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IM. STANISŁAWA STASZICA W KRAKOWIE

Wydział Inżynierii Metali i Informatyki Przemysłowej

MULTISCALE MODELING

„Report II”

Name and surname of the student: **Michał Pożarlik**

Signature of the student: Signature of the reviewer:

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1. Technology

Project was creating using Windows Forms technology. Basic language was C#, application was writing using IDE[1]: Microsoft Visual Studio 2015. UI[2] have been designed using standard editor integrated with VS.

This technology is still popular for Windows desktop application. The most important think about this decision was chose simple and fast technology. Microsoft deliver a lot of libraries integrated with Windows Forms, so it was easy to create user friendly application for simulation of grain growth.

This project is open-source[3], so for repository is using GitHub[4] website with public settings for repository. Visual Studio include tools for using GitGub, so all commits have been created using IDE.

The most important for decision about language was preference for developer. Knowledge is important for choose technology, especially, when project have quick deadline.

Project is continuation of preview grain growth application (CA method), so in theory from code and technology side this project is only extension for old implementation. In real, old code needed refactor to make it more scalable.

1 Integrated Development Environment – software application for software developers.
2 User Interface - interface with which a person may interact
3 More details: https://opensource.org/ (02.01.2019)
4 https://github.com/Micp95/MultiscaleModelling (02.01.2019)

2. User Interface

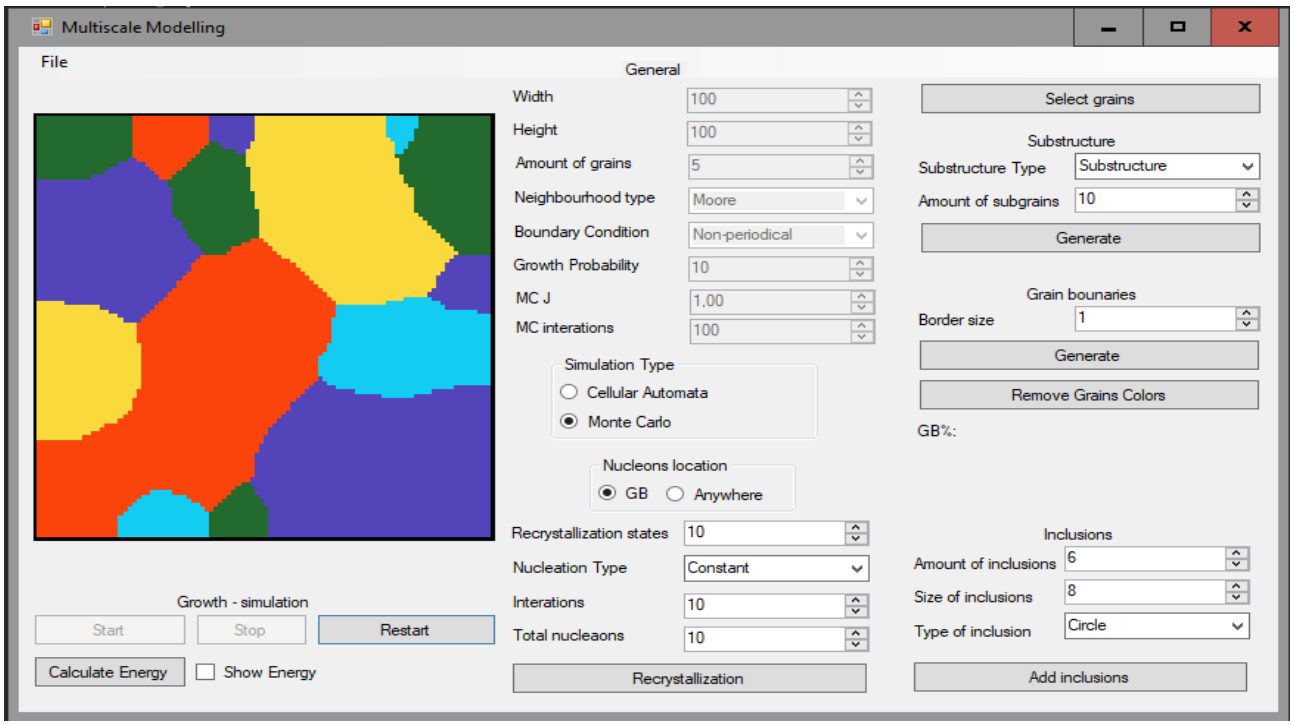

Fig. 1: Application UI

From UI side application include 3 new sections (Fig 1). Currently user have possible to change type of simulation (Cellular Automate or Monte Carlo). After generate grains will be possible to start recrystallize or calculate and show energy for grains structure.

