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MULTISCALE MODELLING

Grain growth project report, part II

Application for simple grains growth and recrystallization simulation (Fig. 1)

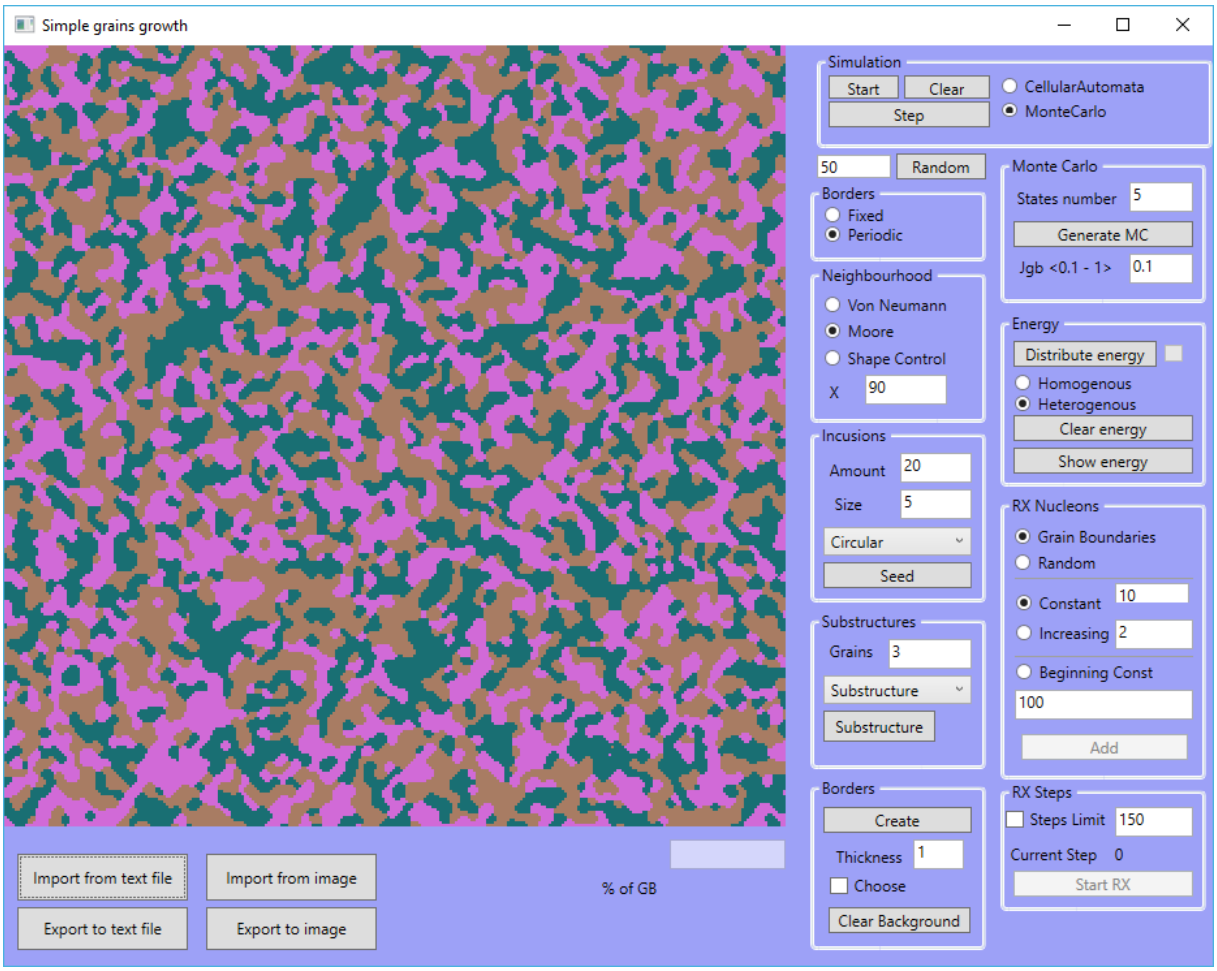

Figure 1. Grains growth application interface

Technologies used:

- .NET 4.7 - is a software framework developed by Microsoft that runs primarily on Microsoft Windows. It includes a large class library named Framework Class Library (FCL) and provides language interoperability (each language can use code written in other languages) across several programming languages.
- WPF - is a graphical subsystem by Microsoft for rendering user interfaces in Windows-based applications.
- C# - is a general-purpose, multi-paradigm programming language encompassing strong typing, imperative, declarative, functional, generic, object-oriented (class-based), and component-oriented programming disciplines.

The reason, why .NET technologies were used for this project, is ther simplicity, quick set-up and transparent API for high-level programming. WPF allows rapid development of desktop applications, and is supported with rich documentation.

Code available at: https://github.com/TMaj/MultiScaleGrainsGrowth

This program is intended to be used for simulating simple grains growth algorithm and recrystallization. It is based on cellular automata and Monte Carlo algorithm, and provides user with possibilities of adjusting simulation parameters such as boundaries, neighbourhood or inclusions. Features regarding Monte Carlo algorithm are listed below:

Application features

1. Monte Carlo area creation (Fig. 2)

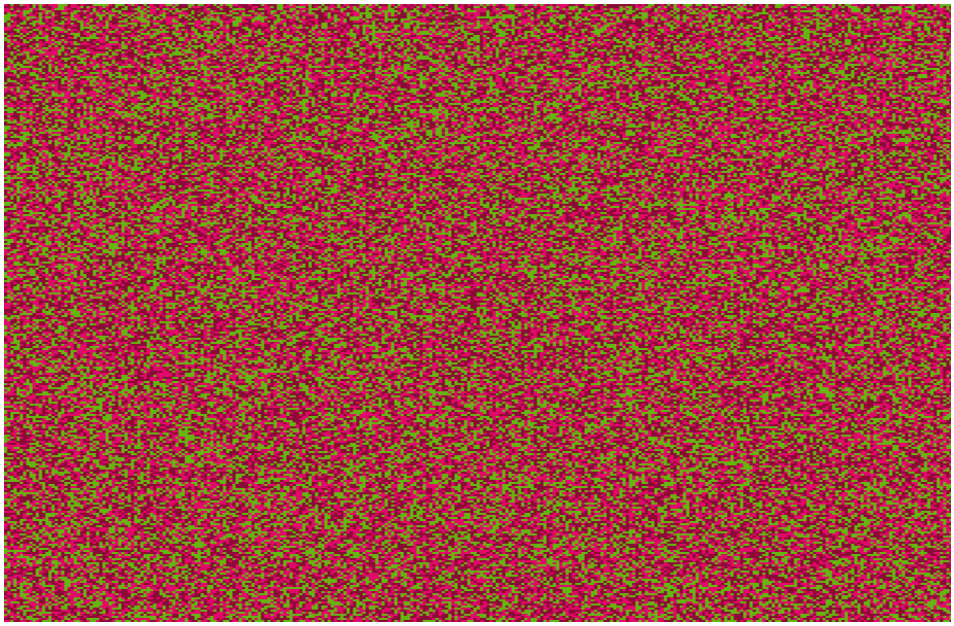

Figure 2. Randomly generated cells for MC simulation

2. Monte Carlo simulation (Fig. 3)

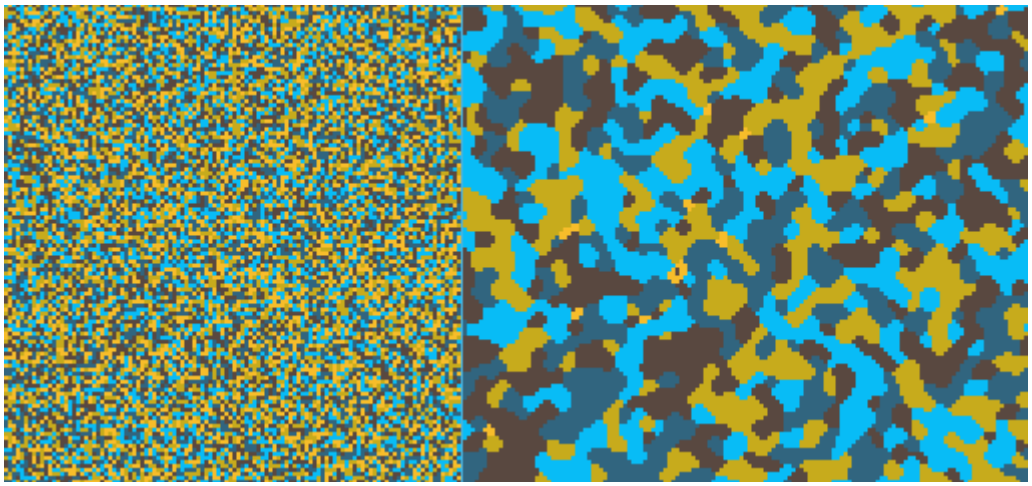

Figure 3. Monte Carlo simulation – before/after.

3. Dual – phase simulation

- *Monte Carlo substructure in Cellular Automata structure (Fig. 4)*

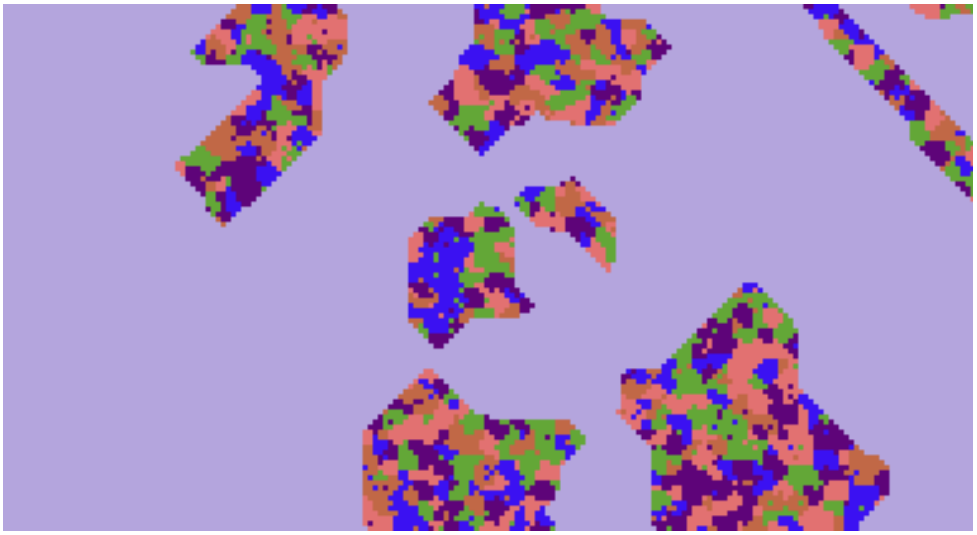

Figure 4.

