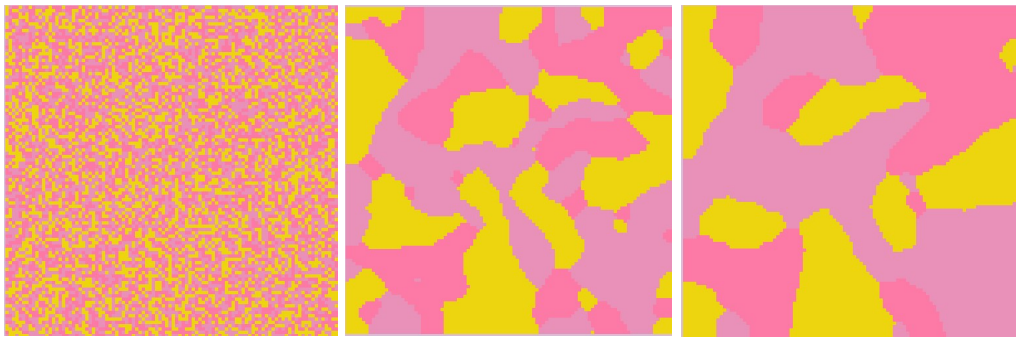
Picture 2 Monte carlo

As You can see on Picture no. 2 Monte Carlo Algorithm starts with 50 Nucleons distributed at all Picture Box, then You can see microstructure after 10 and 20 Steps.

2) Monte Carlo algorithm with 3 ID, Moore neighbourhood



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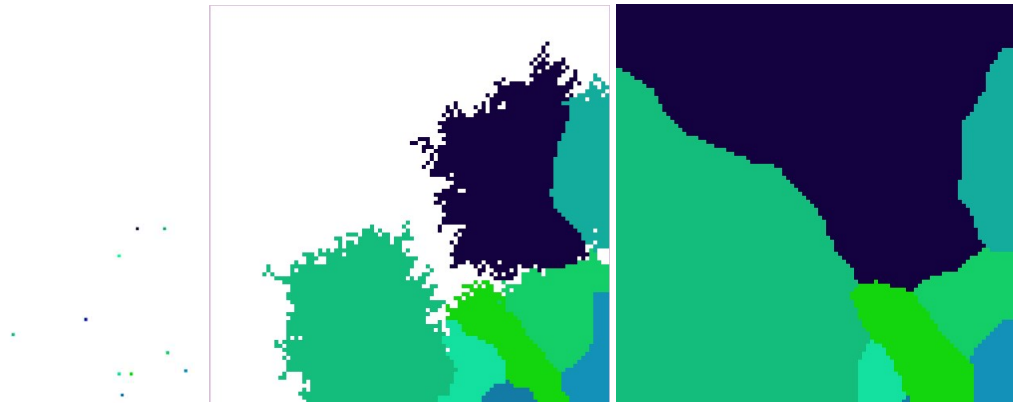
Picture 3 Monte Carlo

On the Picture 3 You can see microstructure generated with 3 different ID, and what happen after 10 or 20 Monte Carlo Steps.

3) Monte Carlo algorithm with 10 ID, Monte Carlo Grain growth, Moore Neighbourhood.



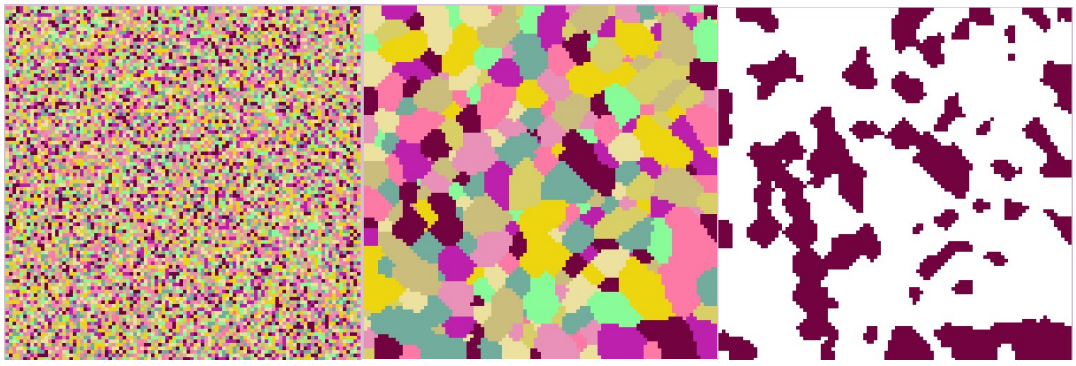
Picture 3 Monte Carlo algorithm from few nucleons

On the Picture 3 You can see Microstructure generated from beginning till end only with grain growth based on Monte Carlo algorithm.

