Multiscale Modelling Raport No 2

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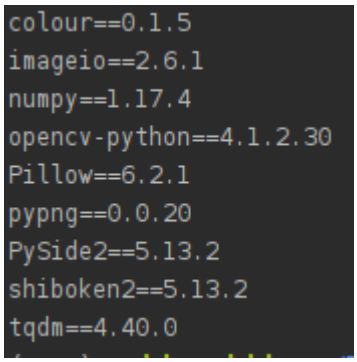
Number of album: 285494

Group number: 1

Repostitory address: https://github.com/Barcol/multiscale

1. Used technology

Entire application was created with Python language. On addition, certain external packages were used. List of them, along with their versions can be found on Picture 1.



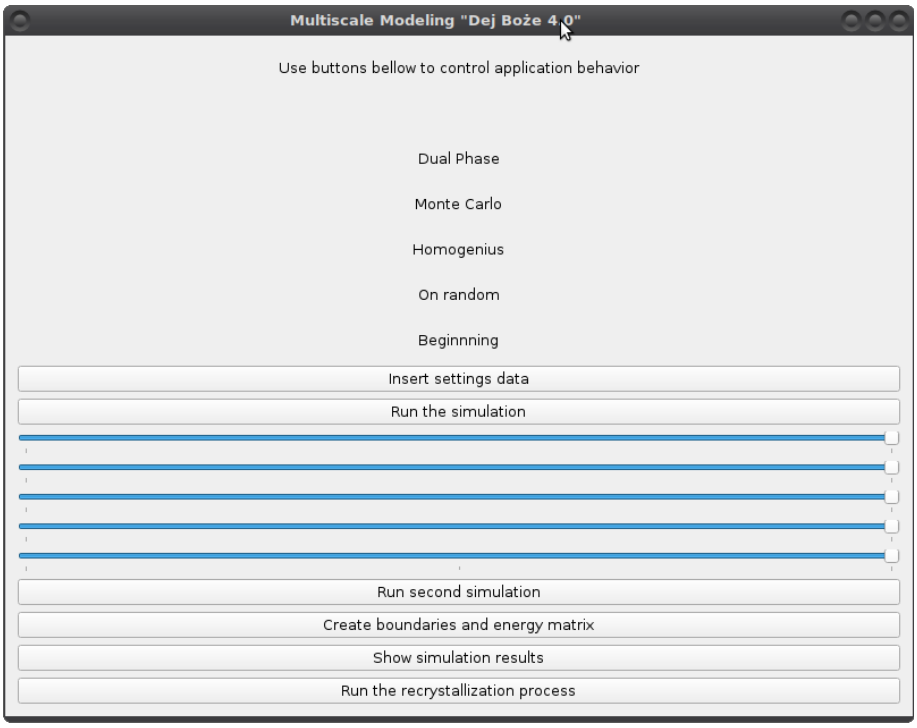
Picture 1. List of used external packages.

The GUI was created with QT librarys implementation, called PySide2.

