	Oliwia Strzelec	Data wykonania 18.12.2018
Mutliscale Modeling	2nd report	Data oddania 20.12.2018

Contents

1. Technologies

This project is a continuation of the project described in the first report. The technology used for this project was described in details in the previous report. It is worth mentioning that the entire backend of the application is maintained in Spring which a web technology based on Java. To support the view Thymyleaf, HTML and JavaScript have been used.

2. Monte Carlo grain growth algorithm

The first functionality that has been implemented is Monte Carlo grain growth algorithm. This method consists in the fact that after defining the number of nucleons by the user the first step is to randomly fill the entire space with nucleons. The user interface for selecting the method of growth and the number of nucleons is shown in Figure 1.2. Randomly filled space is shown in Figure 1.1.

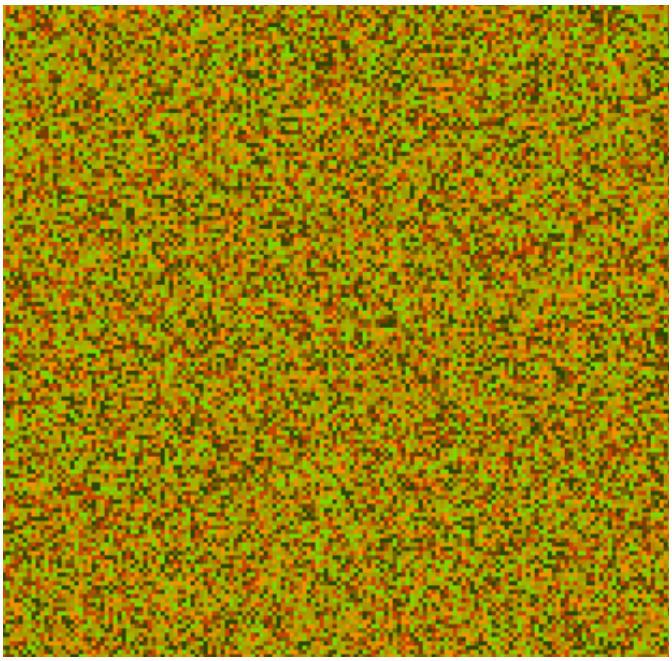

Figure 1.1. The first step of the Monte Carlo method, space randomly filled with nucleons

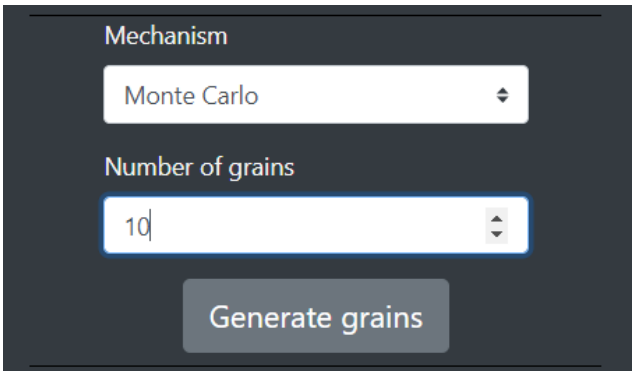

Figure 1.2. *User interface for selecting the method of growth and number of grains*

In the next stage, the user selects the number of iterations, as shown in Figure 1.3. In each iteration, energy is calculated for each cell in a random order based on the neighborhood and the J value. The J value is taken from the user interface, as shown in Figure 1.4. Then the cell is changed to a random neighbor and the energy is recalculated. If the energy decreases, the cell remains changed, otherwise, the changes are withdrawn. The view of the grains after Monte Carlo growth is shown in Figure 1.5.

