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Year 2, IS WIMIIP

05.01.2018

Multiscale Modelling
Report 2

1. Aim of the project

The goal of the second project was to create a program that is able to generate two-dimensional images of statistically representative metallic structure based on the Monte Carlo model and static recrystallization. All of the previous project's functionalities are also present in the current project.

The implemented functions include:

- Monte Carlo grain growth
- Static recrystallization, including:
    - Nucleation – distributing new nuclei in the structure
    - Nucleation – selecting location
    - Energy distribution – homogenous, heterogenous

The project's code can be found at https://github.com/uzikus1/multiscale-project/

2. User interface

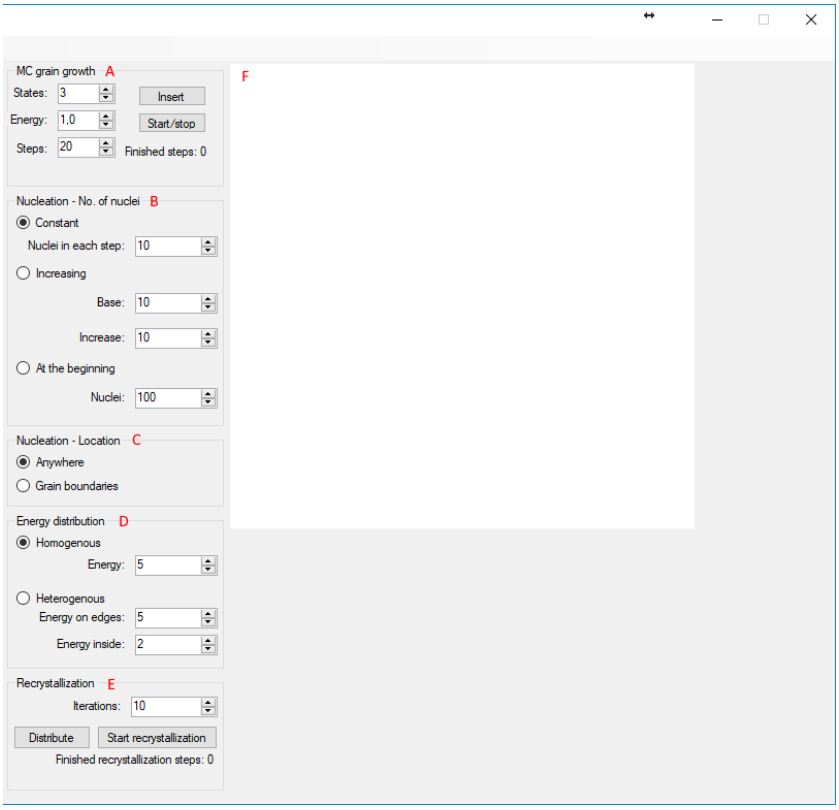


Figure 1. Program's main window with the newly implemented functionalities.

Main interface elements:

A. Monte Carlo grain growth panel
B. Nuclei distribution selection panel
C. Nuclei location selection panel
D. Energy distribution selection panel
E. Recrystallization panel
F. Energy visualization picture box.

3. Descriptions of implemented functions

a. Monte Carlo grain growth

This is the new project's main feature which we can use to generate structures based on the Monte Carlo method. Before the growth, user has to specify the number of states, energy value and number of calculation steps.(Figure 2).

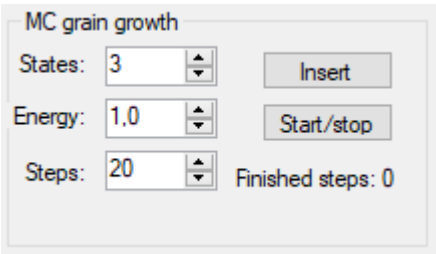


Figure 2. Monte Carlo grain growth panel.

After pressing the *Insert* button, the initial structure will be generated (Figure 3).

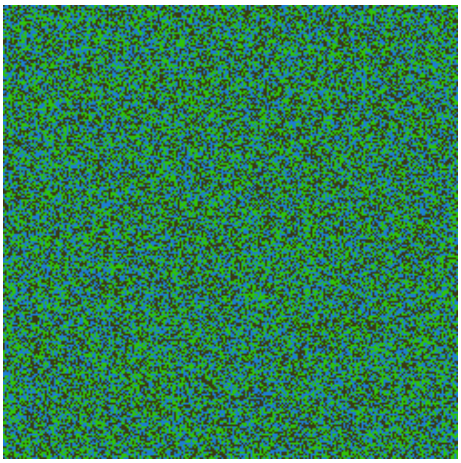


Figure 3. Generated 250x250 size initial microstructure.