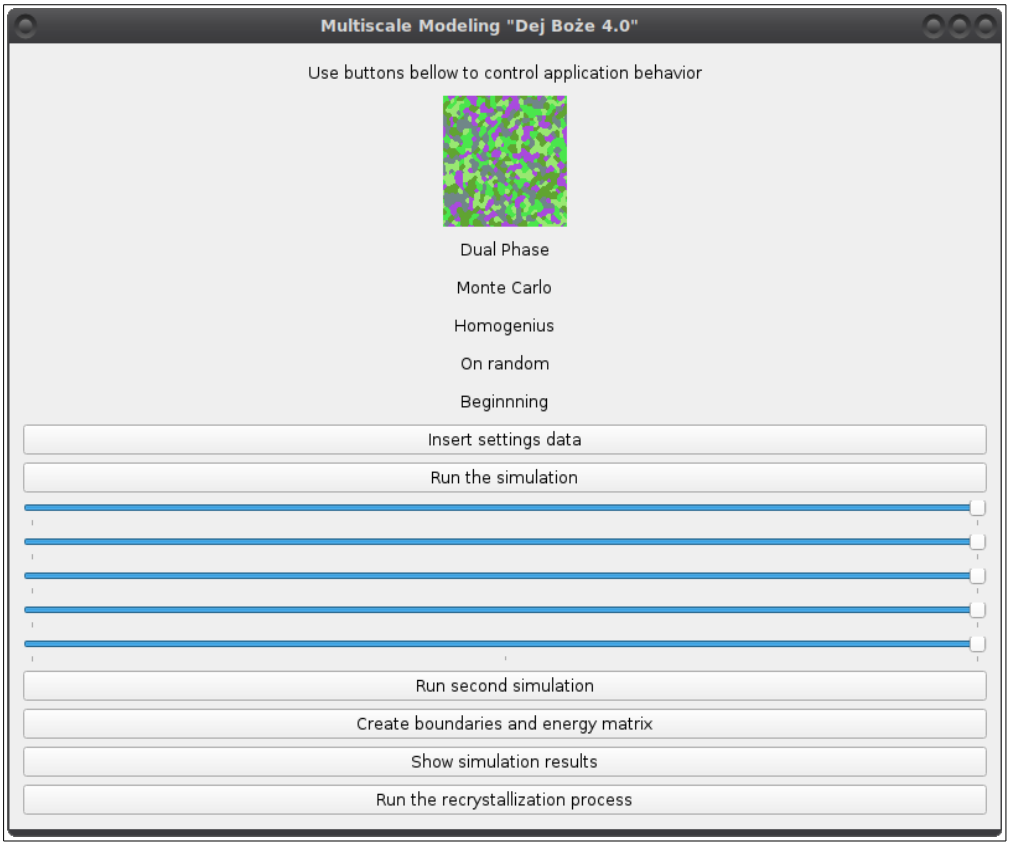
2. Graphical User Interface

On pictures 2 and 3 we can see two basic application windows. Picture 2 shows us the main screen, with its inputs. Picture 3 on addition contain preview of simulation result. We can see on both on them sliders that are used to determine certain simulation parameters, such as place of nucleon generation (on boundaries, or anywhere), number of nucleons added each recrystallization iteration (we can choose constant, growing, or we can specify to only add nucleons at the beginning of simulation).

We can command the program via buttons containg precise labels. Every button is connected only to action it uses as label. The only exception of this, is function to add actual result on preview. There are 3 buttons capable of this functionality: Run the simulation, Create boundaries and energy matrix, and Run the recrystallization.



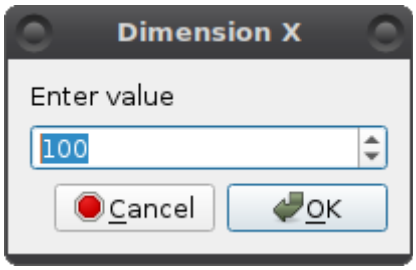
Picture 2. Main application window.



Picture 3. Main application window with preview.

2.1. Basic usage of application

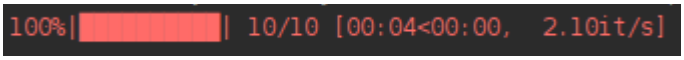
First step user have to take is to pick final dimensions of simulation. To do so, user have to use the “Insert settings data” button. This causes four input boxes to show one after another. Example of such boxes is shown on picture 4.



Picture 4. Example of input box

Beside off box shown on picture 4, the three others are used to collect data about: Dimension Y, Number of grains, and Number of iterations .

After picking all values, user can use “Run the simluation” button, to start simulation and see its preview. User will be informed of simulation progress via TQDM package, shown on picture 5.

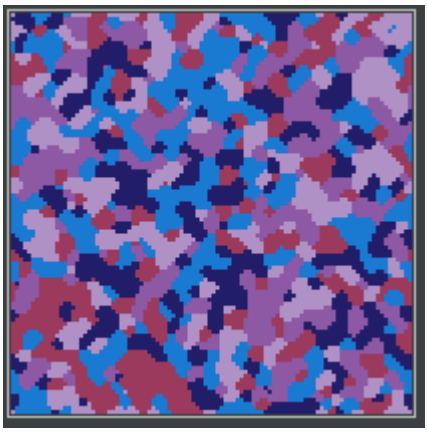


Picture 5. Tqdm progress bar.

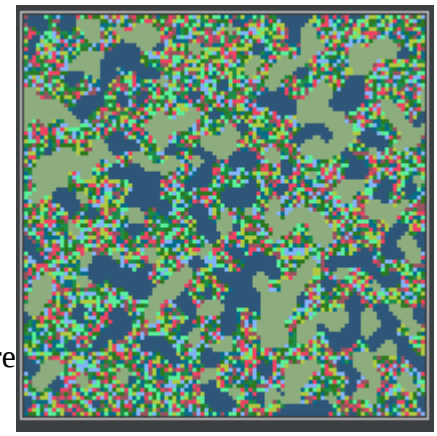
2.2. Second simulation

If the user is willing, he can rerun the simulation, but with Substructure or Dual Phase option.

