Second report

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Multiscale Modeling

In this project I decided to use C# mainly because of ease of creating almost anything in this language. It can be quickly applied to develop Windows desktop applications and games. Also Winforms made it infinitely faster to develop transparent GUI within minutes.

User interface :

User interface consists of few buttons and inputs that are used to control process of grain growth simulation. Window of application have two parts. On left hand side we have simulation board where visualisation of modelled process is performed. On right hand side is simulation control panel where all meaningful parameters of simulations are placed.

Most of those inputs are already named in such way it is very self-explanatory but I will go out of my way to describe it in best manner I can imagine.

Selecting button Grain growth right away is going to start simulation with default parameters what are already set in all fields.

Button reset is as name suggests is used for start simulation over again.

Next up is Neighbourhood type that has two options, either it is von Neumann or Moore. This changes the way that grain growth behaves.

Number of grains is influencing amount of initial grains. This number have to be in range between 1 and 100.

Number of inclusions decides whether there should be any more grains that already are.

This number have to be in range between 1 and 100.

Input called size of inclusion changes how many pixels make each inclusion is made of. This number have to be in range between 1 and 100.

Shape of inclusion governs the way the inclusion is shaped. It is either circle or square.

Last input in this section is changing whether inclusions are added to simulation space before or after grain growth.

New parts to second report are as follows :

Monte Carlo which expands ability of app to also perform Monte Carlo microstructure generation. For this button there are also 2 lists that control amount of States of MC and amount of iterations of MC algorithm. We can compare CA and MC method in Fig 2-3.

Another addition is Dual Phase button and 4 radio buttons that control what kind of Dual Phase we are going to perform.

Last part of new features is Static recrystallization button. This allows to use energy to create new grains and grow them according to energy.

We also gain ability to view either Grains or said Energy.

There is also ability to choose how energy is distributed : Homogenously or Heterogenous.

Another thing is to choose whether Nucleons should stay in constant number or continuously grow.

Lastly there is also field to control amount of recrystallization steps.

Four buttons on the bottom are dedicated to export/import actions. This makes it possible to export simulation space to .txt or .bmp files in any desired location with any name and also import it in the same manner.

Exemplary start up screen of project application.