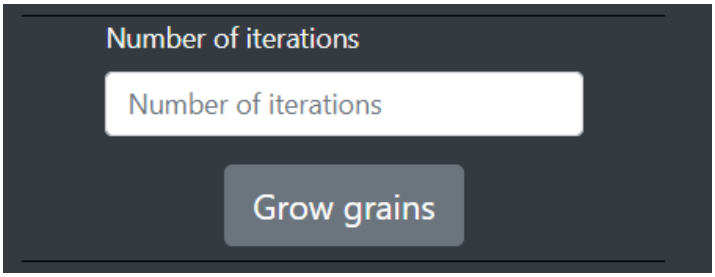

Figure 1.3. *User interface for selecting the number of iterations*

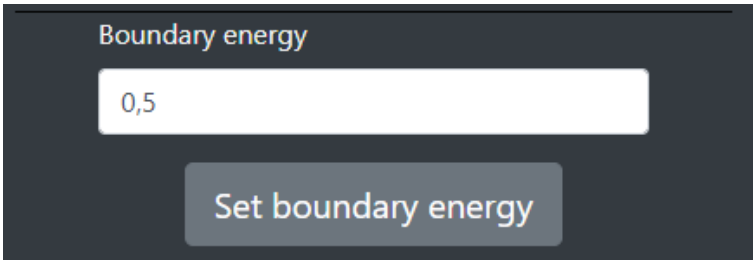

Figure 1.4. User interface for determining the J value

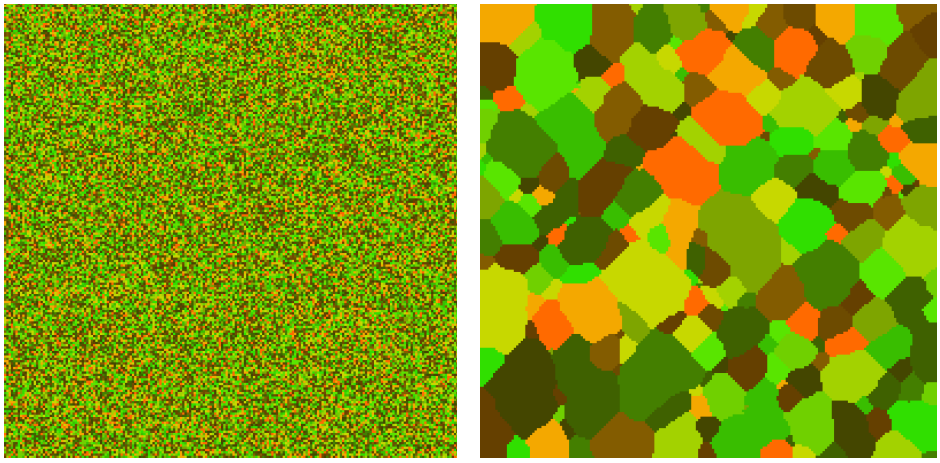

Figure 1.5. *Grains before and after Monte Carlo grain growth*

3. Dual phase microstructure

Another feasibility of the program is the ability of running a second growth and determining how many grains from the previous microstructure should remain unchanged. Grains can take the form of a dual phase and then change color or substructure and retain the original color. The user interface for selecting the amount of grains and the type of microstructure is shown in Figure 2.1. The second growth can be carried out using both Cellular automata and Monte Carlo methods. The view of the grains after the Monte Carlo growth, the view of grains after choosing of microstructure and the microstructure view after the second grow with the cellular automata method are juxtaposed with each other in picture 2.2.

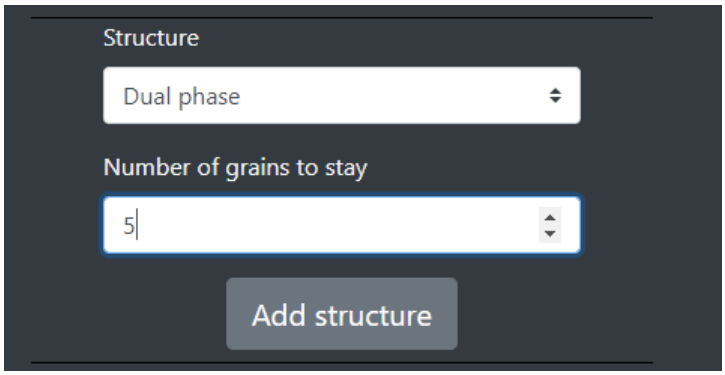

Figure 2.1. *The form to choose the type of microstructure and the amount of grains*

