Second Report

Multiscale Modeling, Maria Krauz

User interface

Presented on the figure 1 user interface contains all updates performed during the whole process of system creation. User can choose between two methods used for microstructure generation, which are Cellular Automata and Monte Carlo.

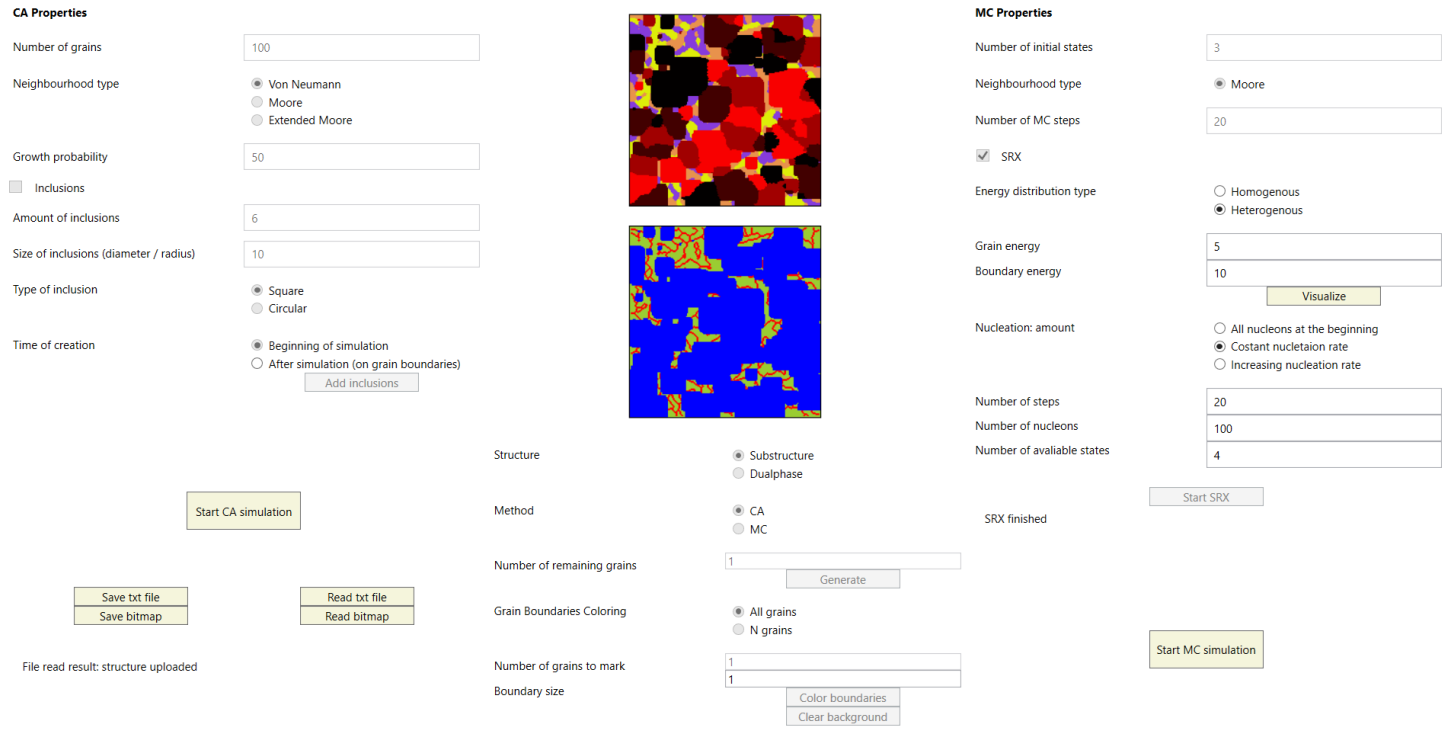

Fig 1: User interface

MC parameters

Basic parameters which user provides are *number of states* and *number of MC steps*. For this method the *Moore neighbourhood type* is a default one for the grain growth process. By pressing the *Start MC simulation* button user can start the process of grains growing. The growth process is carried out in accordance with assumptions of MC method. The resulting structures obtained after each MC step are displayed so the user can see how the whole process is performed.