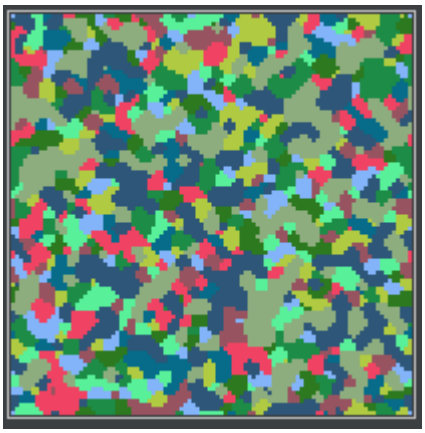
Moment of changing state can be observed on pictures 6, 7, 8, 9.



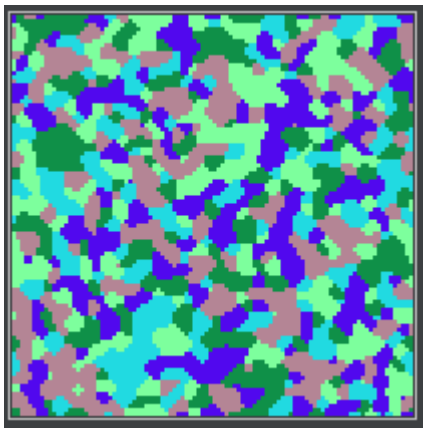
Picture 6. Dual phase before second simulation



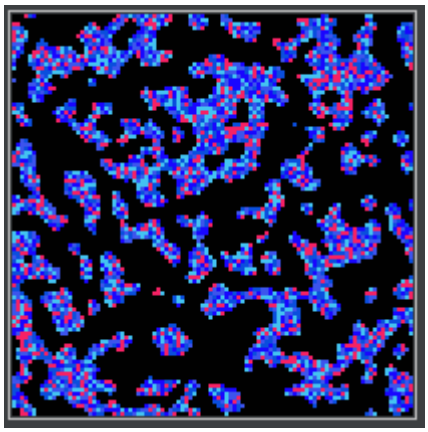
Picture 7. Dual phase after start of new one (we can see colors changed)



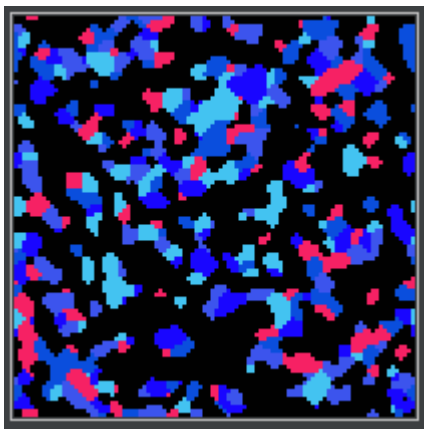
Picture 8. Simulation completed.



Picture 9. Substructure before second simulation



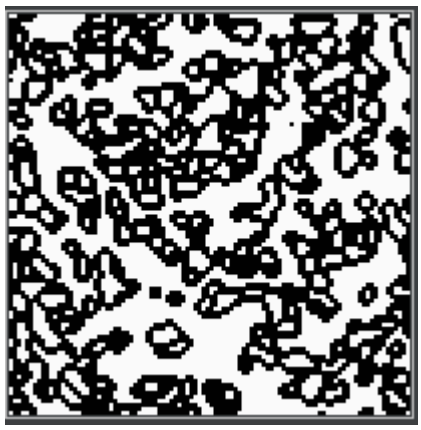
Picture 10. First frame of second simulation.



Picture 11. End of second simulation.

2.3 Boundaries end energy distribution

When simulation is done, user can use program to create boundaries image, and prepare energy matrix. Both of those are shown in Picture 12, Picture 13 and Picture 14.