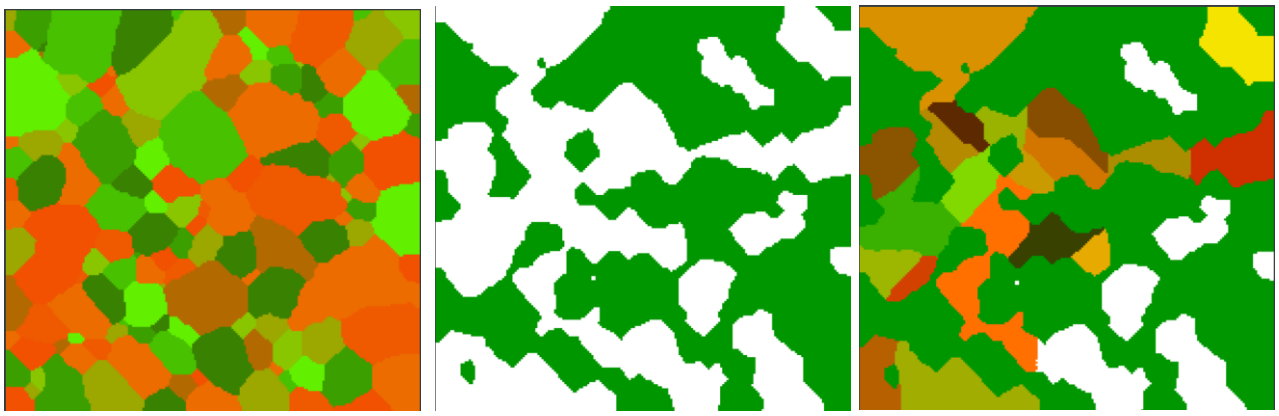

Figure 2.2. Grains after Monte Carlo growth, dual phase type microstructure, grains after second growth with the celular automata method with visible substructure

4. Energy distribution

Another feature is the ability to switch between stored energy views and ordinary structure view. The button for changing the view is shown in Figure 3.2. Initially, energy can be distributed in two ways: homogenous and heterogenous. In the first case, one energy value should be given for all cells, while in the second one - the upper and lower limits of the energy value range. Low energy corresponds to a dark color, and high energy - bright. In the case of heterogeneous energy distribution, the highest energy is accumulated at the grain boundaries. The user form for selecting energy distribution is shown in Figure 3.1. In Figure 3.3. a view of grains and a view of energy were put together.