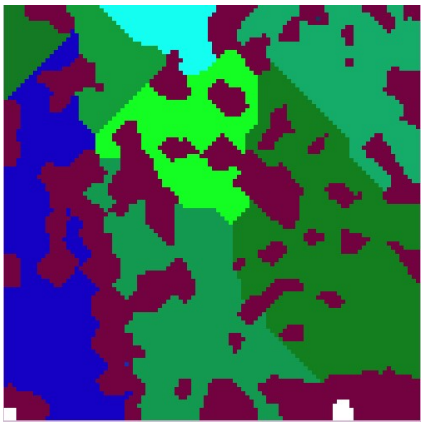
Now You can Use functionality from previous program – Dual phase. Click on it, mark grains and click one more time. You can now generate new microstructure with Cellular automata or Monte Carlo algorithm – see on Picture 4.

Picture 4 Dual phase and new microstructure

Another example on Picture number 5 :



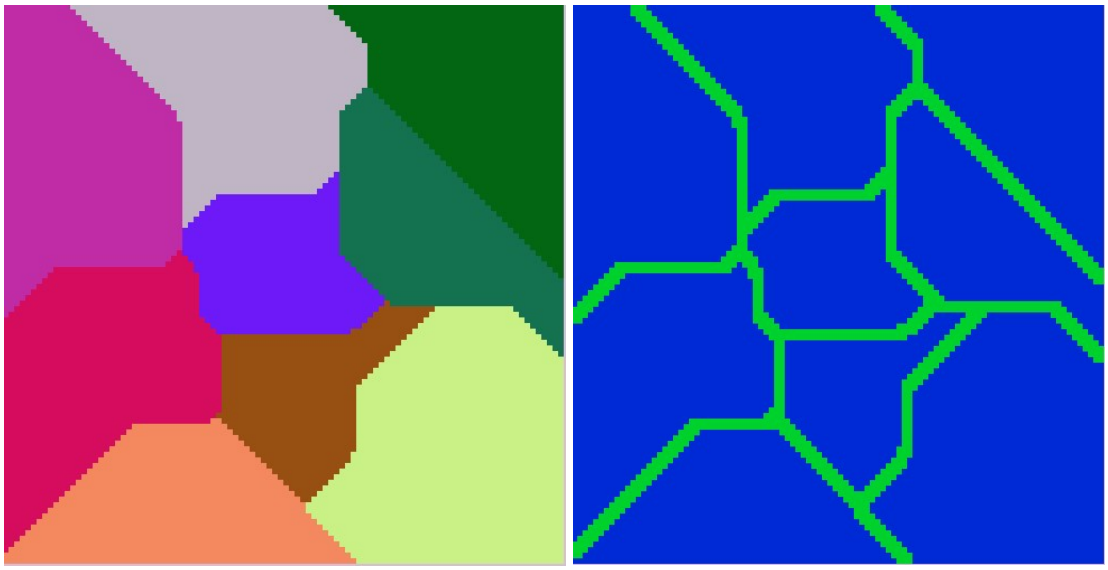
MC – 10 ID MC – 10 ID/ 10 STEPS Dual phase