Picture 12. Boundary image created basing on simulation results from picture 13.

```
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```

Picture 13. Energy matrix debuging display (homogenious distribution of value 15 with 10% of uncertainty)

```
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[15.0, 5.0, 5.5, 13.5, 15.0, 13.5, 15.0, 16.5, 16.5, 4.5, 5.0, 5.0, 5.0, 4.5, 4.5, 16.5, 15.0, 15.0, 16.5, 16.5]
```
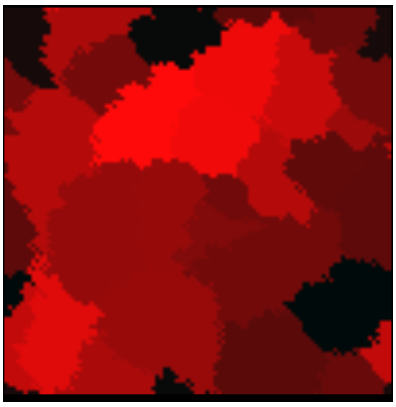

Picture 14. The same situation as in picture 13, but distribution is heterogenious, and the value for grain boundaries is equal to 5.

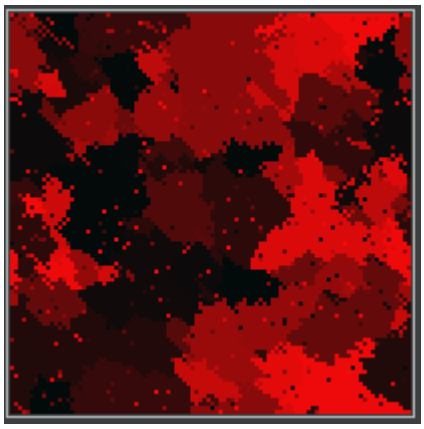
2.4 Recrystallization

Recristallization comes with three options of adding new nucleons:

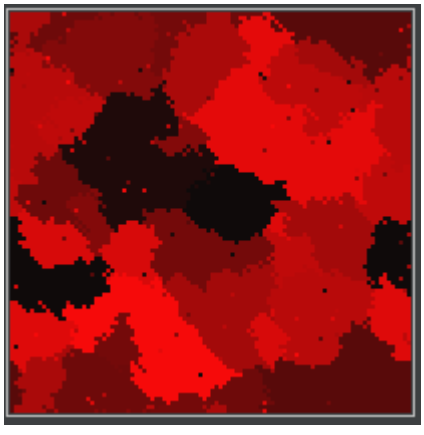
-Just ones, during the first iteration. On every other iteration they just grow. This can be spoted on picture 15.