After pressing the *Start/stop* button, the grain growth proces will commence and will last the amount of steps that was previously specified by the user (Figure 4).

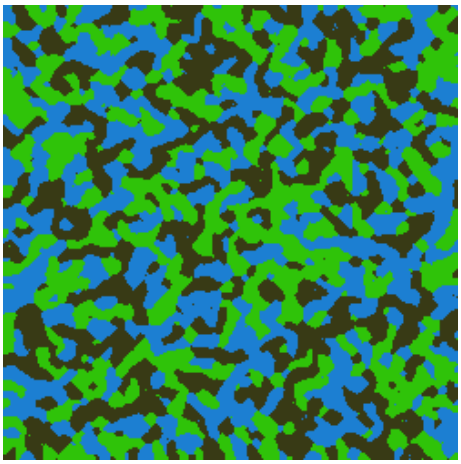


Figure 4. The 250x250 size mictostructure after 20 calculation steps.

b. Nuclei distribution selection panel

Before static recrystallization can be started, user has to select how new nuclei will be distributed. The available options are: added constantly every step, increasing every step or simply added at the beginning of the proces (Figure 5).

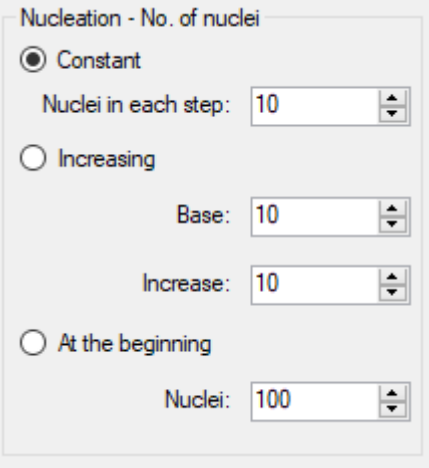


Figure 5. Nuclei distribution selection panel.

c. Nuclei location selection panel

The next step is selecting the location where new nuclei will appear – either anywhere in the structure or only on the grain boundaries (Figure 6).

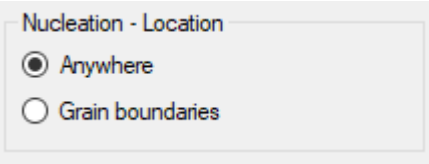


Figure 6. Nuclei location selection panel.

d. Energy distribution selection panel

Before the energy can be distributed, we have to select whether it will be distributed uniformly in the whole area (homogenous) or differently based upon the grain boundaries (heterogenous). User can select the desired energy value for each type (Figure 7).

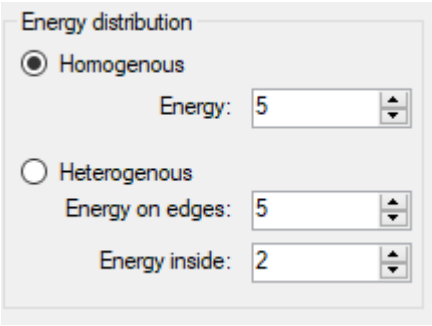


Figure 7. Energy distribution selection panel.

e. Recrystallization panel

This panel allows user to distribute energy based on previous options, specify the number of recrystallization steps and start the simulation (Figure 8).

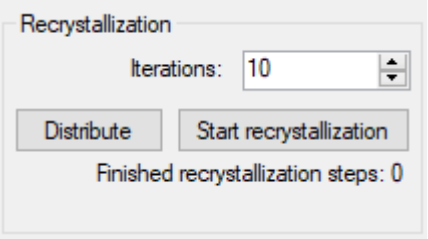


Figure 8. Recrystallization panel.

After pressing the *Distribute* button, new nuclei will be inserted and a energy visualization will be generated (Figure 9).

