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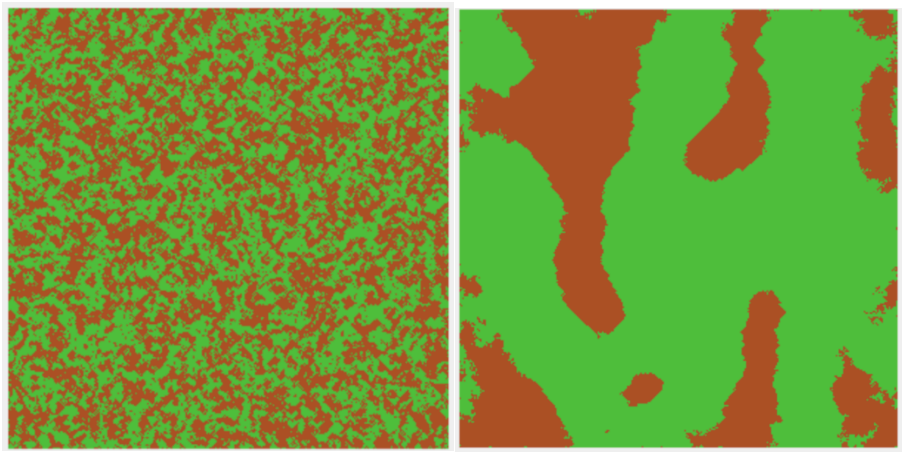
2nd Report – MC Static Recrystallization Algorithm

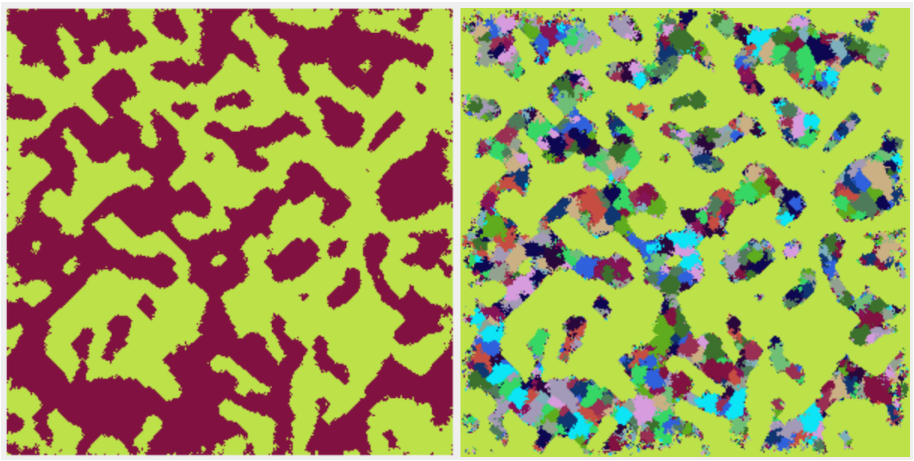
Monte Carlo Grain Growth

Number of states: 2



Picture 1: Monte Carlo at the beginning of the simulation and after 500 iterations

Dualphase MC -> MC



Picture 2: Monte Carlo dualphase

Recrystallization is a process by which deformed grains are replaced by a new set of unreformed grains, that nucleate and grow until the original grains have been entirely consumed. Recrystallization is usually accompanied by a reduction in the strength and hardness of a material and a simultaneous increase in the ductility.
Due to complex structure of metals their behavior depends on many factors like grain size, grain boundaries, dislocation density, stacking fault energy etc.

Initial material morphology:

First step, before we use algorithm, is to generate initial material morphology (CA or MC method). Then we can start with SRX MC. First is to distribute stored energy (H) for each grain. There are two options of energy distribution.

Homogenous (energy of each grain is the same)**:**

Picture 3: Homogenous distribution

Heterogeneous (maximal energy - red is stored only on boundaries between different grains and minimal energy is assigned to other - yellow)**:**

Picture 4: Heterogeneous distribution

Nucleation: next algorithm step is to apply random nucleation on boundaries or anywhere.

Picture 5: Grains are generated on boundaries, where is the highest energy

Picture 6: 60 randomly generated grains

Neighbors check: after nucleation, next step is like standard Monte Carlo Algorithm. Firstly, we are selecting site randomly. If in our selected site is recrystallized neighbor, we compute energy for our site from eq. 1

$$E_i^{beforeSRX} = J\sum_{j=1}^{Z}(1-\delta_{SiSj}) + H_i \qquad \text{Eq. 1}$$

Then we place recrystallized element on our current space and compute energy for it from equation 2.

$$E_i^{afterSRX} = J\sum_{j=1}^{Z}(1-\delta_{SiSj}) \qquad \text{Eq. 2}$$

Last step is to check if computed energy for equation 3 is lower or equal zero. If it's true we change current element to recrystallized, else we replace element to old one.

$$\Delta E_i = E_i^{afterSRX} - E_i^{beforeSRX} \qquad \text{Eq. 3}$$

All steps above repeat for all sites. Whole algorithm stops after number of iterations assumed by user.

Results

Neighborhood: Moore
Simple Grain Growth: 20 grains

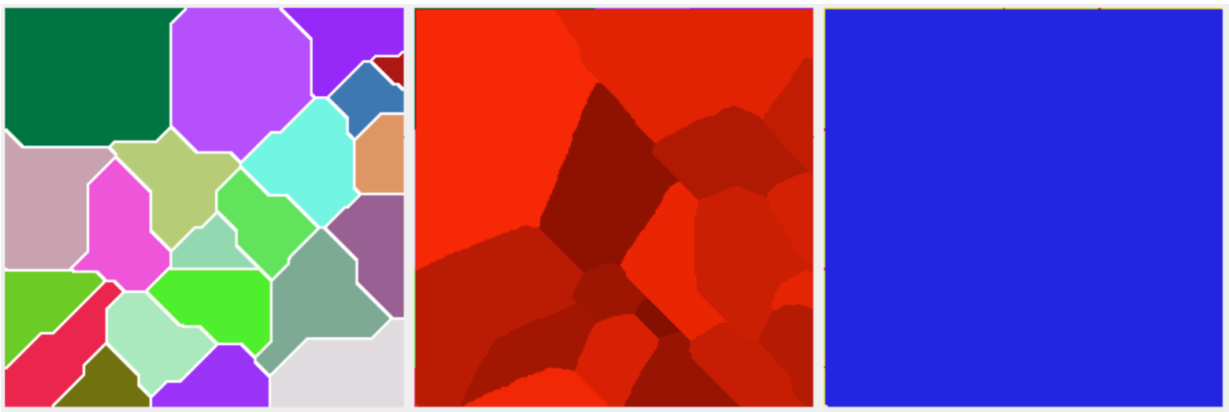
Monte Carlo SRX:
Min. energy: 2
Max. energy: 6
Grains amount: 20

0 MCS

20 MCS

60 MCS

120 MCS



In the last step, whole previous structure is covered by the new one.

Conclusion

Recrystallization is defined as the process in with grains of a crystal structure come in new structure or crystal shape. As we can notice our algorithm works the same. We have got deformed microstructure on very beginning and then by MCSRX we are trying to reduce deformation by replacing old grains by the new one. After a certain amount of steps our old microstructure is completely replaced.