2.1. Simulation output – grains structure and energy

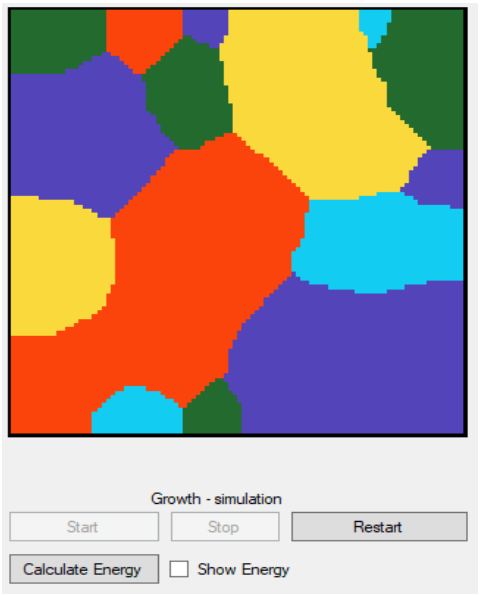

Fig. 2: Output window

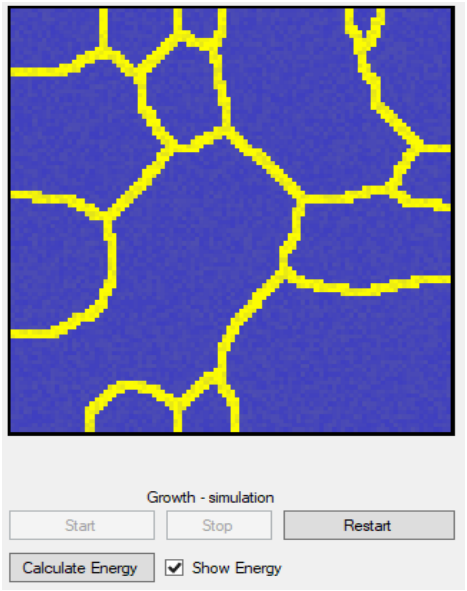

Fig. 3: Output window – show energy

Main of them is simulation output on left side of application. Nucleons are represented by colorful pixels, user can change simulation size, but always will see bitmap in one size. It is possible, because application rescale generated map to bitmap in application. After generate structure (Fig 2) it is possible to calculate energy (by click button - “Calculate Energy”), and show it by select checkbox - “Show Energy” (Fig 3).

2.2. Basic simulation parameters

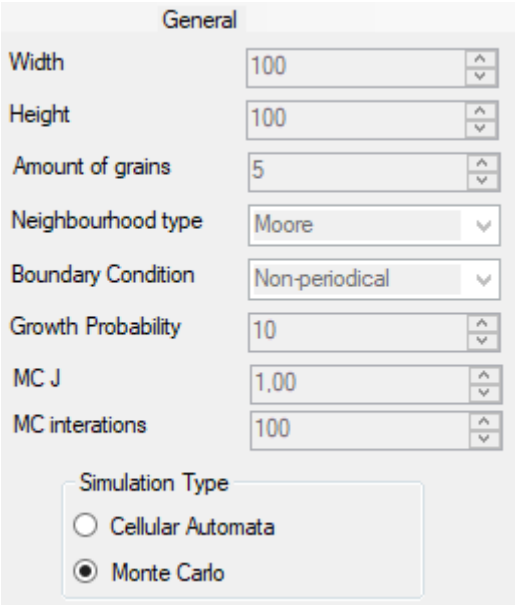

Fig. 4: General parameters

Next section [Fig. 4] is about change mainly settings for growth simulation simulation.
More about each fields:

1. Width – width of simulation map (output bitmap),
2. Height – width of simulation map (output bitmap),
3. Amount of grains – number of grains in map,
4. Neighborhood type – type of grains neighborhood:
    1. Von Neumann
    2. Moore
    3. Moore 2 - extension of Moore neighborhood
5. Boundary Condition - currently unused – only implemented one option: Non-periodical BC
6. Growth Probability – parameter for Moore extension neighborhood type
7. MC J – physical value “J” for Monte Carlo simulation
8. MC iterations – amount of Monte Carlo iterations
9. Simulation Type – type of simulation: Cellular Automate or Monte Carlo

2.3. Recrystallization

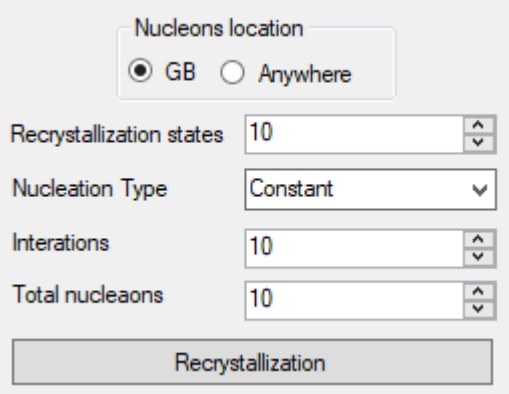

Fig. 5: Recrystallization settings

Recrystallize section [Fig. 5] contain parameters for recrystallize process.

1. Nucleons location – place for seeding new grains. We can seed new nucleons on Grains Boundaries, or Anywhere,
2. Recrystallization states – amount of new grain states,
3. Nucleation Type – type of grains seeding: Constant, Increasing, Begin Of Simulation,
4. Iterations – number of Monte Carlo iterations,
5. Total nucleons – total nucleons on the end of simulation.

Section include button to initialize recrystallization process - “Recrystallization”.

3. Application outputs

The application allows generate a lot of complex grains structure. This chapter contains basic capabilities with descriptions, how to use them.

3.1. Monte Carlo grain growth

For Monte Carlo simulation is important to setts three basic parameters: MC J, MC Iterations and select Simulation Type to “Monte Carlo”. The most important for Monte Carlo simulation is set iterations of simulation. For small value of this parameter (Fig 6.) we will generate a lot of small grains. When we will set higher number of iterations, we will see less grains (Fig 6). On extreme case, when we will set a large number we will see only one grain (Fig. 7).

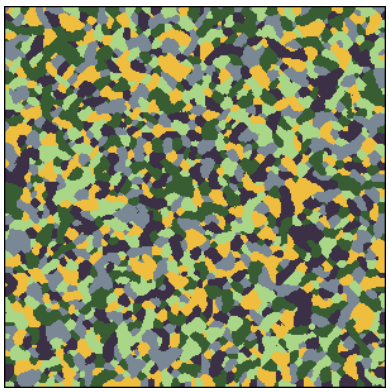

Fig. 6: MC 10 iterations (300x300)

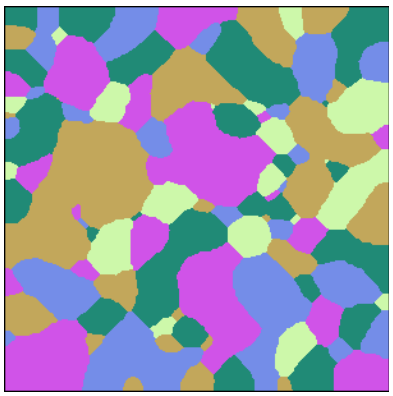

Fig. 7: MC 100 iterations (300x300)

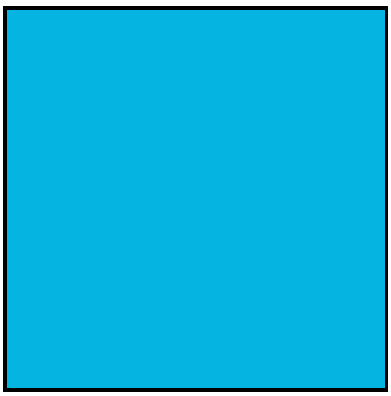

Fig. 8: MC 1500 iterations (100x100)

3.2. Dual phase microstructure

After generate grains structure, will be possible to generate substructure or dual phase. User need to select remaining grains, write amount of grains to generate and select type of new structure. Additional step is select type of simulation (MC or CA). Next step is click generate button and start simulation.