CA grain growth after dual phase

Picture 5 Dualphase

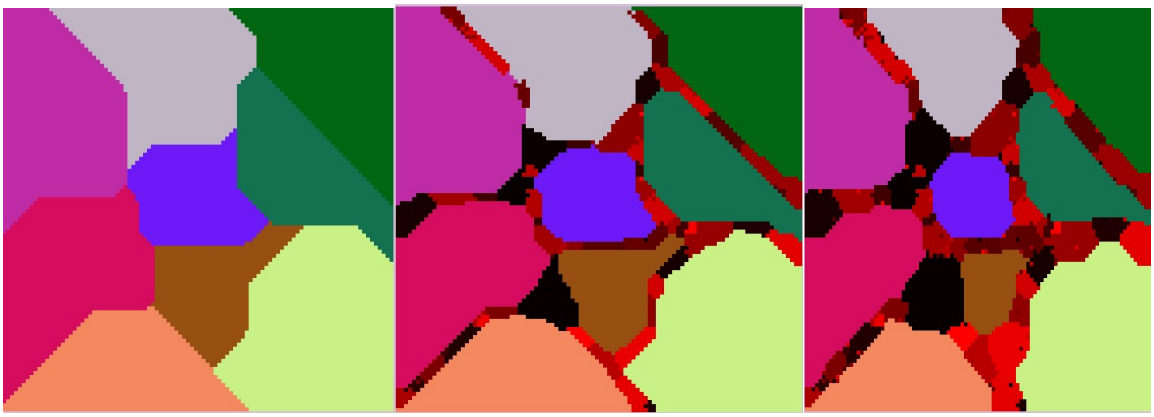
Recrystallization requires calculation of energy of lattice site surrounding elements of simulation. Level of energy to distribute can be set, also type of energy distribution can be selected from homogeneous and heterogeneous.



Picture 6 Preview of distributed energy

Picture 2 shows energy after distribution. Simulation where done with heterogeneous type of energy distribution. Blue color symbolized places with minimum amount of energy and green with maximum. Energy was stored near grain boundaries.

Now we can start recrystallization on grain boundaries with Constant nucleation = 10

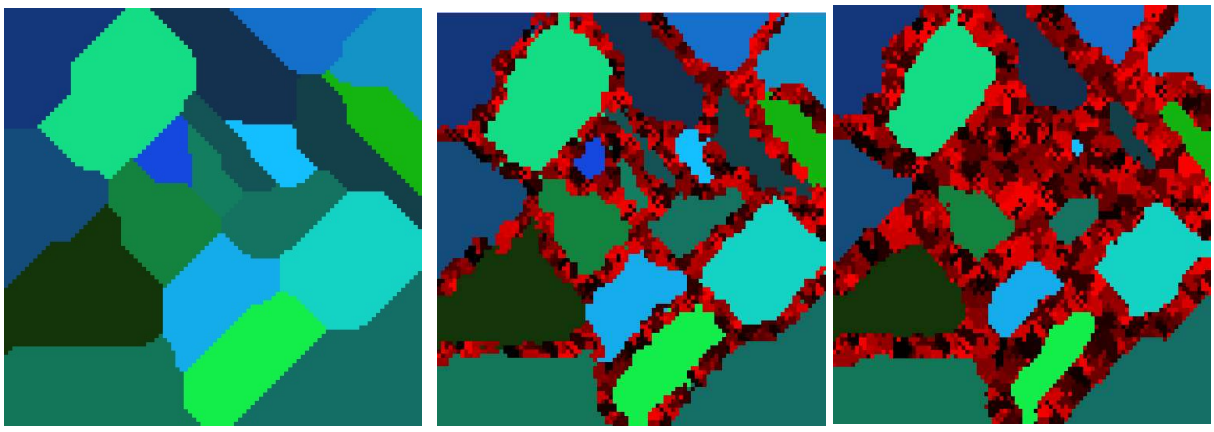


0 Steps 10 Steps 20 Steps

Picture 7 Constant Recrystallization

Picture No. 7 show us Recrystallization algorithm, first we have to calculate energy and distribute to each cell. After 20 steeps we can se that recrystallize only grains on boundaries.

Increasing method, 20 more nucleons at each step of SRX.