-Add constant amount of nucleons every iteration. This is shown on picture 17.
-Add growing amount of nucleons every iteration (for examle 10, 20, 30, etc.) This situation is presented on picture 16.



Picture 15. Nucleons added once.

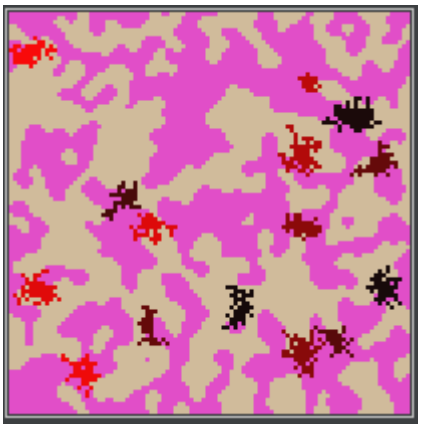


Picture 16. Growing number of nucleons every iteration.

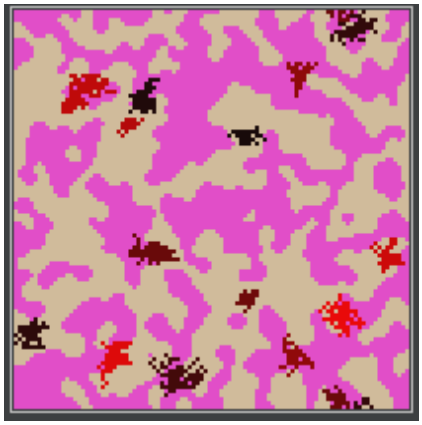


Picture 17. Constant number of nucleons added every iteration.

On addition to those 3, the nucleons also have the option of being placed anywhere, or just on grain boundaries. These two variants are shown on pictures 18 and 19.



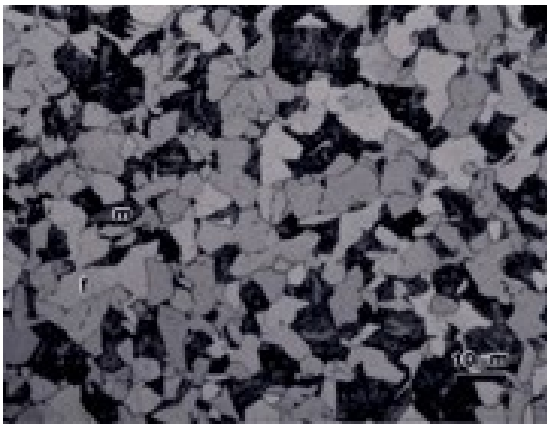
Picture 18. Nucleons on grain boundaries



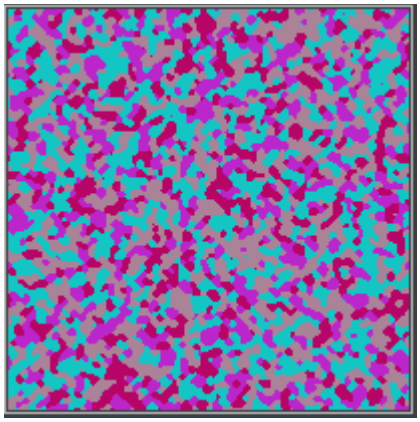
Picture 19. Nucleons positioned randomly.

3. Summary

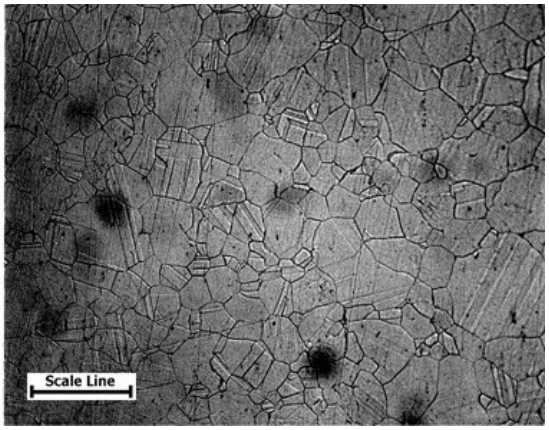