- *Cellular Automata substructure in Monte Carlo structure (Fig. 5)*

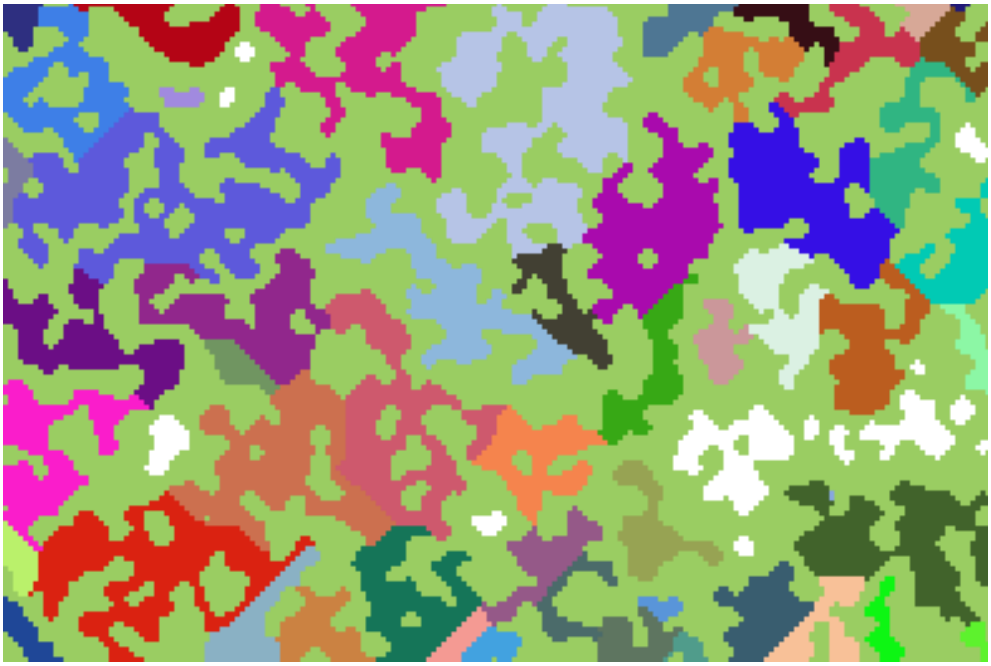

Figure 5.

4. Energy distribution

User can choose whether to apply heterogeneous (bigger energy on grain borders) or homogeneous energy distribution.

- *Heterogeneous energy distribution inclusions (Fig. 6)*

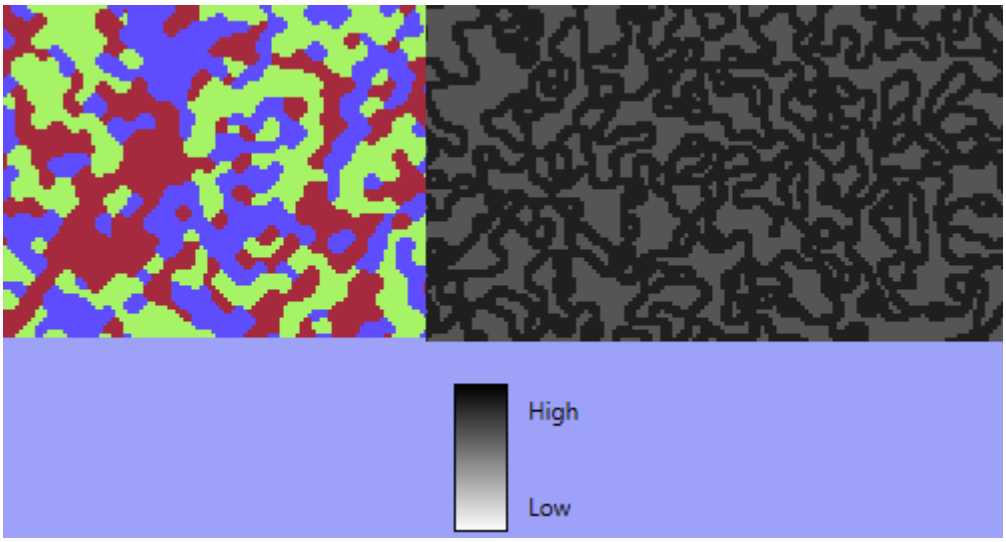

Figure 6.

- *Homogeneous energy distribution (Fig. 7)*

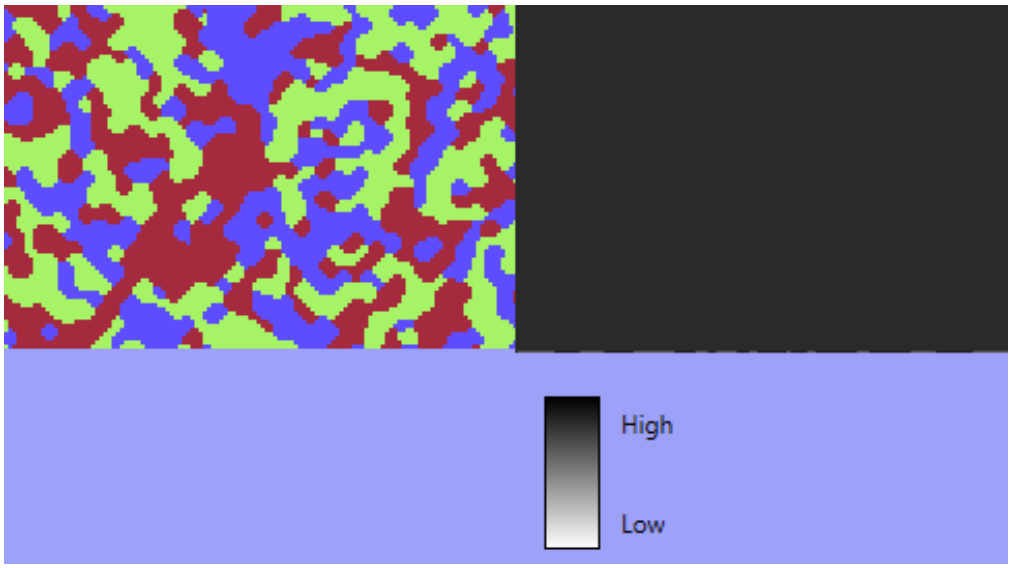

Figure 7.