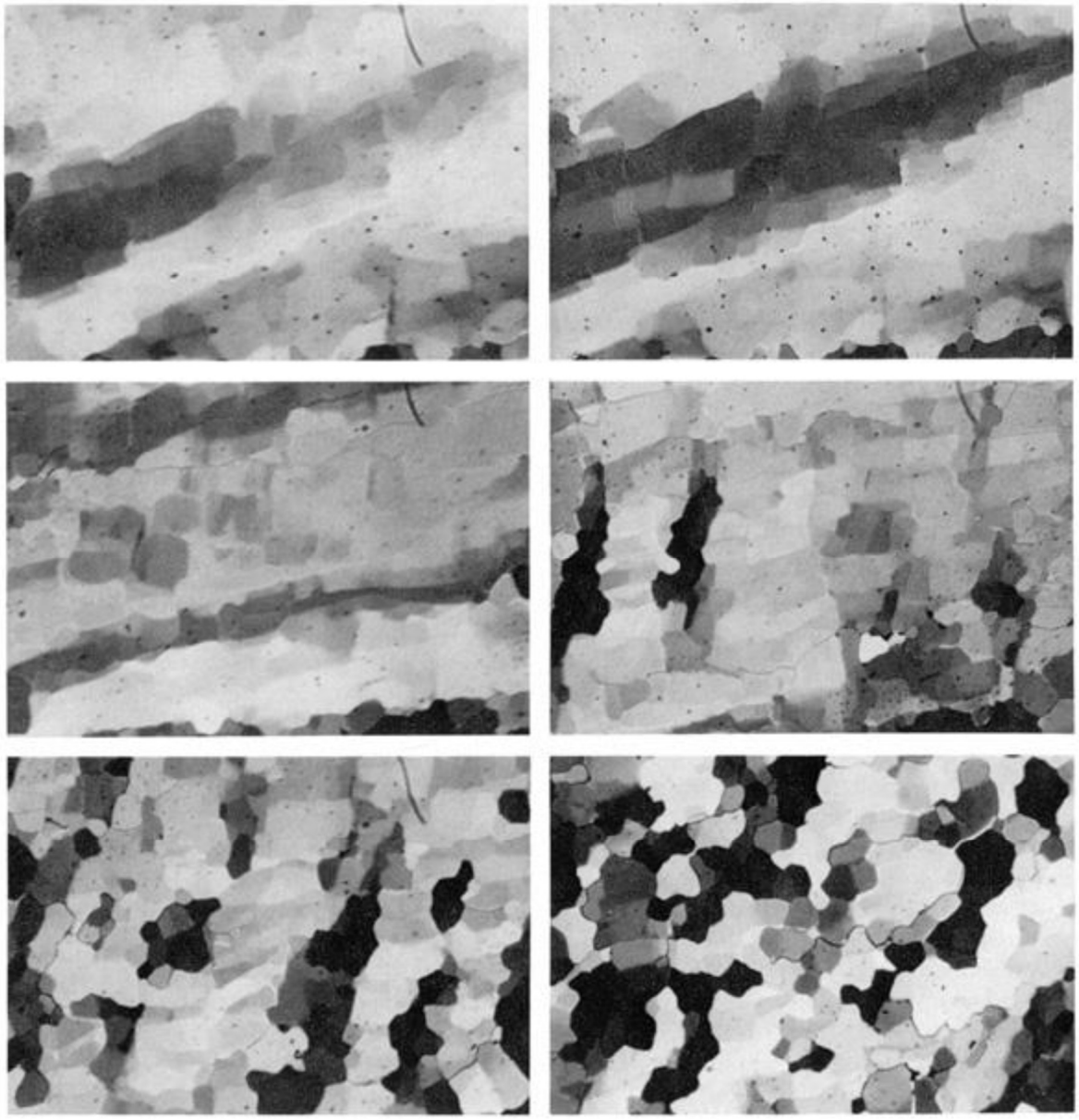


0 Steps 10 Steps 20 Steps

Picture 8 Increasing Recrystallization

Picture No. 8 show us Recrystallization algorithm, first we have to calculate energy and distribute to each cell. As You can see with Increasing method we recrystallize more cells than constant so that method is implemented correctly.

Picture no 9 show real recrystallization :



Picture 9 Real examples of recrystallization[1]

Transformations during static recrystallization presented on real microstructures is located on sixth picture. Initial and final steps of this mechanism can be linked with output presented at previous screens, especially with method using random nucleation. This report shows that nowadays multiscale modelling is very important area of material science. Result from my application are similar to real microstructures. Output can be better, but it costs a lot of time to develop software fulfilling industry requirements. For academic purposes this application fits correct. Certainly the development of this application is helpful to learn a lot about construction of materials.

[1] http://www.ged.rwth-aachen.de/Ww/projects/rexx/DruryUrai90Recrystallization/DruryUrai90DefMech5.htm