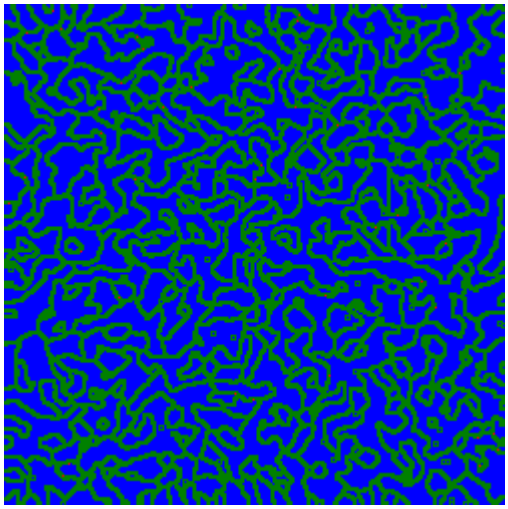


Figure 9. Heterogenous energy distribution based on the Figure 5.

After pressing the *Start recrystallization button*, the static recrystallization will commence. Both the grain and energy visualization is updated each step (Figure 10a, 10b, 10c, 10d, 10e, 10f).

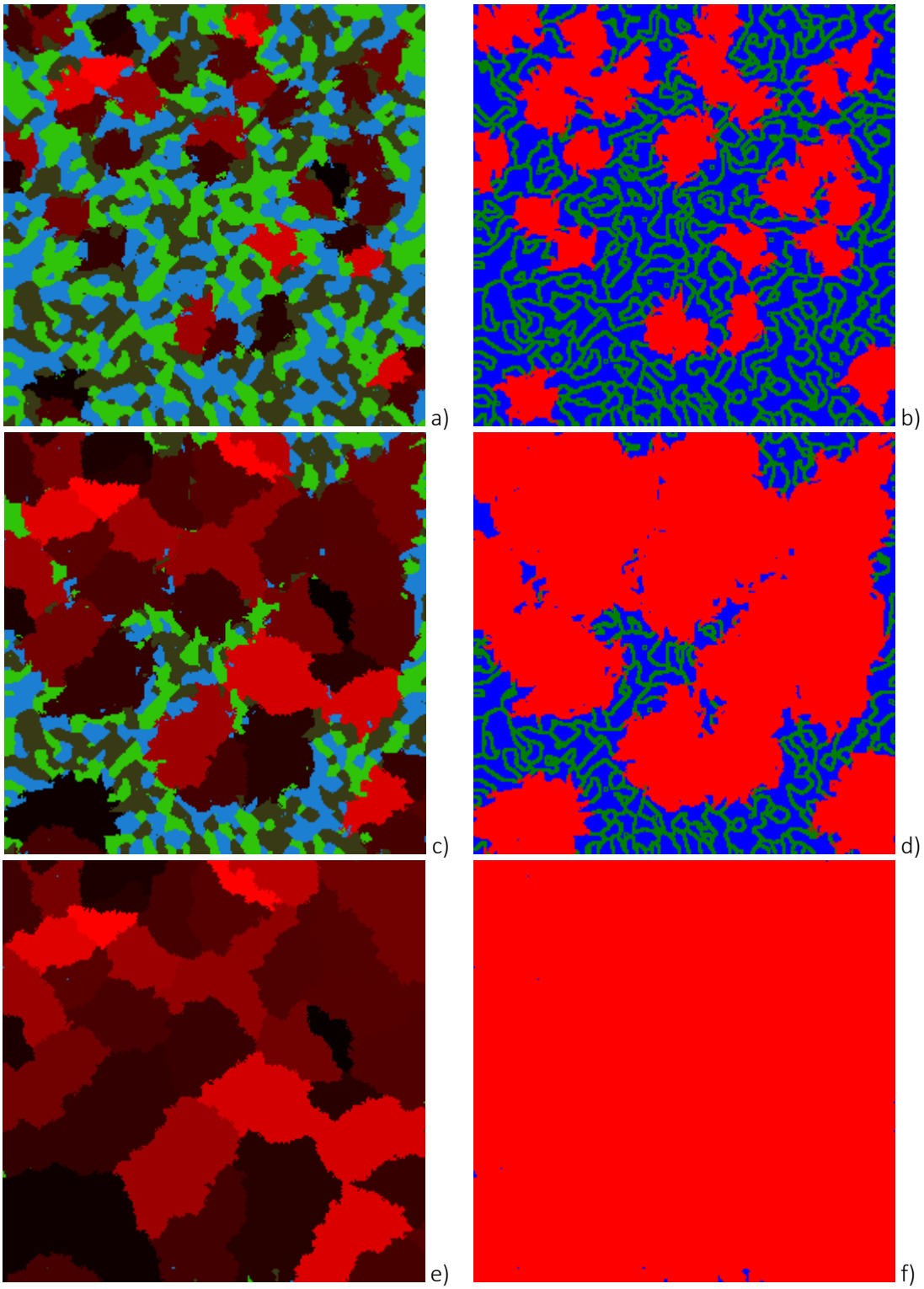
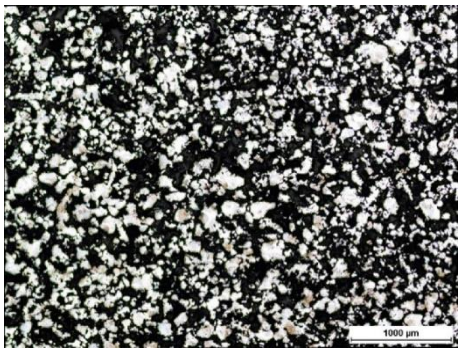