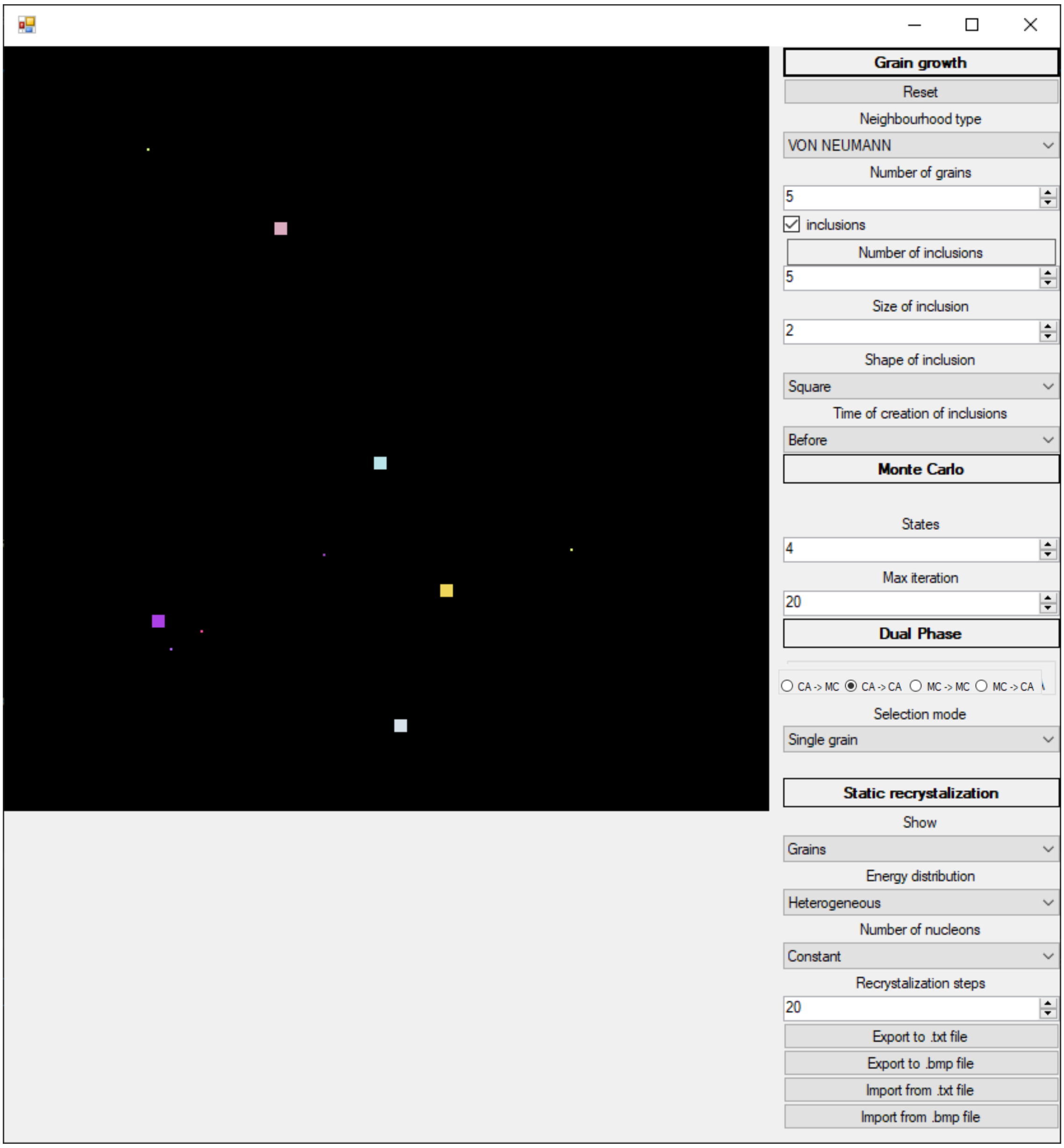


Fig. 1 User Interface

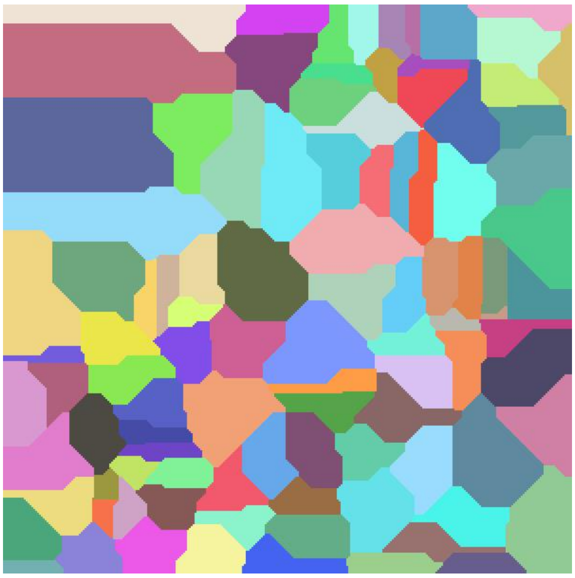


Fig. 3 Structure generated with CA method.

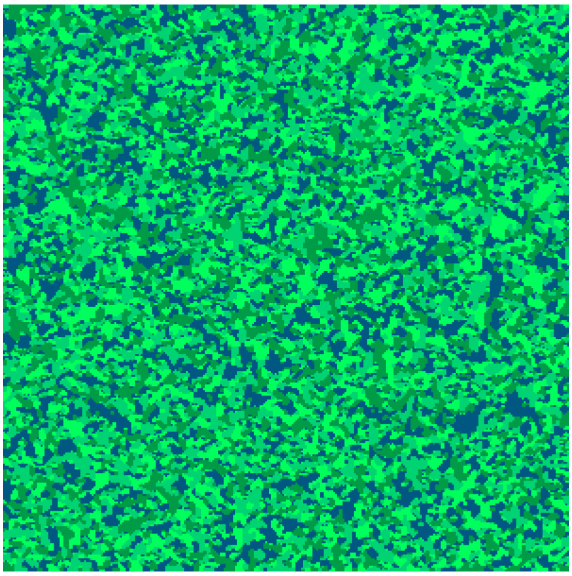


Fig. 2 Structure generated with MC method.