The application allows user to generate many different mincrostructures. Most of them are similar to the real-life misrostructures. Pictures 20, 21, 22, 23 shows example simulations along with their genuine real-life microstructures.



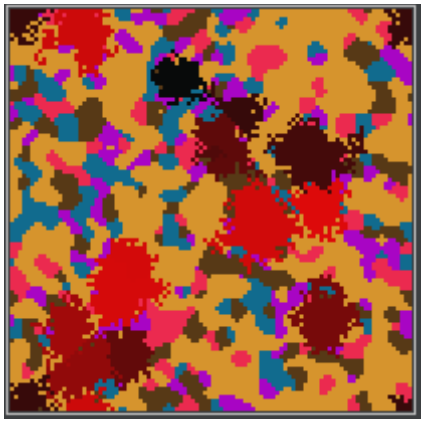
Picture 20. Steel [1]



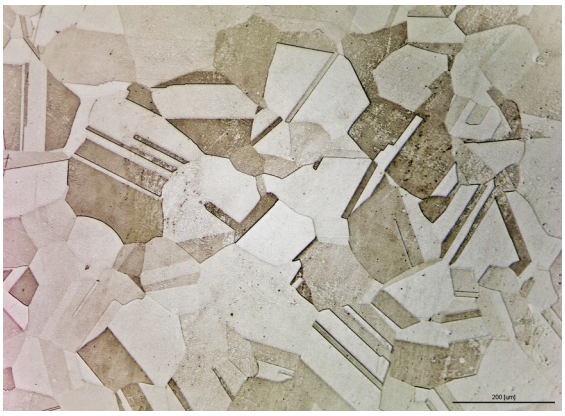
Picture 21. Simulation



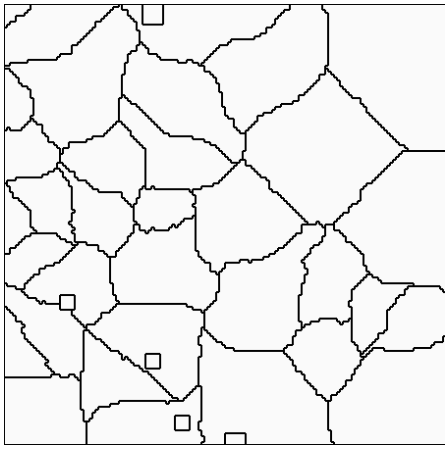
Picture 22. Another steel [2]



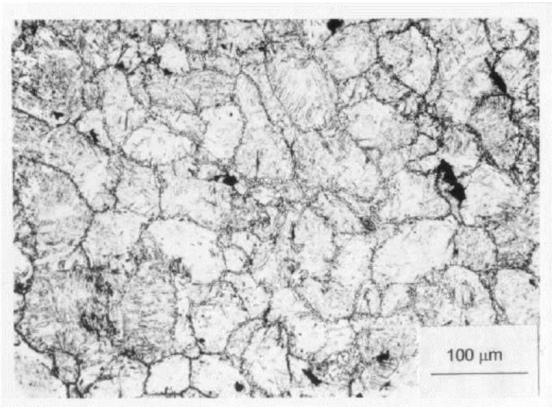
Picture 22. Simulation with recrystalization



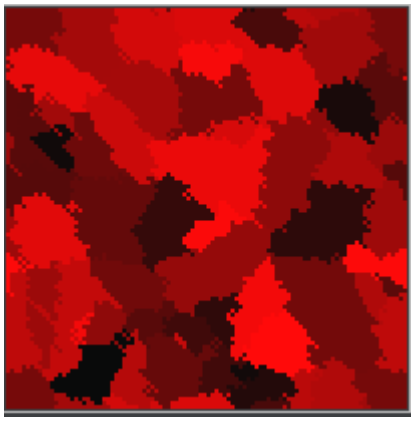
Picture 23. Stainless steel microstructure



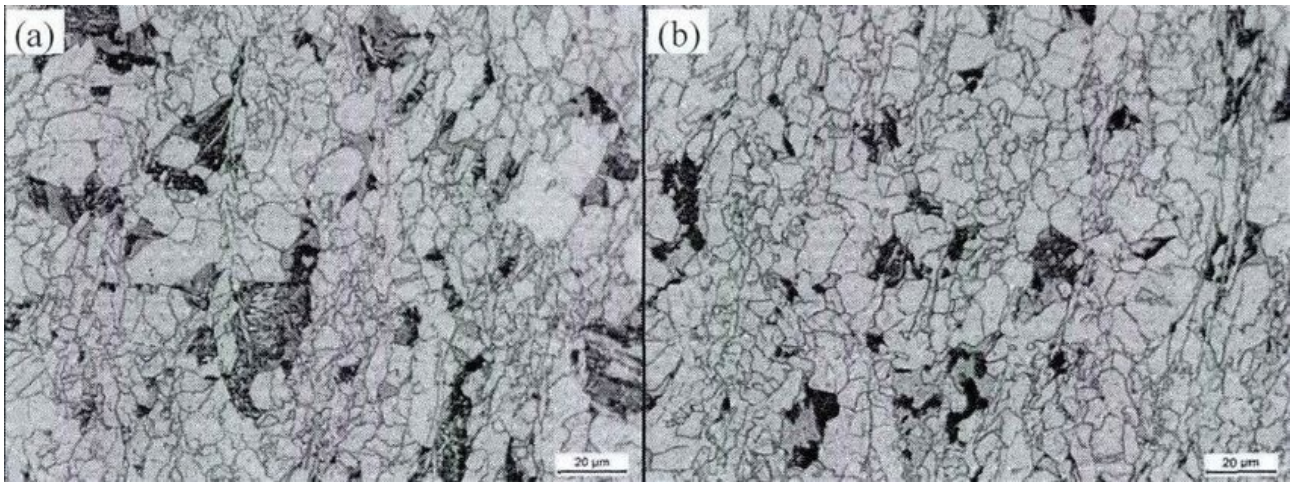
Picture 24. Boundaries of CA simulation



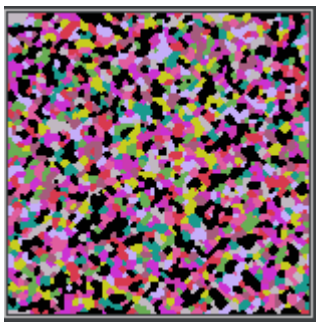
Picture 25. Recristallized austenite steel



Picture 26. Recristallized simulation



Picture 27. Microstructure od Nb-Ti steel.



Picture 28. Simulation with inclusions made as substructure.

4. Bibliography

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