The following illustrations shows resulted structures processed accordingly to the certain parameters configuration. Structures presented on figures 2 and 3 are the basic onces obtained respectively for the following configurations: CA method, number of grains: 100, neighbourhood type: Von Neumann and MC method, number of states: 3, number of steps: 30.

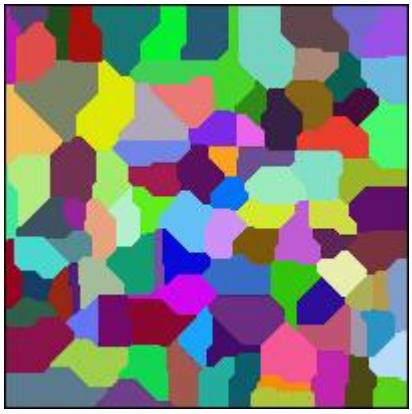

Fig 3: Base structure generated with CA method

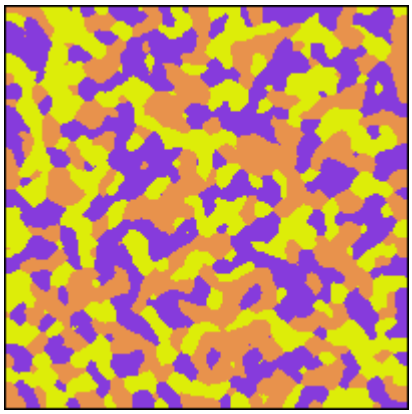

Fig 2: Base structure generated with MC method

Advanced DP

When structure generation (based on MC or CA method) is finished user can choose parameters of its modification. The dual phase structure can be generated using CA or MC method. User can also specify number of remaining grains, which will become a second phase in resulted structure. After pressing *Generate* button, user obtains the resulted structre on which he can observe new grains and the sacond phase corresponding to several grains of the base structure.

Figures 4-7 presents dual phase structures generated as a modifications of based structures presented on figures 2 and 3. The following values of individual parameters of structure modification were set: Fig. 4 – remaining grains: 10, CA method, number of grains: 300, neighbourhood type: Von Neumann, Fig. 5 - remaining grains: 10, MC method, number of states: 3, number of steps: 20, Fig. 6 - remaining grains: 1, CA method, number of grains: 300, neighbourhood type: Von Neumann, Fig. 7 - remaining grains: 1, MC method, number of states: 3, number of steps: 20.