Dual Phase

When user wants to add dual phase it is possible to click Dual Phase button which will check whether structure is already there if so, it will prompt user to select grains to stay till next phase. There is possibility to choose with single grains or all grains in given color. Figures 5-7 showcase each of Dual Phase modes.

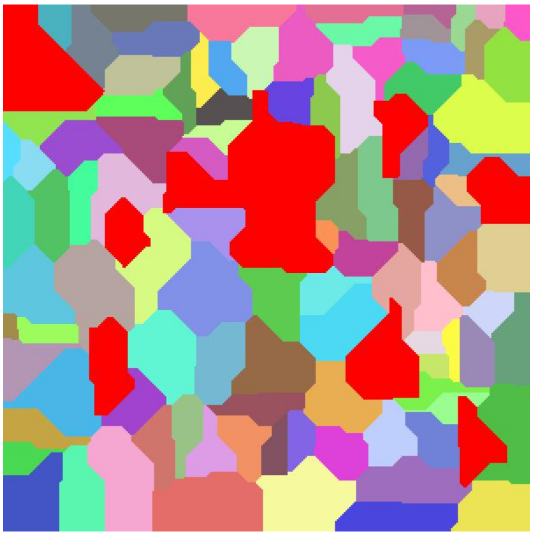


Fig. 5 CA-CA

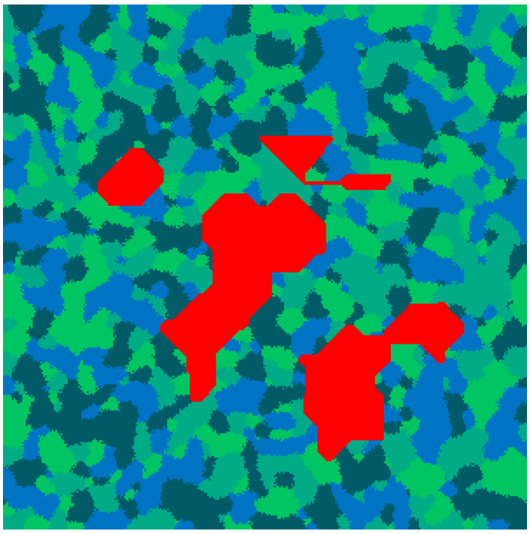


Fig. 4 CA-MC

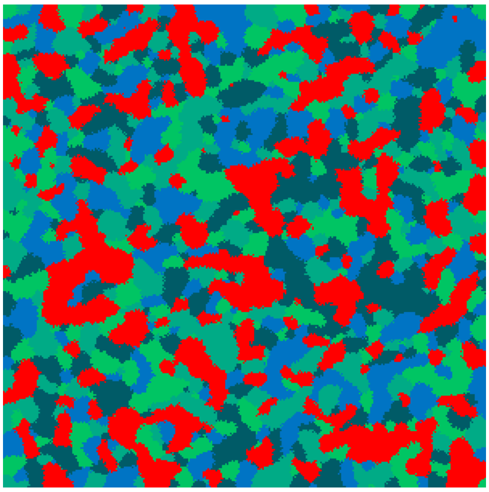


Fig. 7 MC-MC

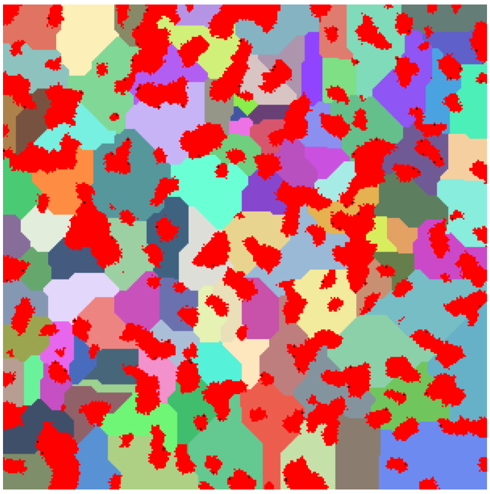


Fig. 6 MC-CA

Monte Carlo SRX – Static Recrystallization

Distribution of energy can be visualized with previously generated structure. User can choose to show energy distribution changing from view on Grains to Energy. All of them are shown in Figures 8-10.

