Fully automated orientation relationship calculation and prior austenite reconstruction by random walking clustering

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Outline

Introduction

OR calculation

Clustering of product grains

Results

- Validation based on the retained Austenite
- Validation based on the same area

Conclusions

Motivation

- In-house development of reconstruction[1234] software
- Fully automated
- Fast

[1] C Cayron, B Artaud, and L Briottet. "Reconstruction of parent grains from EBSD data". In: *Materials characterization* 57.4 (2006), pp. 386–401.

[2] Goro Miyamoto et al. "Mapping the parent austenite orientation reconstructed from the orientation of martensite by EBSD and its application to ausformed martensite". In: *Acta Materialia* 58.19 (2010), pp. 6393–6403.

[3] Pierre Blaineau et al. "A new approach to calculate the γ orientation maps in steels". In: *Solid State Phenomena* 160 (2010), pp. 203–210.

[4] V Tari, AD Rollett, and H Beladi. "Back calculation of parent austenite orientation using a clustering approach". In: *Journal of Applied Crystallography* 46.1 (2013), pp. 210–215.

Calculating the real OR

- Improves the accuracy during reconstruction.
- BUT ... current methods[5][6] are based on semi automated procedures where the user has to manually select parent phase grains.

[5] G Miyamoto, N Takayama, and T Furuhara. "Accurate measurement of the orientation relationship of lath martensite and bainite by electron backscatter diffraction analysis". In: *Scripta Materialia* 60.12 (2009), pp. 1113–1116.

[6] M Humbert et al. "Refinement of orientation relations occurring in phase transformation based on considering only the orientations of the variants". In: *Scripta Materialia* 64.2 (2011), pp. 114–117.

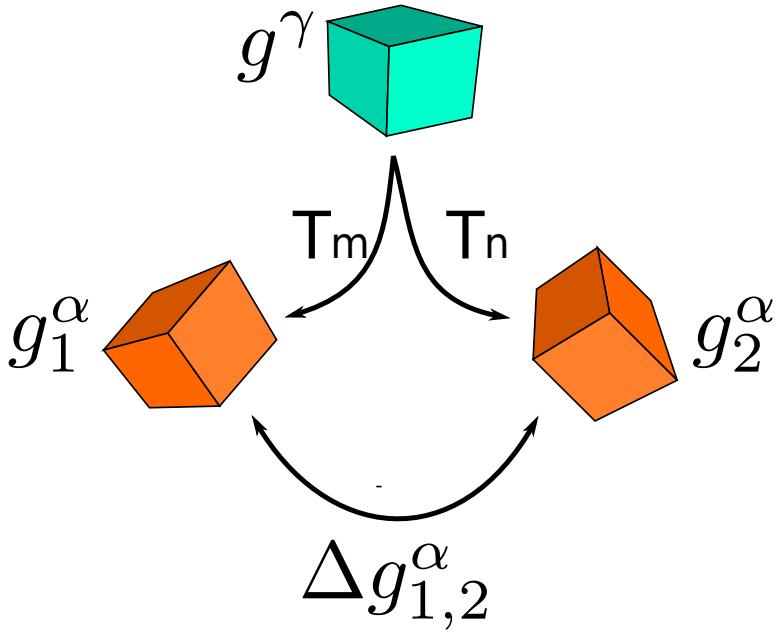
OR deviation

$$T_m^{a' \leftrightarrow \gamma} g^{\gamma} \left(g_a^{a'}\right)^{-1} = 0$$

$$T_m^{a' \leftrightarrow \gamma} T_n^{\gamma \leftrightarrow a'} g_a^{a'} \left(g_b^{a'}\right)^{-1} = 0$$

$$T_m^{a' \leftrightarrow \gamma} T_n^{\gamma \leftrightarrow a'} \Delta g^{a'} = 0$$