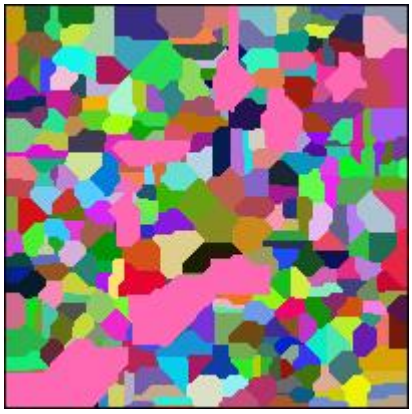

Fig 4: CA-CA

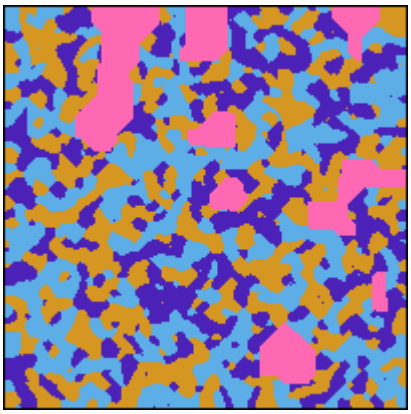

Fig 5: CA-MC

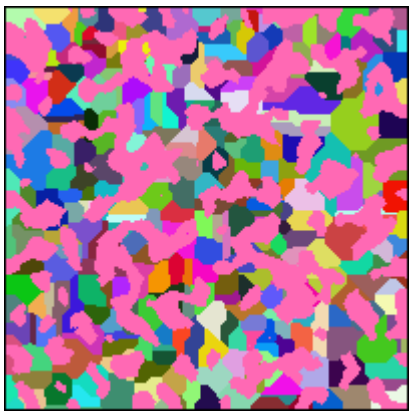

Fig 6: MC-CA

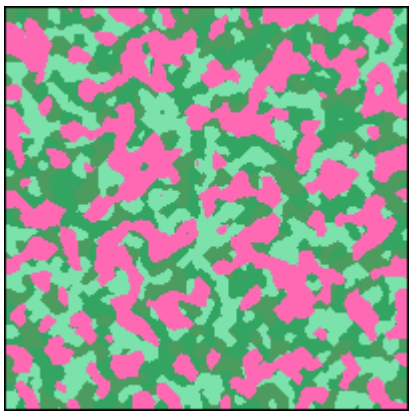

Fig 7: MC-MC

Monte Carlo SRX – Static Recrystallization

- Energy distribution

Energy distribution can be vizualized on the previously generated structure. User can choose if energy distribution is *homogenous* or *heterogenous* an provide such information as *grain energy* and *boundary energy*. After pressing *Vizualize* button, the figure presenting energy distribution is displayed. Figures 8-11 presents respectively homogenous and heterogenous energy distribution of structures presented on figures 2 and 3. To vizualize energy three colors were used: blue – represents zero energy in cell, green – one to five energy rate and red – higher energy.

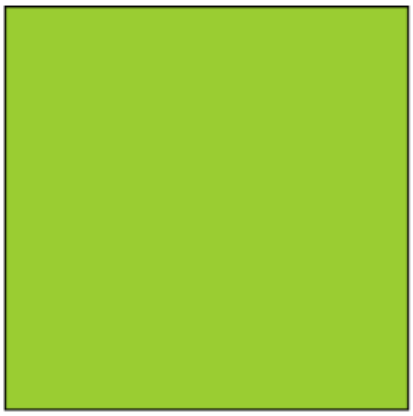

Fig 8: Homogenous energy distribution generated for first base microstructure

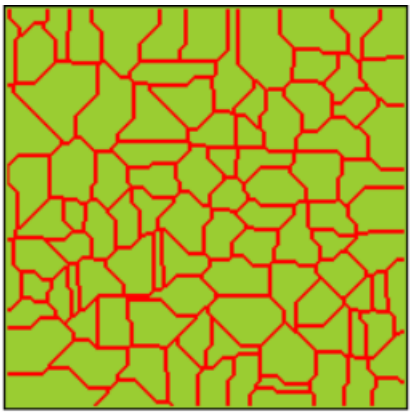

Fig 9: Heterogenous energy distribution generated for first base microstructure

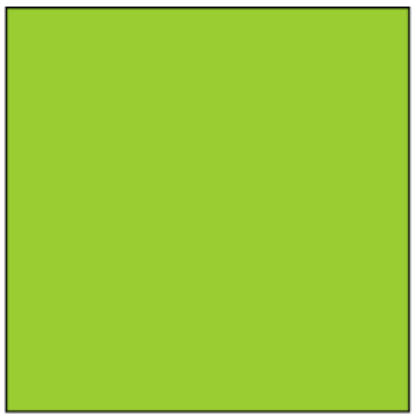

Fig 10: Homogenous energy distribution generated for second base microstructure

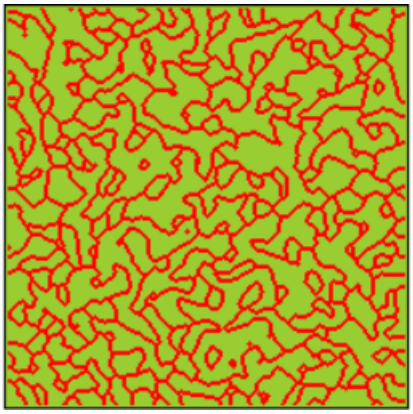

Fig 11: Heterogenous energy distribution generated for second base microstructure

- Nucleation

Nucleation phase starts after user press the *Start SRX* button. New grains can appear in places int the microstructure where the energy is higher. If the homogenous energy distribution was choosen, as the energy rate is constant in the whole structure, nucleons can appear anywhere. In case of hererogenous energy distribution, nucleons can be observed on the grains boundaries where the energy is the highest. User can choose between three types of nucleons distribution in time: adding all of them at the beginning of simulation, through all the process with constant nucleation rate or with increasing nucleation rate. What is more, user can also define *number of nucleons* and *number of avaliable grains states*. New, recrystallized grains are visualized in the red color to make it easier to differ them from the non-recrystallized onces.