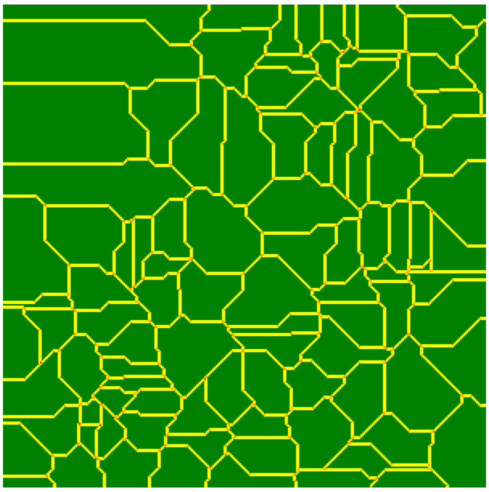


Fig. 9 CA Hetergenous energy Distribution

Fig. 8 Homogenous energy distribution

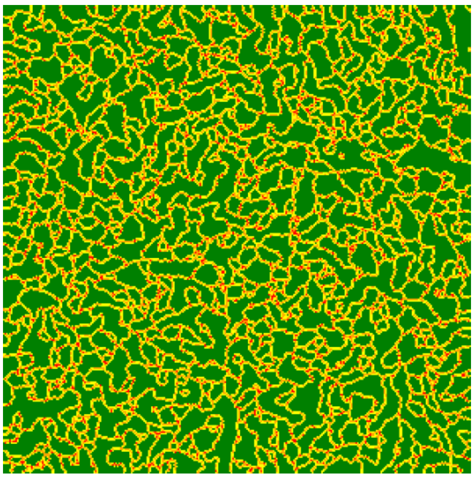


Fig. 11 MC Hetergenous energy Distribution

Fig. 10 Homogenous energy distribution

SRX Recrystallization stats when so called button is clicked. New grains have possibility to appear only in places where energy high. Homogeneous energy distribution allows grains to grow anywhere in structure. Heterogeneous energy distribution allows only on grain boundaries because energy is higher there. We can choose if we want them to grow on constant rate or keep increasing. Figs 12-18 showcase various option tested in this module.