Possible is to generate dual phase structure between two different type of simulations: Monte Carlo and Cellular Automate. It is possible to generate complex combination between simulation, for example CA → MC (Fig 9.) or MC → CA (Fig 10.).

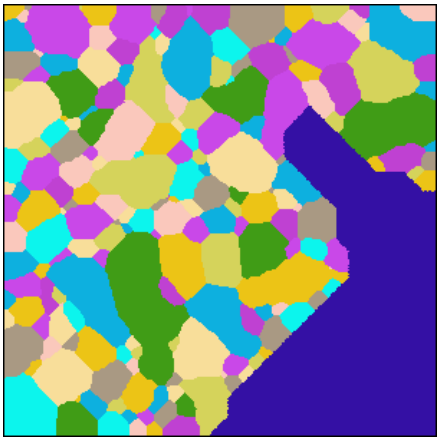

Fig. 10: CA -> MC

Fig. 9: MC -> CA

3.3. SRX Monte Carlo

3.3.1. Nucleation and growth

After generate base structure (Fig 12) it is possible to simulation recrystalization process. User need to write parameters for simulation, like number of iterations (20 in example) and number of states (10 in example) Important is select type of nucleation, application have implementation for three nucleation methods:

1. Constant – create new grains in constant batch per iteration (Fig 11),
2. Increasing - create new grains in increasing batch per iteration (Fig 13),
3. Begin Of Simulation – create all grains in first iteration (Fig 14).

Fig. 12: Base structure

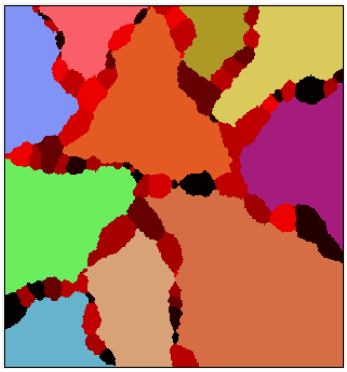

Fig. 11: Constant nucleations (100 nucleaons)

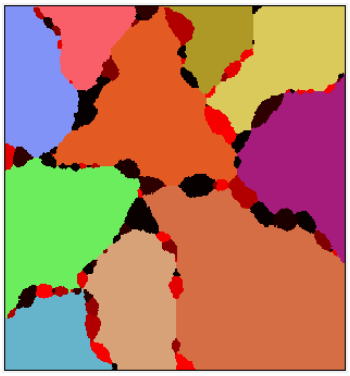

Fig. 13: Incresing nucleations (100 nucleaons)

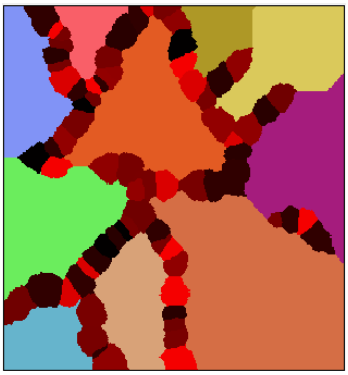

Fig. 14: Begin Of Simulation nucleations (100 nucleaons)

3.3.2. Energy distribution

Application possible to calculate and show energy in structure. Energy for Fig. 16, you can see on Fig. 15. After 20 iterations of recrystalization (Fig. 17) process we have other energy distribution (Fig. 15).

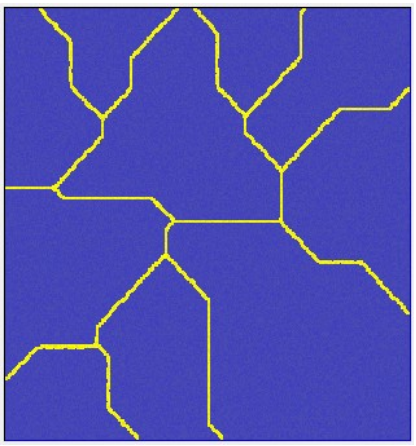

Fig. 16: Energy for base structure

Fig. 15: Structure after 20 iterations of recrystalization (Begin Of Simulation nucleations)