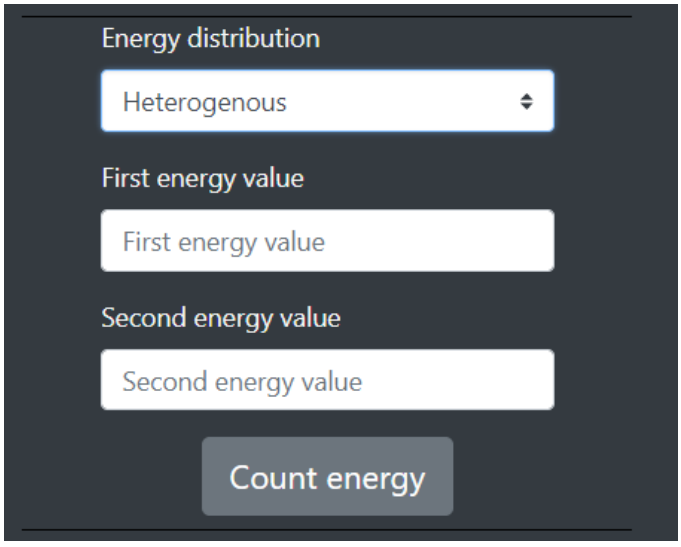

Figure 3.2. *The form for choosing energy distribution*

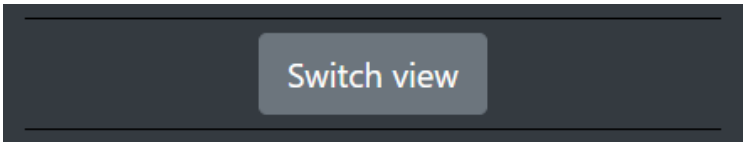

Figure 3.2. *Button for changing the view*

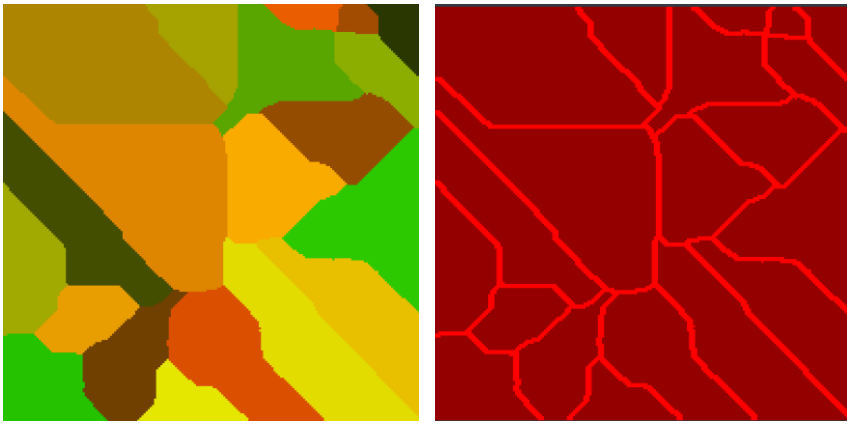

Figure 3.3. *View of grains and the view of heterogeneous energy distribution*

5. Recrsatlization

The last implemented functionality was the ability to perform the recrystallization process. Recrystallized nucleons can be placed on the grain boundaries, or randomly on the entire space. The user form for adding recrystalized nucleons is shown in Figure 5.1. Figure 5.2. shows a grain view and energy view after 10 iterations of recrystallization with nucleons at grain boundaries with heterogeneous energy distribution. As can be seen, recrystallization occurs faster at the grain boundaries because they have a higher initial energy. Figure 5.3. state of the grains after 20 iterations of recrystallization is presented. As can be seen, recrystallization also started in the grain volume. Figure 5.4. shows the view after another 10 iterations, and in Figure 5.5. state of grains and energy after the recrystallization process is presented. It can be seen that everywhere the energy is 0 and the whole space is filled with recrystallized grains.

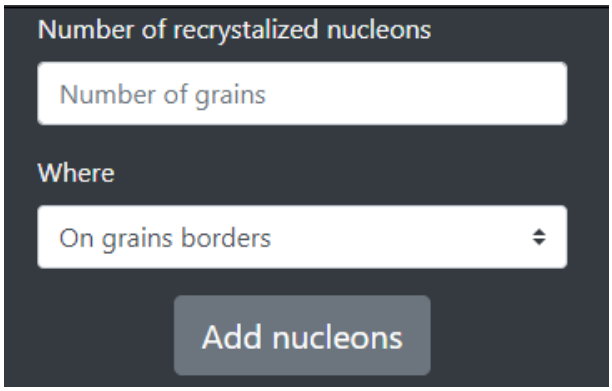

Figure 5.1. *The user form for adding recrystalized nucleons*

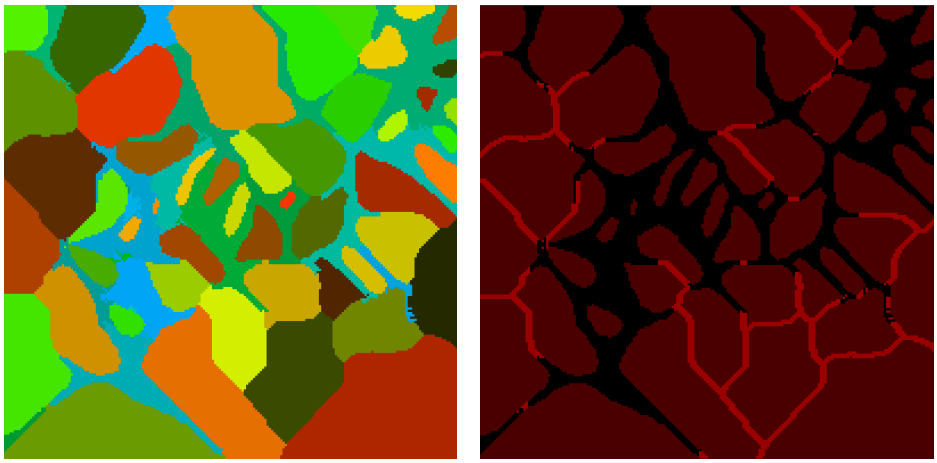

Figure 5.2.G*rain view and energy view after 10 iterations of recrystallization with nucleons at grain boundaries with heterogeneous energy distribution*