5. Various nucleation modules

User can use three methods of generating new nucleons during each step of recrystallization, multiplied by two areas in which they shall appear (grain boundaries or random). Amount of new nucleons is configurable.

- *Constant at the beginning of simulation (Fig. 8)*

  In this method, new nucleons appear once, at the beginning of simulation.

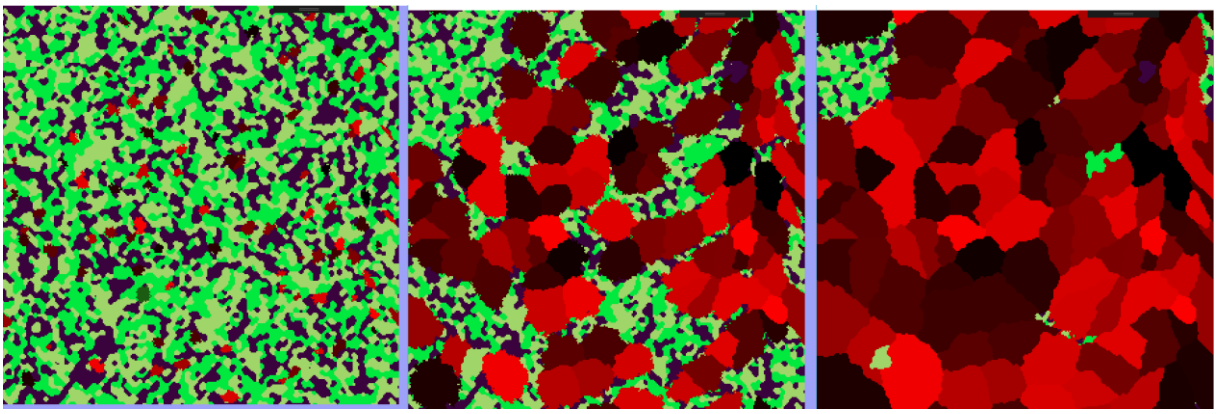

Figure 8. 100 nucleons at steps 5, 30, 60 of MC recrystallization (grain boundaries appearing).

- *Constant (Fig. 9)*

  This method creates fixed amount of nucleons at each step.

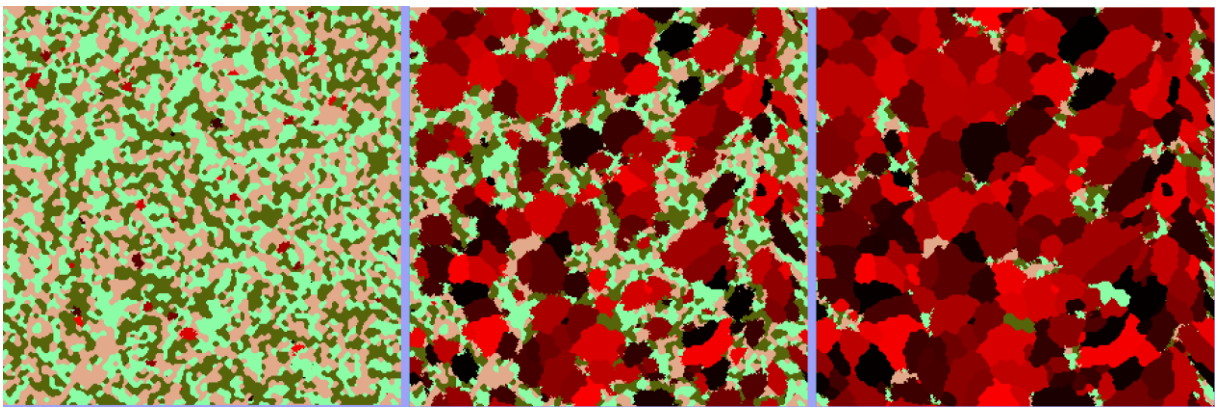

Figure 9. Constant appearing of five nucleons per step, at steps 5, 20, 40 of MC recrystallization (grain boundaries appearing).

- *Increasing (Fig. 10)*

  This method generates increased amount of nucleons at each step.

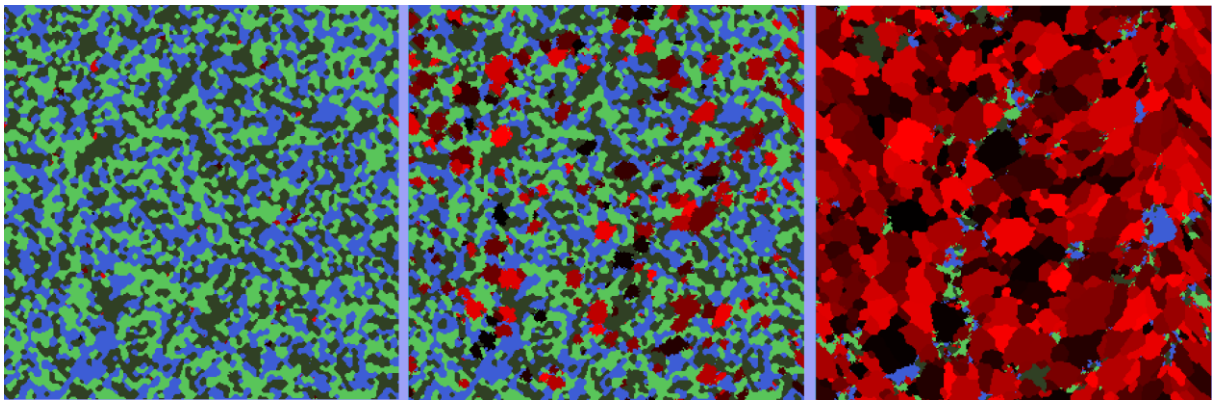

Figure 10. Increased appearing of two nucleons times step, at steps 5, 20, 40 of MC recrystallization (grain boundaries appearing).