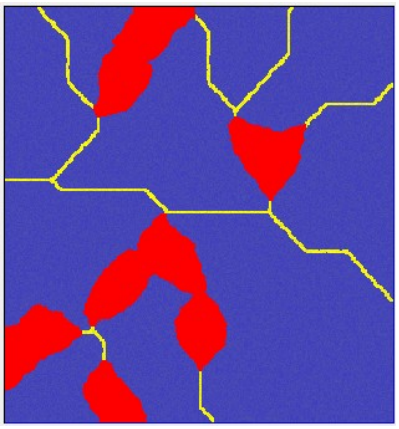

Fig. 17: Energy after 20 iterations of recrystalization

Where yellow color means more energy than blue. Red color means structure without energy. The simulation tends to lowest energy, after rectystalization (Fig. 18) we haven't energy in simulated system (Fig 19).

Fig. 18: Structure after recrystalization

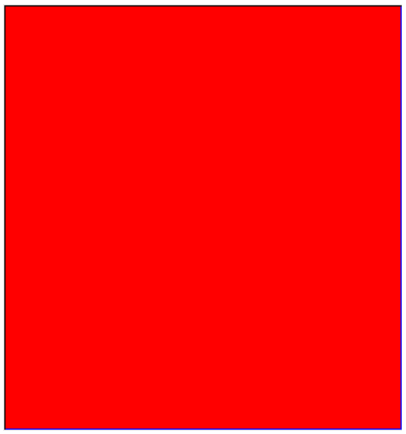

Fig. 19: Energy after recrystalization

4. Real structure compare

Monte Carlo method can be used to generate very similar structure like really photos. For example Fig 20 present steal structure[5] and in right side (Fig 21) we have structure generated by simulation.

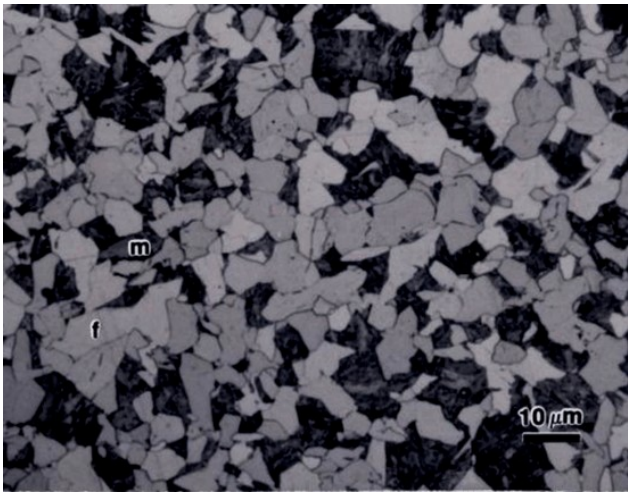

Fig. 21: Microstructure of 8620 alloy steel austenitized at 927 ºC, isothermally transformed at 677 ºC for 1 minute and water quenched after etching in 10% sodium metabisulfite.

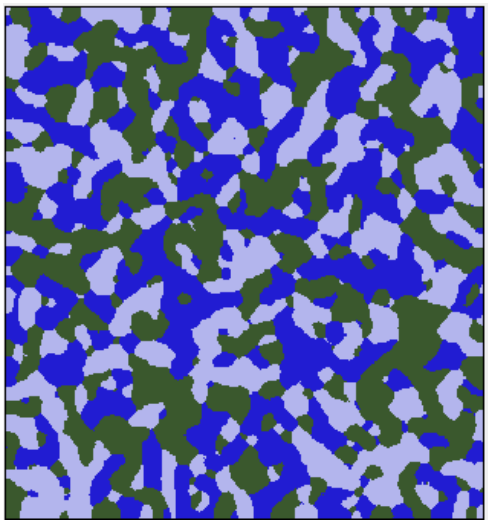

Fig. 20: Generated structure using MC growthing

Better result we can achieve, when we will use dual-phase structures, because we can regenerate and create substructure. It is possible to generate structure (Fig 23) looks like real DP steal (Fig 22)[6].