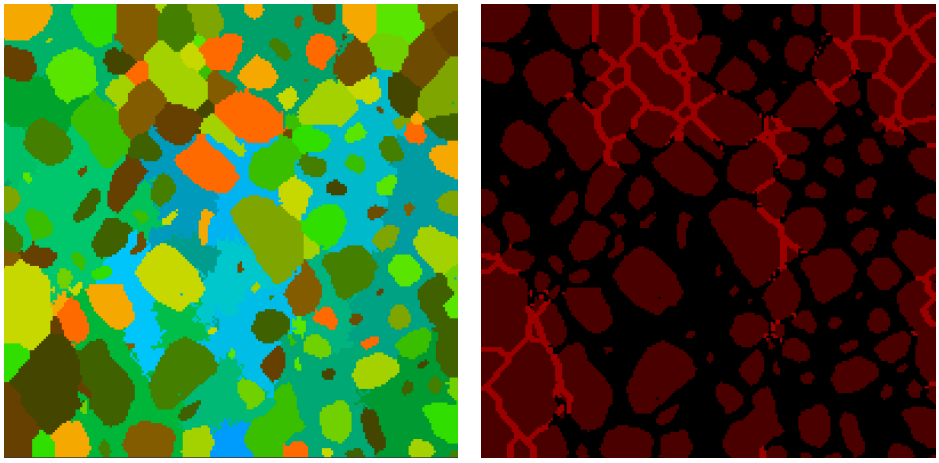

Figure 5.3. Grain view and energy view after 20 iterations of recrystallization with nucleons at grain boundaries with heterogeneous energy distribution

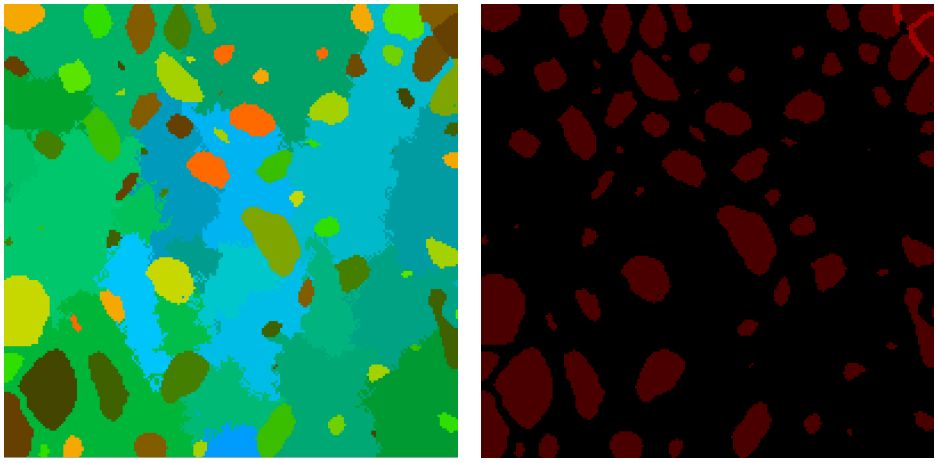

Figure 5.4.G*rain view and energy view after 30 iterations of recrystallization with nucleons at grain boundaries with heterogeneous energy distribution*