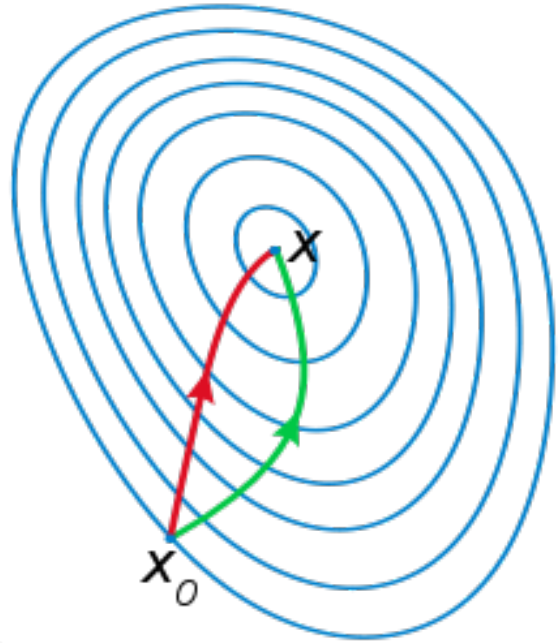
$T = [T_0, T_1, \ldots. T_K]$



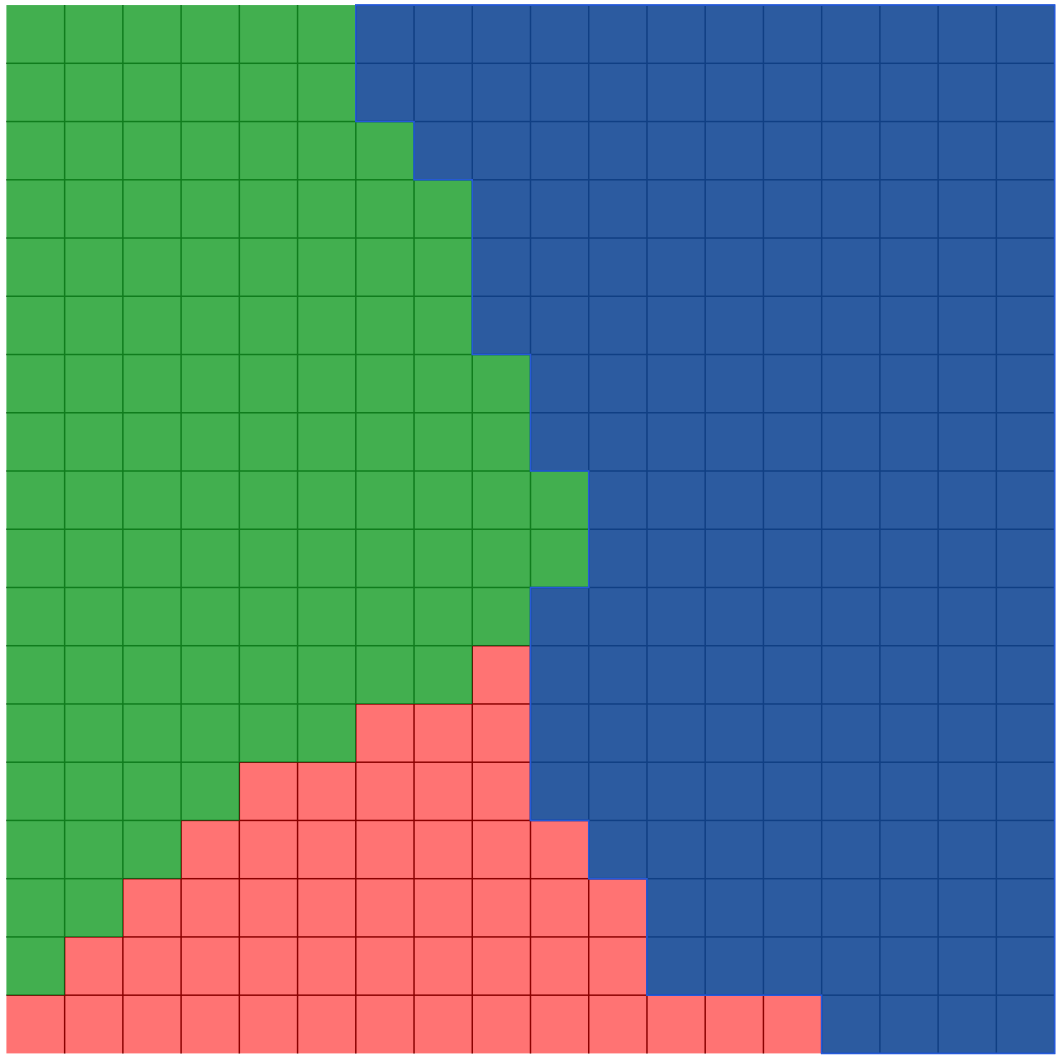
OR optimization

$$\Delta OR = T_m^{a' \leftrightarrow \gamma} g^{\gamma} \left(g_a^{a'} \right)^{-1}$$