- Growth

In every simulation step, after nucleation phase, the growth phase occur. The growth process is performed accordingly to MC assumptions, using modifications to take into account a new parameter that tells whether grains cell have already been recrystallized. User can provide the *number of MC simulation steps*. This parameter is also used to calculate ammount of nucleons which should be added in the particular steps. Each step result is visualized on the microstructure image and energy image.

Following figures 12-17 presents resulted microstructures (a), and visualization of resulted energy distributions (b), generated for the second base microstructure [Fig. 3] for different energy distribution types and with individual SRX simulation parameters.

Fig. 12 – homogenous energy distribution, number of MC steps: 20, all nucleons at the beginning of simulation, number of nucleons: 100, number of states: 4, Fig. 13 - heterogenous energy distribution, number of MC steps: 20, all nucleons at the beginning of simulation, number of nucleons: 100, number of states: 4, Fig. 14 - heterogenous energy distribution, number of MC steps: 20, constant nucleation rate, number of nucleons: 100, number of states: 4, Fig. 15 - heterogenous energy distribution, number of MC steps: 20, increasing nucleation rate, number of nucleons: 100, number of states: 4, Fig. 16 - heterogenous energy distribution, number of MC steps: 40, constant nucleation rate, number of nucleons: 100, number of states: 4, Fig. 17 - heterogenous energy distribution, number of MC steps: 60, constant nucleation rate, number of nucleons: 100, number of states: 4.