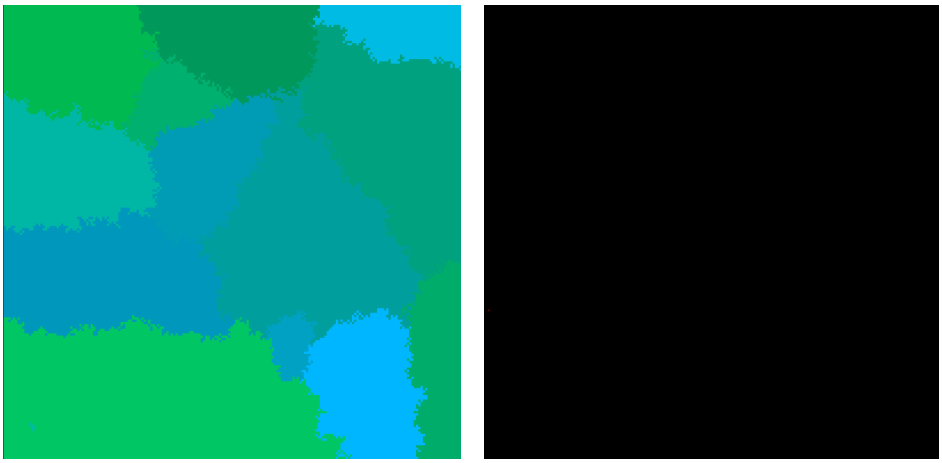

Figure 5.5.G*rain view and energy view after completed recrystallization process*

6. Comparison with literaturę

The deformed microstructures of steel after metadynamic recrystallization are shown below in Figure 6.1.

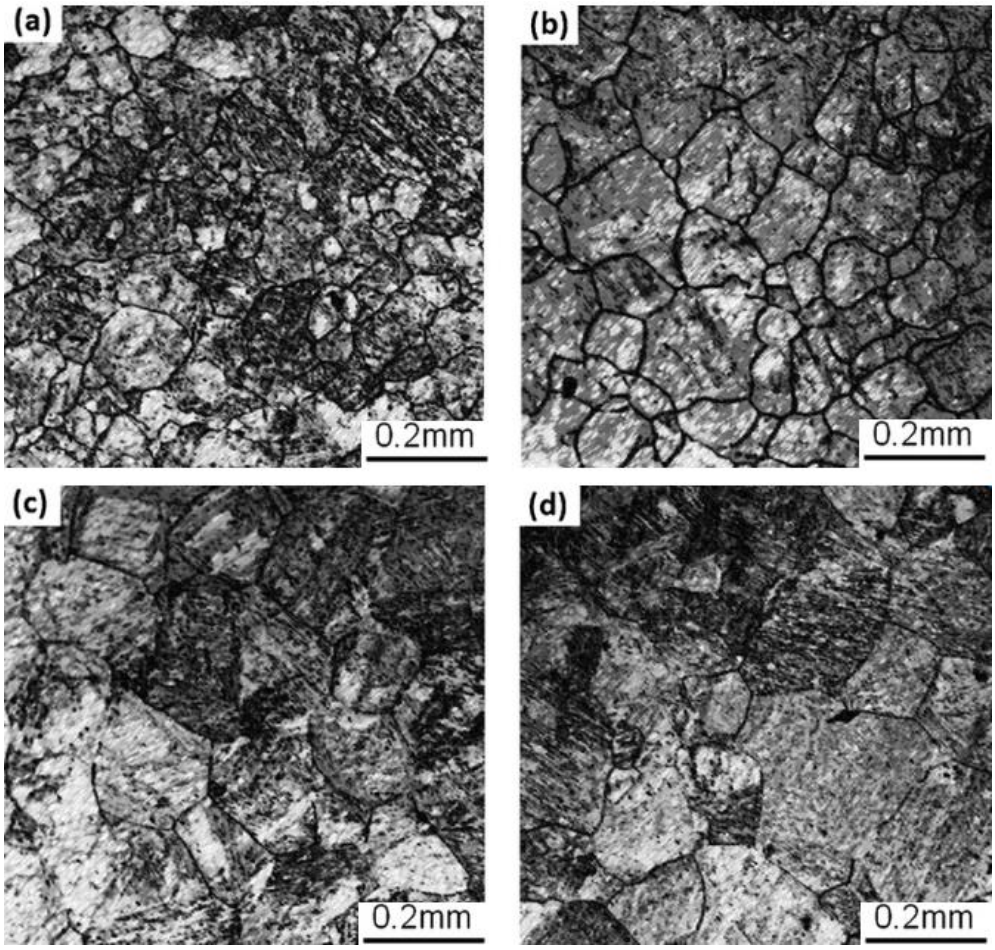

Figure 6.1. *Optical deformed microstructures of 30Cr2Ni4MoV steel after metadynamic recrystallization with forming temperatures of (a) 970 @BULLET C; (b) 1070 @BULLET C; (c) 1170 @BULLET C* [1]