6. Heterogeneous energy simulation

Examples presented above contain simulations with homogenous energy distribution. Example output with heterogeneous energy distribution is presented on Fig. 11. and Fig. 12.

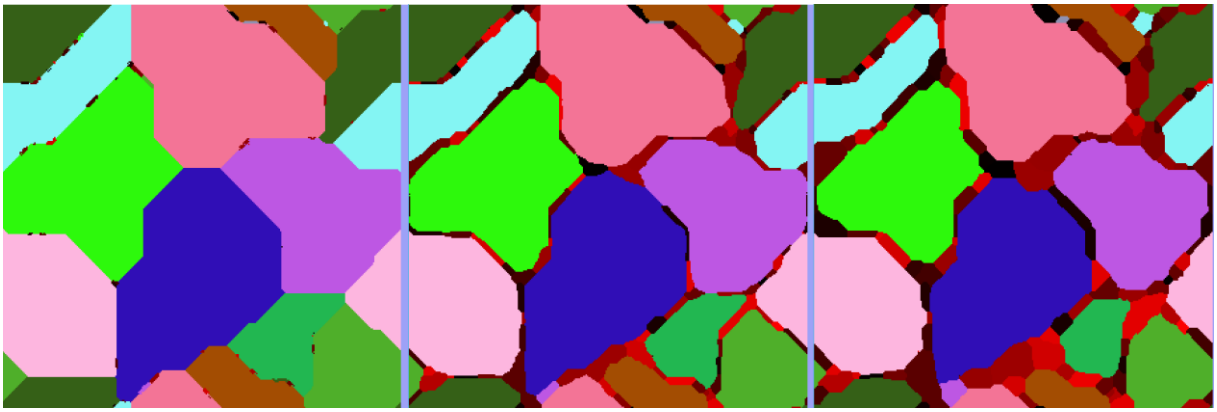

Figure 11. Constant appearing of five nucleons per step, at steps 20, 50, 100 of MC recrystallization (grain boundaries appearing)

Figure 12. Energy distribution after 100 steps of recrystallization (White field means 0 energy).

User Interface manual

User interface is presented on Fig. 13.

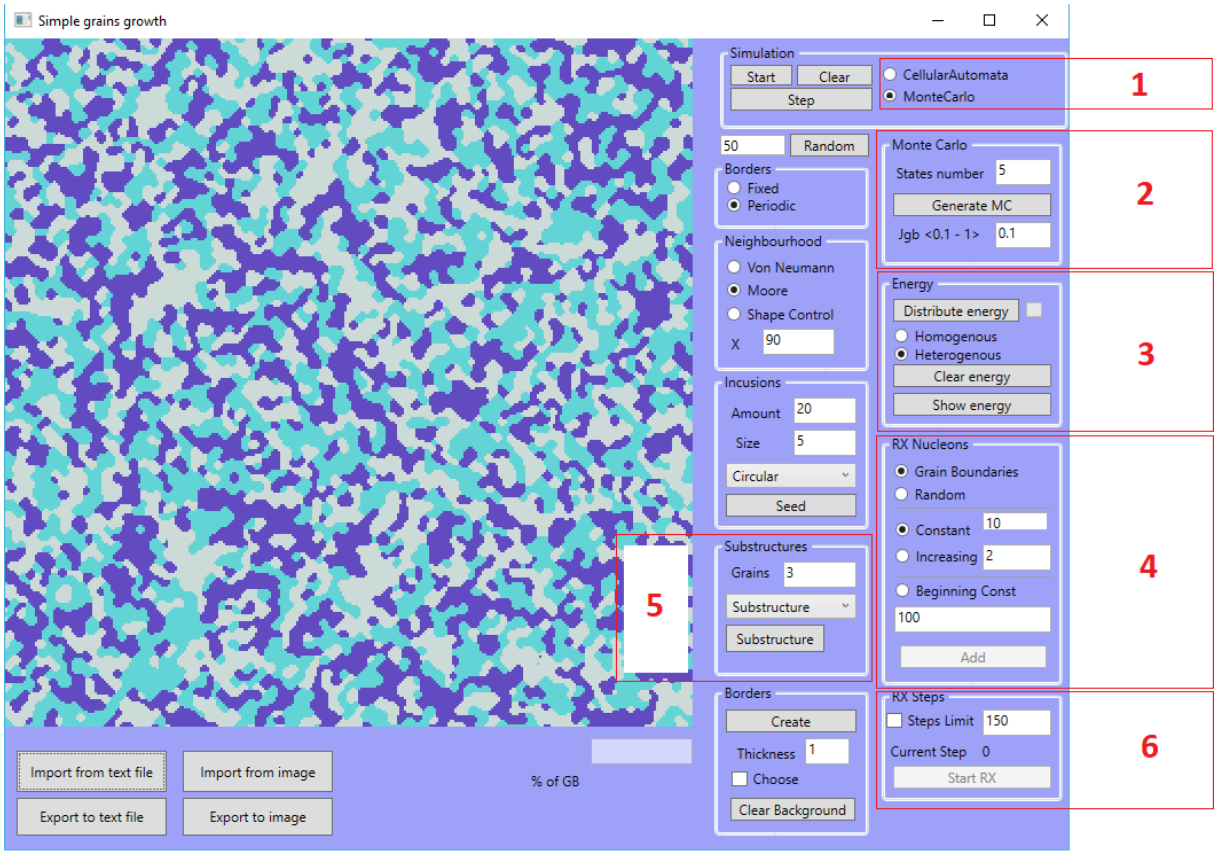

Figure 13. User interface.