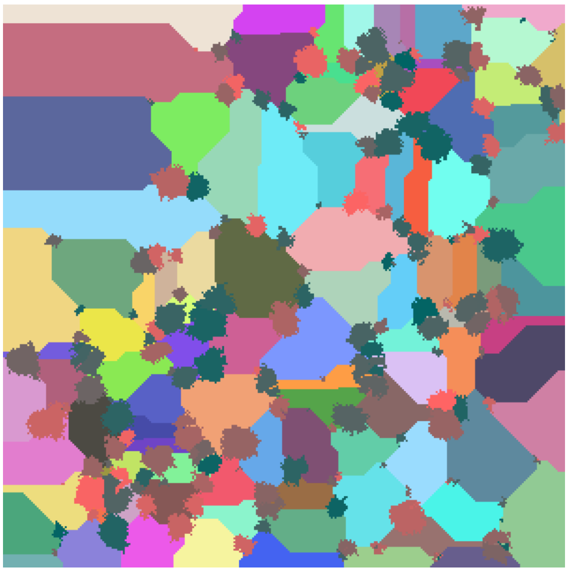


Fig. 12 CA SRX Grains

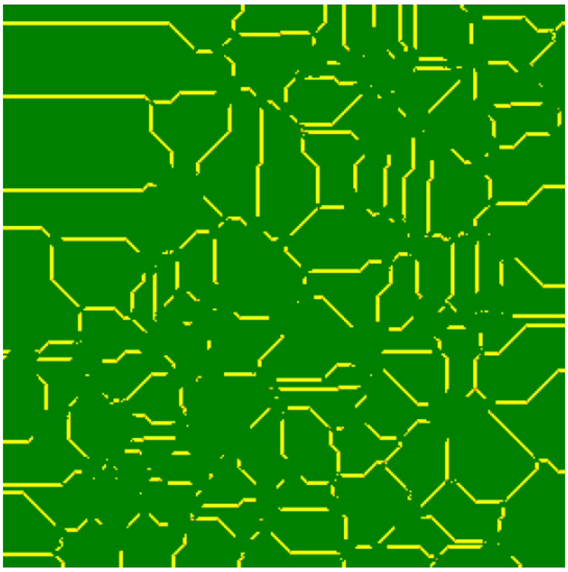


Fig. 13 CA SRX energy

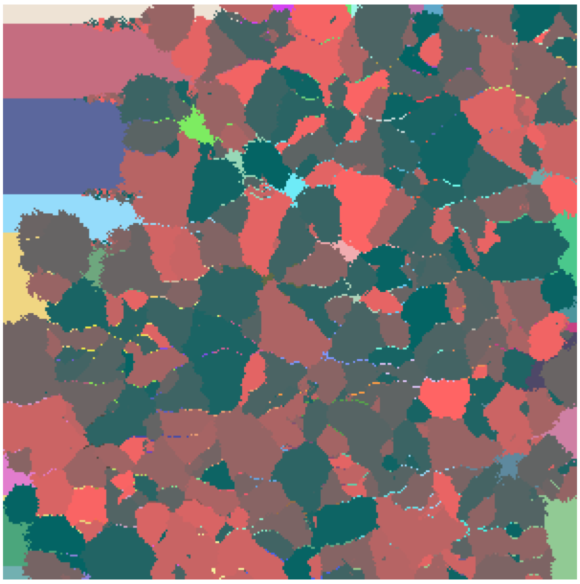


Fig. 15 More CA SRX Grains

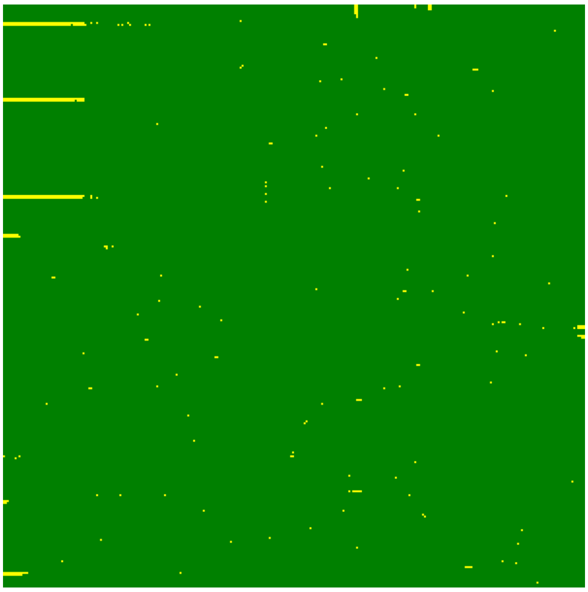


Fig. 14 CA SRX energy

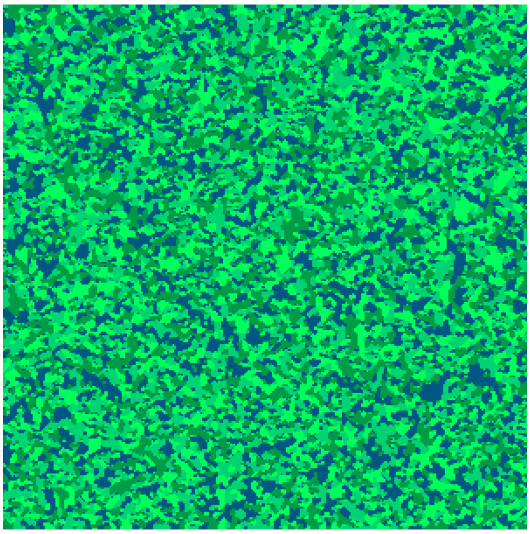


Fig. 17 MC Grains

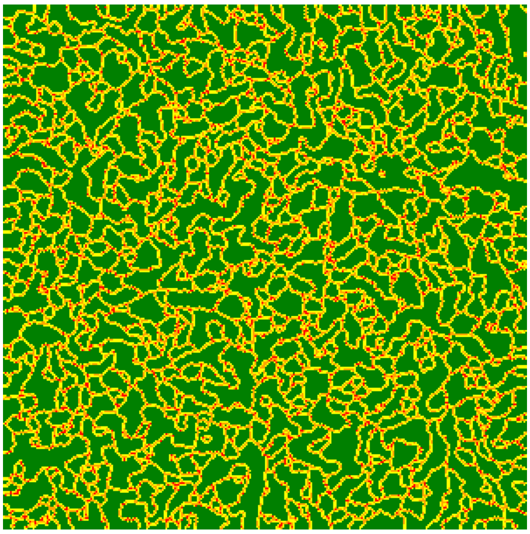
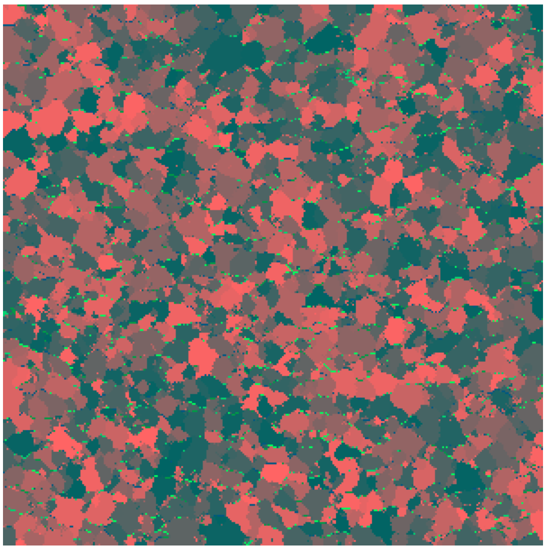


Fig. 16 MC energy



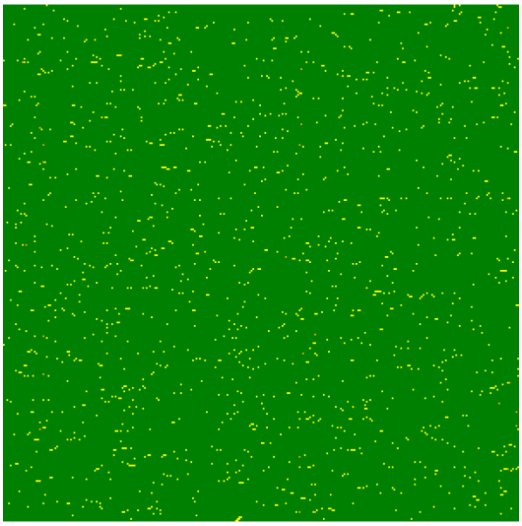


Fig. 18 MC energy after SRX

Fig. 19 MC SRX

Real structures