Figure 10. Comparison of a static recrystallization of a structure based upon the Figure 4 with distribution of 40 nuclei added at the beginning of the process. Energy was distributed homogenously (5 on borders, 1 inside). Compared here are newly recrystallized grains after 10 steps (Figure 10a, 10b), 20 steps (Figure 10c, 10d), after 40 steps (Figure 10e, 10f).

4. Real structure comparison and conclusion

The generated microstructure using the Monte Carlo grain growth method closely represents the structure, which has been created from a real sample (Figure 11).



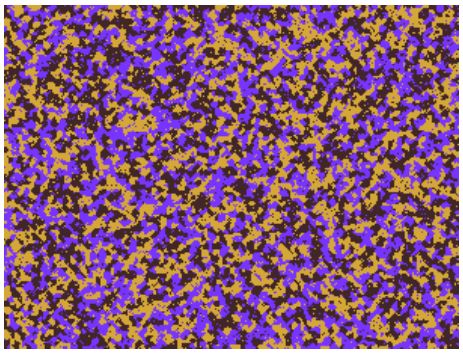
a)

b)

Figure 11. Comparison of a) ASC 100.29 metallic foam (Depczynski, Kazala, Ludwinek i Jedynak, 2016) and b) similar generated microstructure.

The same applies to the implemented static recrystallization feature (Figure 12).

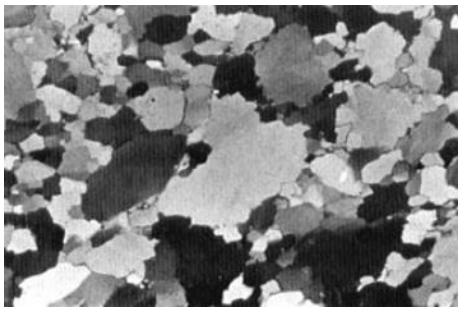
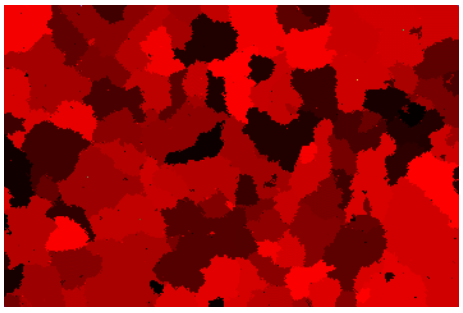

a)

b)

Figure 12. Comparison of a) rock microstructure after static recrystallization (Plaphol, 2018) and b) similar generated microstructure.

Users can utilize the parameters provided by the program to achieve a similar result that is statistically representative to the real sample, e.g. number of states present in the microstructure in the case of Monte Carlo or the nuclei location and distribution in the case of static recrystallization..

Using created software to generate microstructures is much cheaper and quicker method of generating valid structure images which can be used in further research with similarly effective results, which applies to all of the methods implemented in the project. However, each method has different usage, which is clearly visible in Figure X and X – user must carefully select which method will be used to generate a specific microstructure, for the results can be vastly different from the original sample.

5. Bibliography

Depczynski, W., Kazala, R., Ludwinek, K. i Jedynak, K. (2016). Modelling and Microstructural Characterization of Sintered Metallic Porous Materials. *Materials*, 567.

Plaphol, K. (2018, January 05). ***พฤติกรรมเชิงกลและกลไกการเสียรูปของหิน***. Downloaded from http://slideplayer.in.th/slide/2030086/