1. User can choose between ***Cellular Automata*** or ***Monte Carlo*** simulation.
2. ***Monte Carlo*** group box allows to specify number of states present on simulation area **(*States number)*** and constant value ***Jgb*** describing grain boundary energy. Button ***Generate MC*** creates random MC simulation area on canvas.
3. Energy group box:
    a. ***Distribute energy*** button, distributes energy on simulation area in a way chosen with radio buttons below (***Homogenous*** or ***Heterogenous***). ***Checkbox*** placed next to button indicates whether energy was distributed.
    b. ***Clear Energy*** button removes previously assigned energy values.
    c. ***Show Energy*** button toggles view of canvas from normal to energy view with energy scale (Fig. 14.)

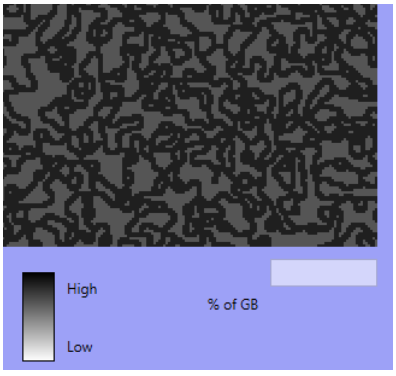

Figure 14.

4. ***RX Nucleons*** group box displays options used for recrystallization phase nucleation.
    a. ***Grain boundaries*** or ***Random*** options specify areas in which new nucleons will appear.
    b. ***Constant, Increasing*** or ***Beginning Const*** specify method and amount of spawning new nucleons (as presented in chapter 5.)
    c. ***Add*** button adds nucleons to simulation area when ***Beginning Const*** option is chosen.
5. ***Substructures*** specifies how many grains should be used to create substructure or dual phase (this is determined by combo box).
    a. Button ***Substructure*** generates substructure.
6. ***RX Steps*** group box allows to set recrystallization steps limit.
    a. Button ***Start RX*** starts and stops recrystallization process.

Comparison of simulation results and real material

The purpose of grains growth simulation is to predict phenomenons occuring in real materials. After proper adjustment of simulation parameters, it is possible to generate structure which is quite similar to real material, for example statically recrystallized steel.

Attempts of re-creating real substance was aimed at S405 steel (Composition presented in table 1.) This material was cooled from 1200ºC to 1000ºC. The recrystallization occurred during time needed to cool material.

C	Mn	Si	P	S	Ni	Cr	Ti	Mo	Al
0,11	1,97	0,95	0,022	0,006	–	–	0,120	0,22	0,025

Table 1. Chemical composition of steel S405

First structure to recreate was mentioned steel after 0,13 seconds of recrystallization (Fig. 15.).

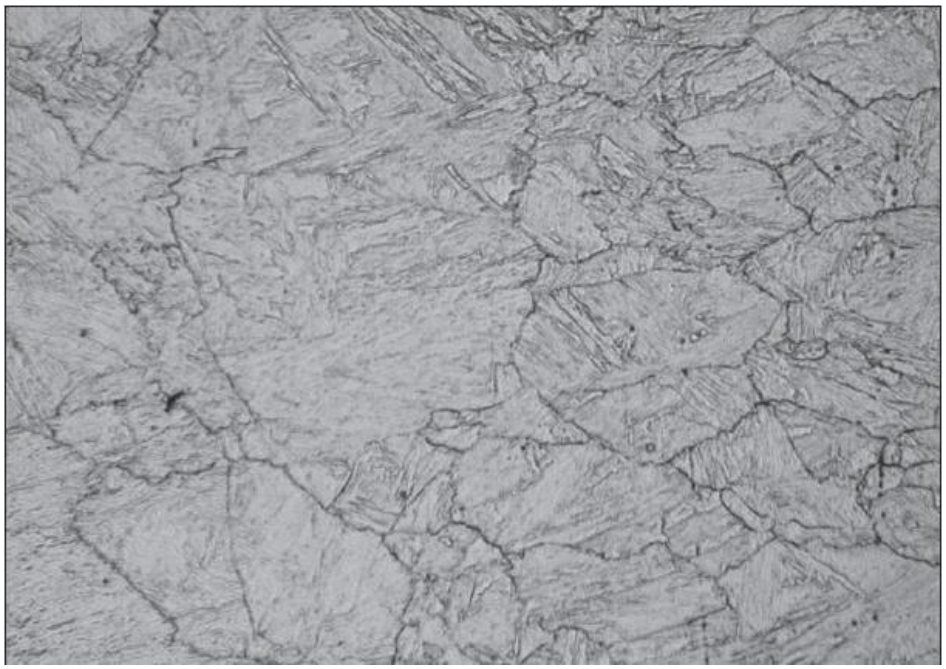

Figure 15. S405 after 0,13 seconds of recrystallization

To recreate material at this state, the best result was achieved after using 50 random nucleons, and performing Cellular Automata Moore Neighbourhood simulation (Fig. 16).