The attempts on comparing real structures with generated ones gives us a hint that our simulation is just an approximation of what is really happening in those structures. Even though MC method in some cases gives closer approach on what nature is producing it still is not good enough [Fig 22 and 24]. Recrystallization depends how user is going to choose grains. Dual Monte Carlo in my opinion is closest one to be relevant in material modelling [fig 20-21.] . SRX like in fig 23 and 25 also need some improvements in state of growing and expansion.

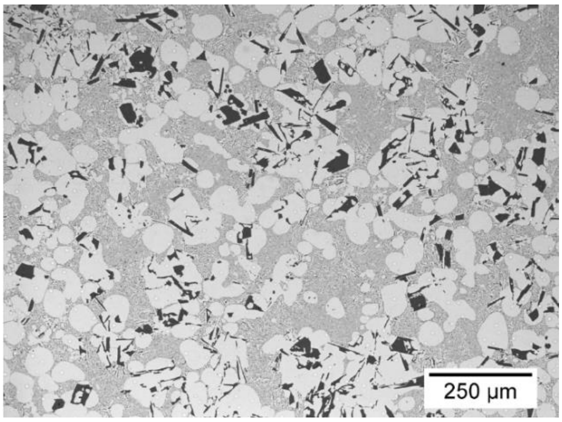


Fig. 21 As-cast microstructure of a CSIR R-HPDC unmodified Al-Si binary eutectic. [1]