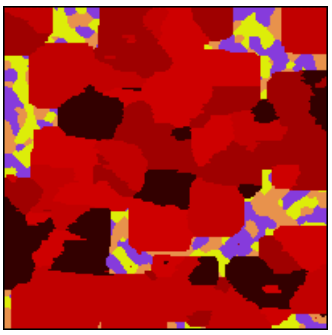

Fig 12.a: Structure image

Fig 12.b: Energy distribution

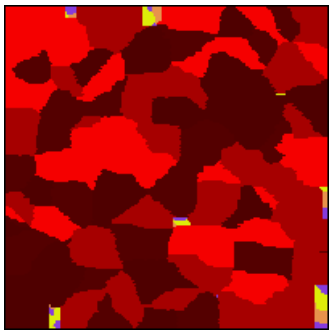

Fig 13.a: Structure image

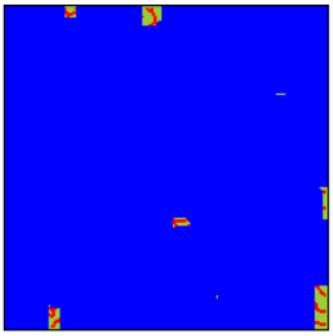

Fig 13.b: Energy distribution

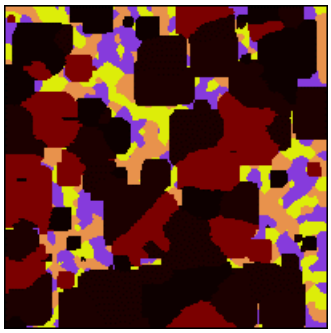

Fig 14.a: Structure image

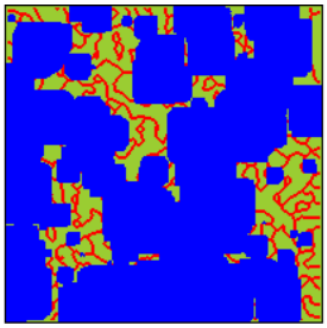

Fig 14.b: Energy distribution

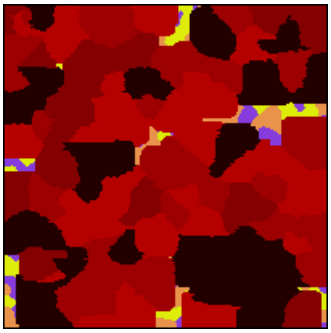

Fig 15.a: Structure image

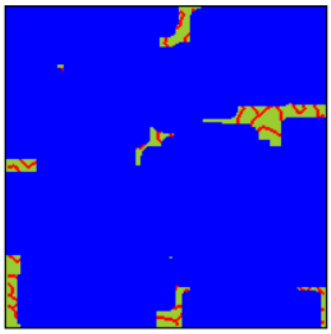

Fig 15.b: Energy distribution

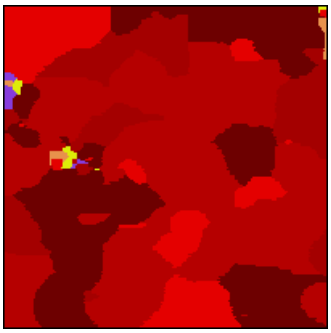

Fig 16.a: Structure image

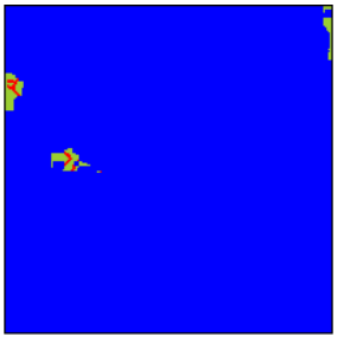

Fig 16.b: Energy distribution

Fig 17.a: Structure image

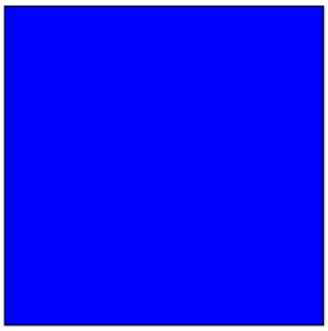

Fig 17.b: Energy distribution

Comparing structures presented on figures 13-15, the impact of nucleons distribution in time can be observed on the resulted structures. If all nucleons are distributed at the beginning of simulation, on the resulted structure we can see that recrystallized grains have similar size. In case of adding new nucleons during the next steps, the size of recrystallized grains is significantly different. Also, for those simulations 20 steps was not enough to obtain fully recrystallized structure. The dependence of resulting structure on the number of simulation steps can be seen by following the changes shown in figures 14, 16 and 17. Increasing the number of simulation steps to 60, for the specified parameters, was enough for the structure to be completely restructured.

Technology

This project is a continuation of already existing one. To create the application the C# programming language was used. The user interface was based on WPF Form. This technology is absolutely sufficient for this type of applications and allowed the author of this paper to create fully interactive user interface, as well as transparent implementation of algorithms.

Real structures

Comparing generated microstructures to the real onces it can be observed that they are just an approximation. Although, the structure generated with MC method (presented on Fig. 18) is more similar to the real one (presented on Fig. 19 [1]) than the structutre generated with CA metod (which can be seen in the first report), it is still the approximation. The same can be observed regarding dual phase microstructure (generated is presented on Fig. 20, real one on Fig. 21 [2]). When it comes to the recrystallization, the whole structure is rebulid to minimalize material internal energy. However, the grains can also have different sizes and forms, which can be seen on Fig. 23 [3] and have been imitated on Fig. 22. This occurs due to the fact that this process can took the process can take different time and run at different speeds.