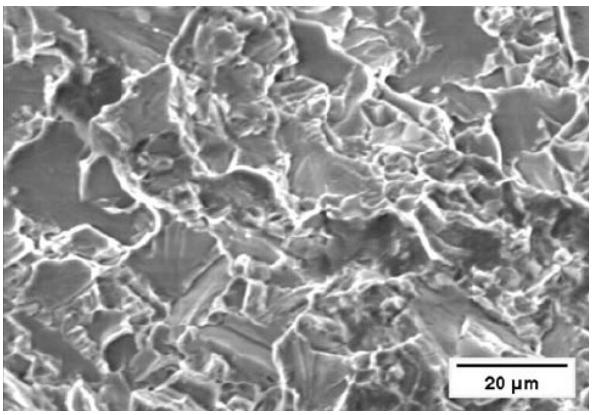

Fig. 23: DP steel Al-0.5 A: Cleavage fracture; specimen's centre; B3 × 15 unnotched specimen.

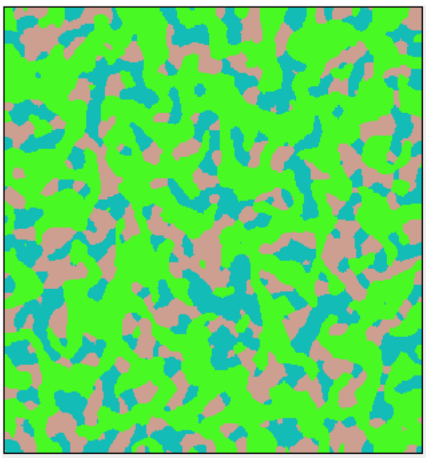

Fig. 22: Generated Dual-Phase structure

ography-with-george-vand
isothermally-treated-steels.html (02.01.2019)

6 https://www.researchgate.net/figure/DP-steel-Al-05-A-Cleavage-fracture-specimens-centre-B3-15-unnotched-specimen_fig14_273693273 (02.01.2019)

Interesting effect we will see after recrystallized process, where we can observe similar structure between simulation effect (Fig 24), and photos of recrystallized grains (Fig 25)[7].

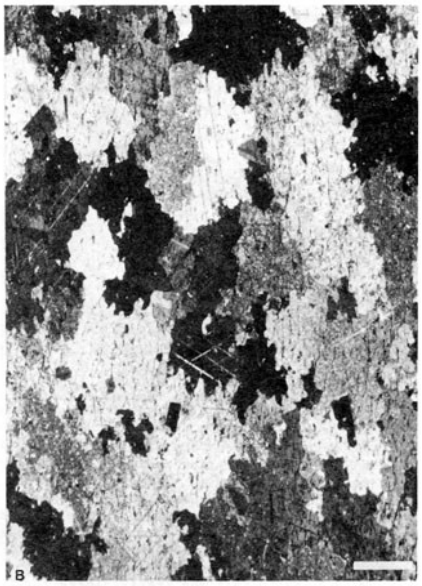

Fig. 24: Recrystallized grains in marble, growing Crossed polarizers, scale bar is 0.2 mm.

Fig. 25: Generated grains after recrystalization

5. Conclusions

Monte Carlo simulation is different method than Cellular Automate and it's possible to generate more realistic results.

Monte Carlo method is very slowly with basic assumptions, but in application applied some improvements like: skip inside grain nodes, random only neighbors for new state. Performance of algorithm still isn't the best, because application doesn't use parallel calculations. It could be next step of application development.

Static recrystallization generating new nucleons, where energy is highest with more probability and process trying to minimalize energy in structure. Recrystallized grains haven't energy so these can't be seeds for new nucleation. We can observe this same process in really structures. Application possible to show energy in structure whenever it will be possible.

Monte Carlo method is working completely random. We can generate a lot of complex structures, but the most important parameter is number of iterations. The parameter is proportional to size of grains. After a large number of iterations simulation will generate only one big grain – it will be stable state, without energy.

Combination MC and CA methods allows to generate realistic structures, and it is a key to get the best results. In nature we can observe random structures like in MC, but some of them are more predictable.

For MC simulation Moore neighborhood will be batter than Von Neumann, because generate more stable results.

7 http://www.ged.rwth-aachen.de/Ww/projects/rexx/Urai+86Recrystallization/Urai+86Recrystallization5.htm (02.01.2019)

Illustration Index