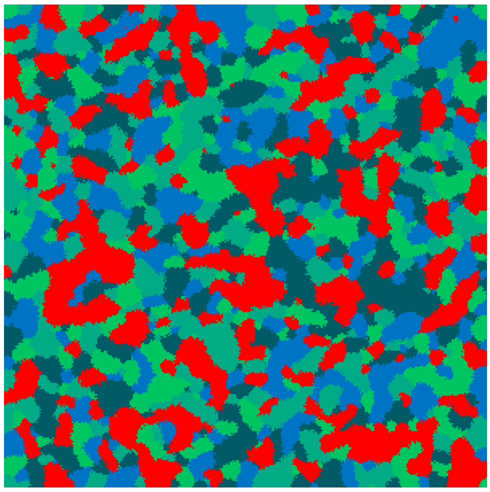
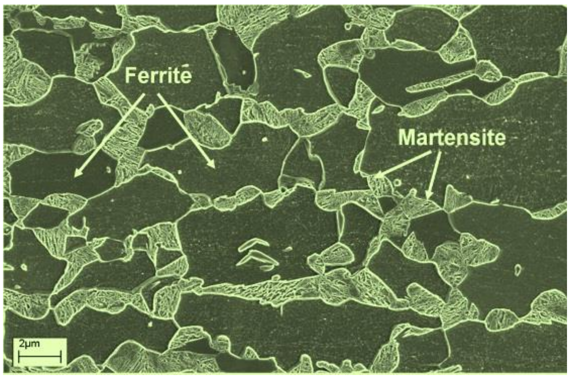


Fig. 20 Generated microstructure



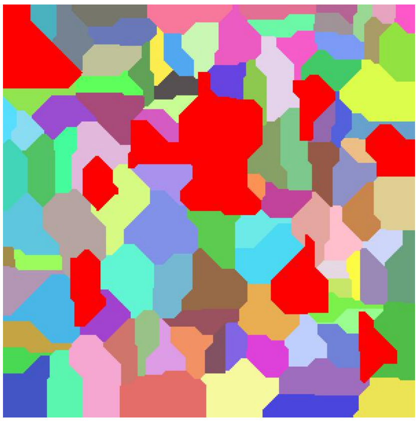


Fig. 22 Generated microstructure

Fig. 24 Micro structure of DP steel [2]

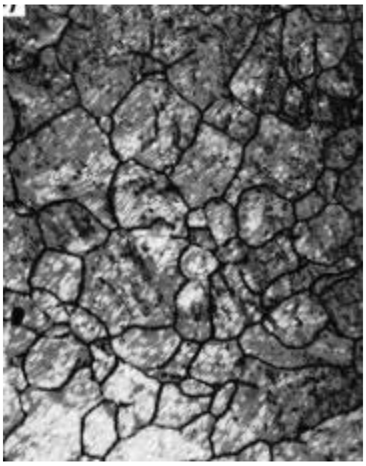


Fig. 25 SRX real life example [3]

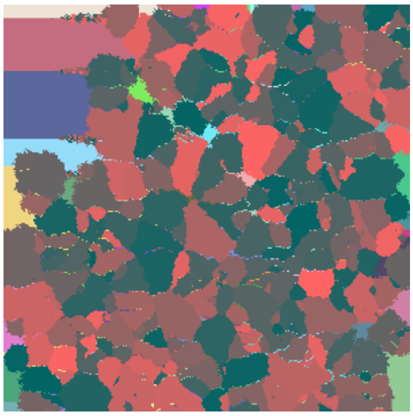


Fig. 23 Generated microstructure

[1] https://www.researchgate.net/figure/As-cast-microstructure-of-a-CSIR-R-HPDC-unmodified-Al-Si-binary-eutectic-11-Metal_fig4_271570890
[2] http://ispatguru.com/dual-phase-steels/
[3] https://www.researchgate.net/figure/Optical-deformed-microstructures-of-30Cr2Ni4MoV-steel-after-metadynamic-recrystallization_fig4_251608599