1 https://www.phase-trans.msm.cam.ac.uk/2008/Steel_Microstructure/SM.html, 11.12.2018
2 https://www.worldautosteel.org/steel-basics/steel-types/dual-phase-dp-steels/, 11.12.2018
3 https://www.researchgate.net/figure/Optical-microstructures-annealed-at-a-250-C-b-300-C-c-350-C-and-d-400-C-for_fig10_259173367, 11.12.2018

Microstructure

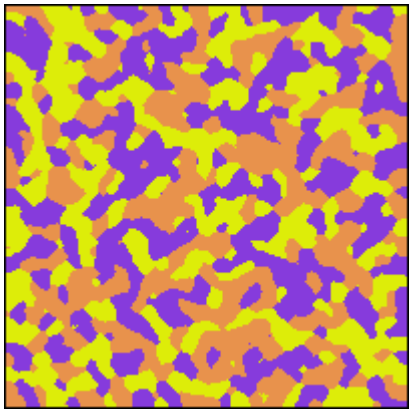

Fig 18: Generated microstructure

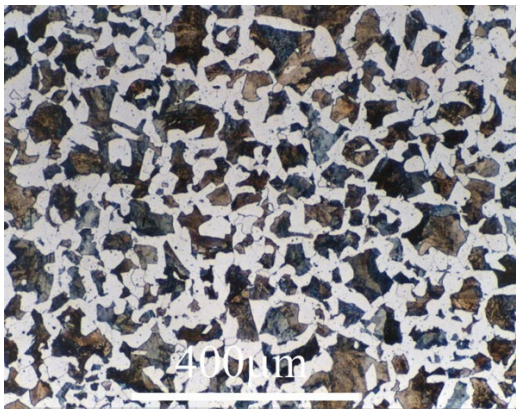

Fig 19: Allotriomorphic ferrite in a Fe-0.4C steel

Dual-phase

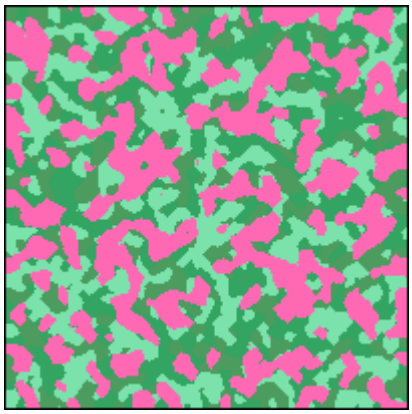

Fig 20: Generated dual phase microstructure

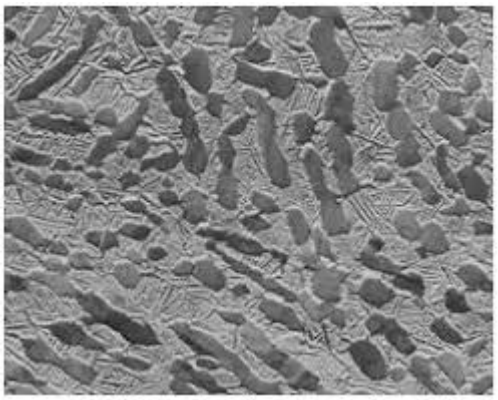

Fig 21: Photomicrograph of DP steel

Microstructure after static recrystalization

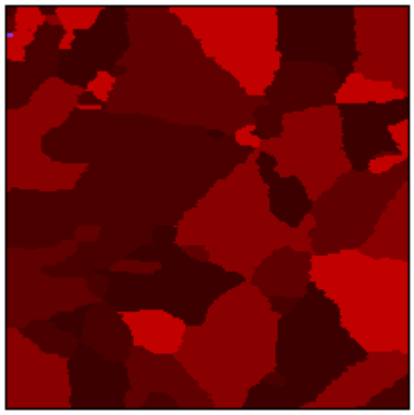

Fig 22: Generated structure after SRX

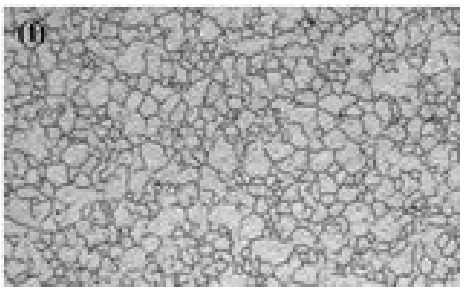

Fig 23: Static recrystallization and grain growth during annealing of an extruded Mg–Zn–Zr–Er magnesium alloy