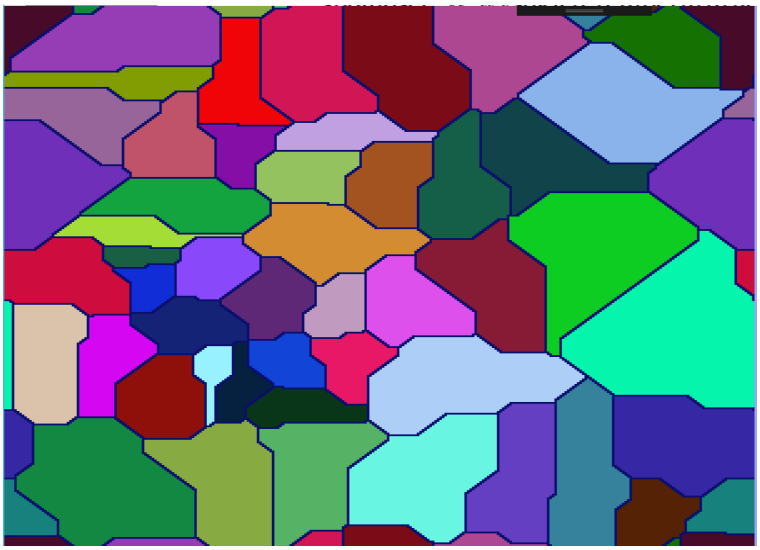

Figure 16.

This configuration managed to achieve similar grains shape and size. It did succeed to recreate smaller grains cumulated at several spots. Overall, the created image seems to be quite accurate attempt of simulating this kind of material.

Second material was same steel after 2,9 seconds of recrystallization (Fig. 17).

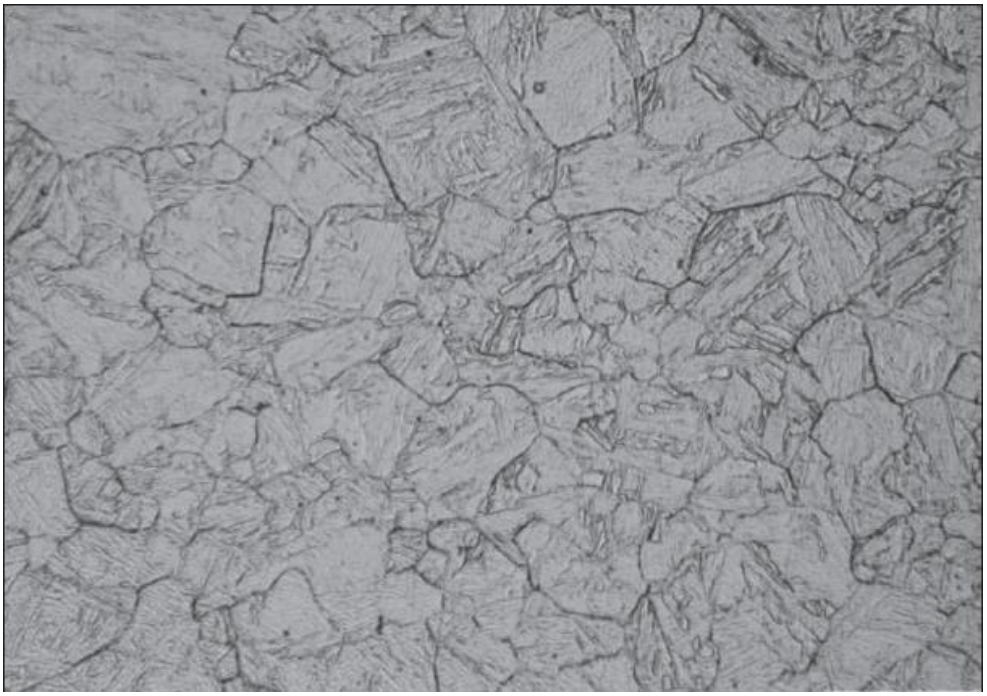

Figure 17. S405 after 2,9 seconds of recrystallization

To create this material by simulation, several steps were made. Firstly, 600 nucleons were chosen and grown (extended Moore neighbourhood, X = 50%). Then, homogenous energy was distributed and increased nucleation module was set (nucleons amount = 2). Final result appeared after 50 steps of recrystallization (Fig. 18).

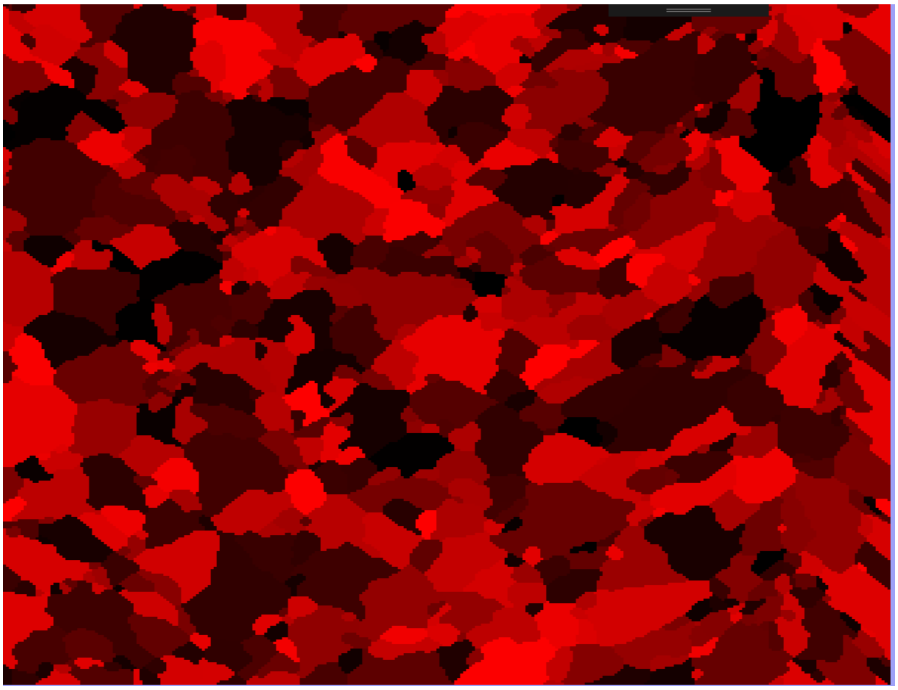

Figure 18.. Second simulation result.