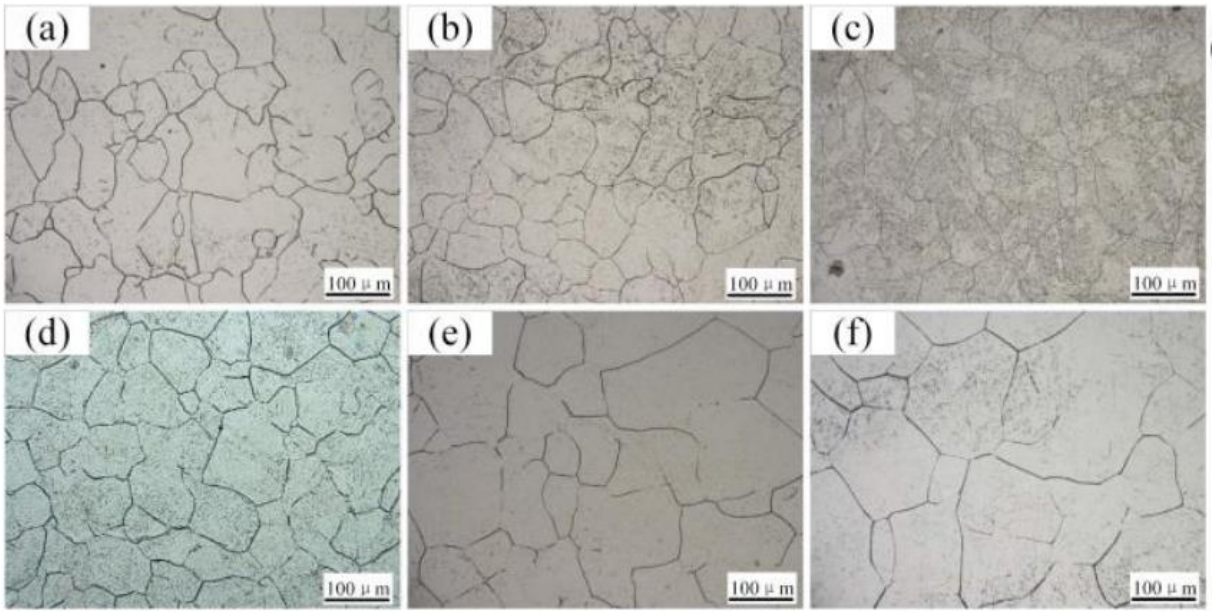

Figure 6.2. *300M steel microstructures after heat treated at (a) 900°C, (b) 950°C, (c) 1000°C, (d) 1050°C, (e)1100°C, (f) 1150°C for 40 minutes of heat treatment at different temperatures* [2]

Figure 2 shows the microstructures of 300M steel after heat-treated at different temperatures for 40 minutes.

It can be seen from Figure 6.1 that the recrystallization process takes place faster at the grain boundaries and the smaller grains recrystallises faster. The picture clearly shows darker places with a more irregular structure and lighter places. This state can be quite well represented by the simulation view during recrystallization process, eg in Figure 5.3. However, it should be noted that grains after recrystallization are characterized by high inhomogeneity inside grains, which significantly differs from the presented model. As can be seen in Figure 5.5. the recrystallized grains in the simulation are uniform inside the boundaries.

Greater similarity can be found in the case of microstructures from Figure 6.2. Simulated microstructures both before and after the recrystallization are characterized by a homogeneous interior and clearly marked grain boundaries.

7. Literature

[1] F. Chen, Z. Cui, D. Sui, B. Fu, *Recrystallization of 30Cr2Ni4MoV ultra-super-critical rotor steel during hot deformation. Part III: Metadynamic recrystallization,* 2012

[2] 1. R. C. Chena, C. Honga, J. J. Lia, Z. Z. Zhenga, P. C. Lib, *Austenite grain growth and grain size distribution in isothermal heat-treatment of 300M steel,* 2017