The result seems to imitate real structure quite accurately.

The last re-created material was S405 steel after 45 seconds of recrystallization. (Fig. 19)

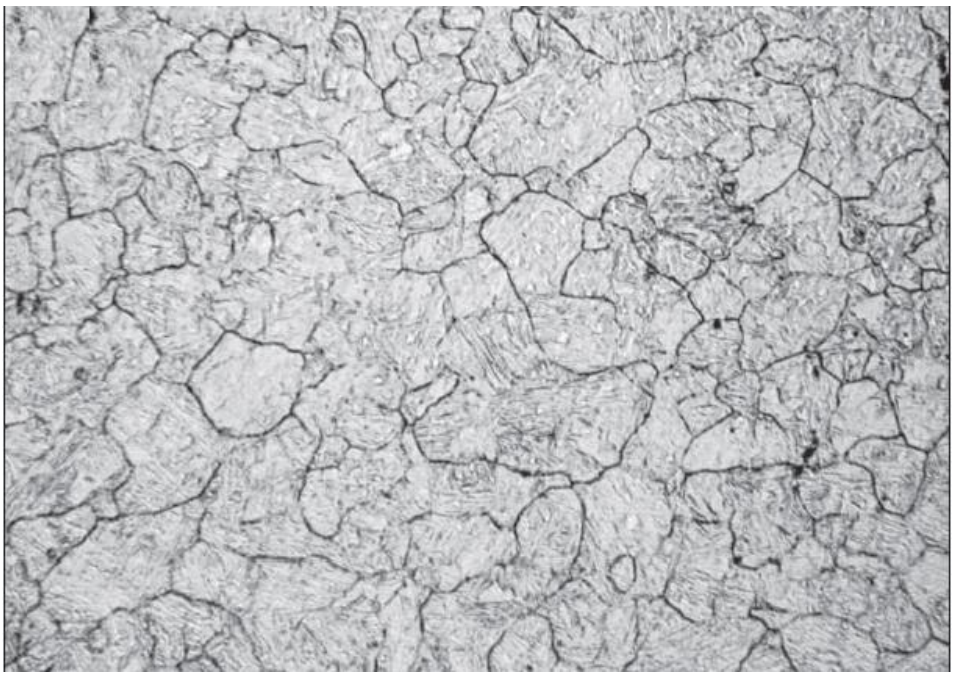

Figure 19. S405 after 45 seconds of recrystallization

Simulation was conducted with growing 800 nucleons (extended Moore neighbourhood, X = 50%), then (Fig. 28). Then, homogenous energy was distributed and constant at beggining nucleation module was set (nucleons amount = 300). Final result appeared after 60 steps of recrystallization (Fig. 20).

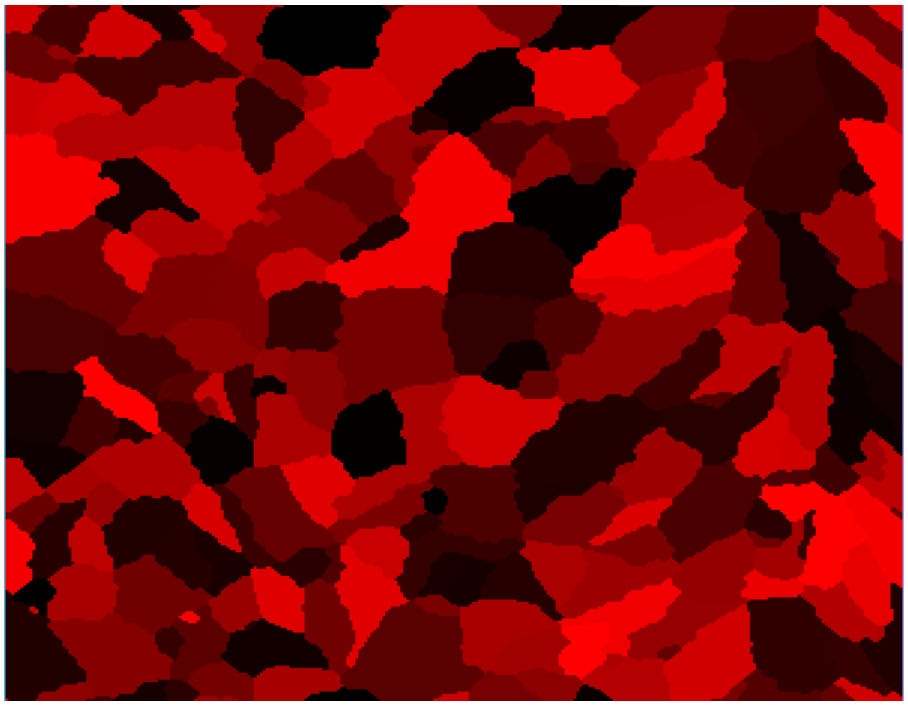

Figure 20. Third simulation result.

This attempt also properly imitates small structures of this recrystallized steel.

Sources:

S405 steeel:

Valeriy PIDVYSOTS'KYY, Roman KUZIAK, Prace Instytutu Metalurgii Żelaza nr 2/2016, tom 68, *ANALIZA KINETYKI REKRYSTALIZACJI PO ODKSZTAŁCENIU ZA POMOCĄ METODY RELAKSACJI NAPRĘŻENIA*