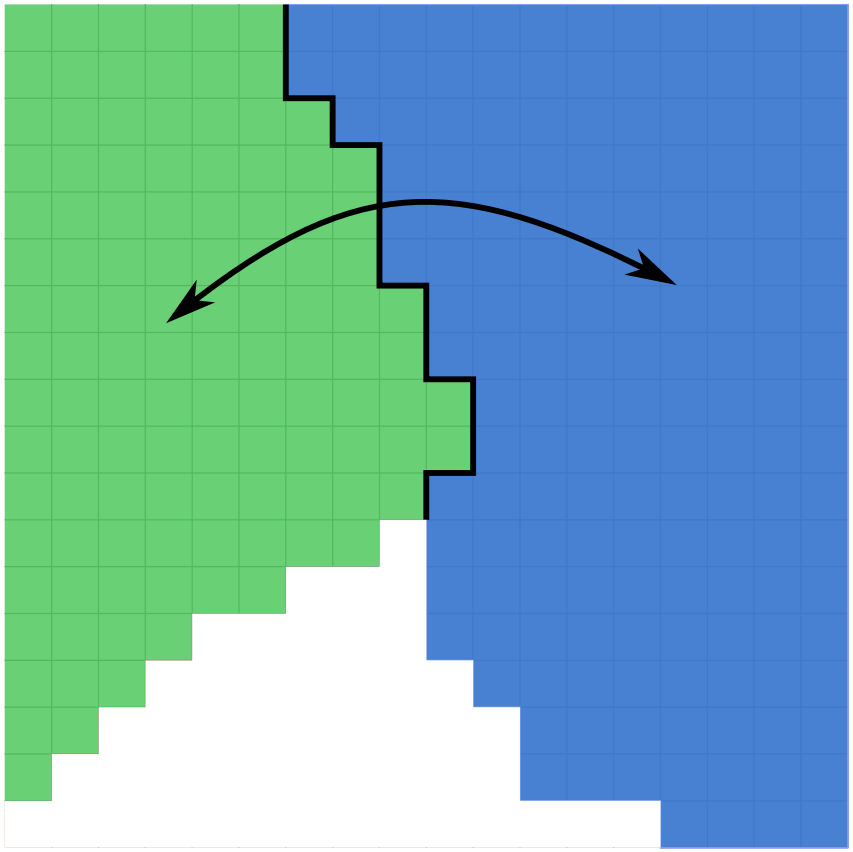
$$\Delta OR = T_m^{a' \leftrightarrow \gamma} T_n^{\gamma \leftrightarrow a'} \Delta g_{1,2}^{a'}$$



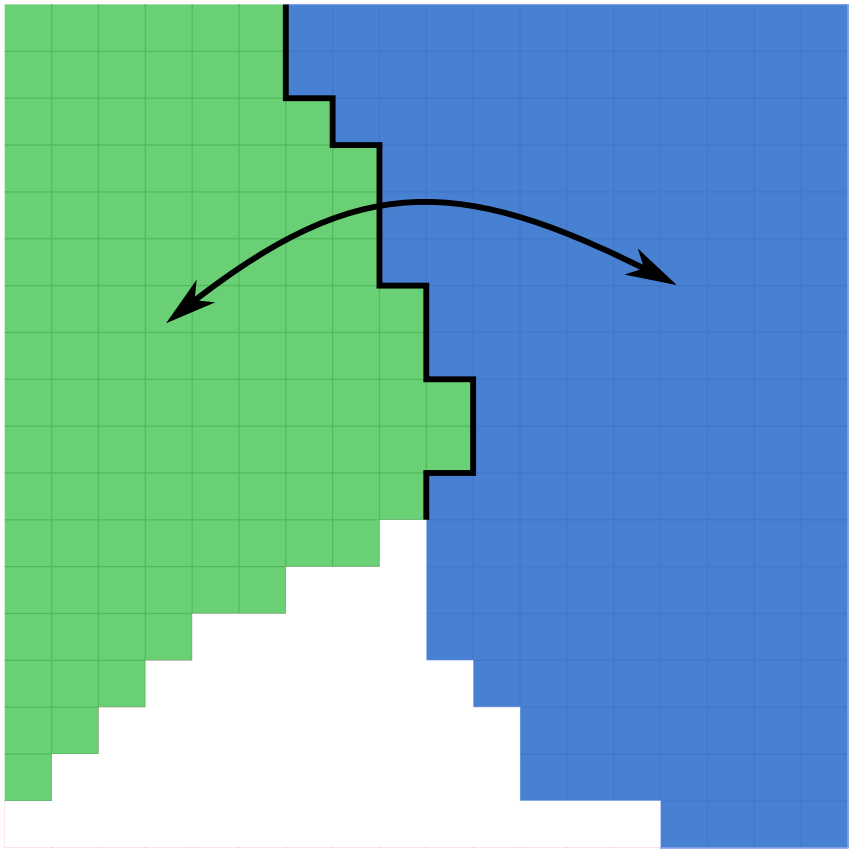
OR region

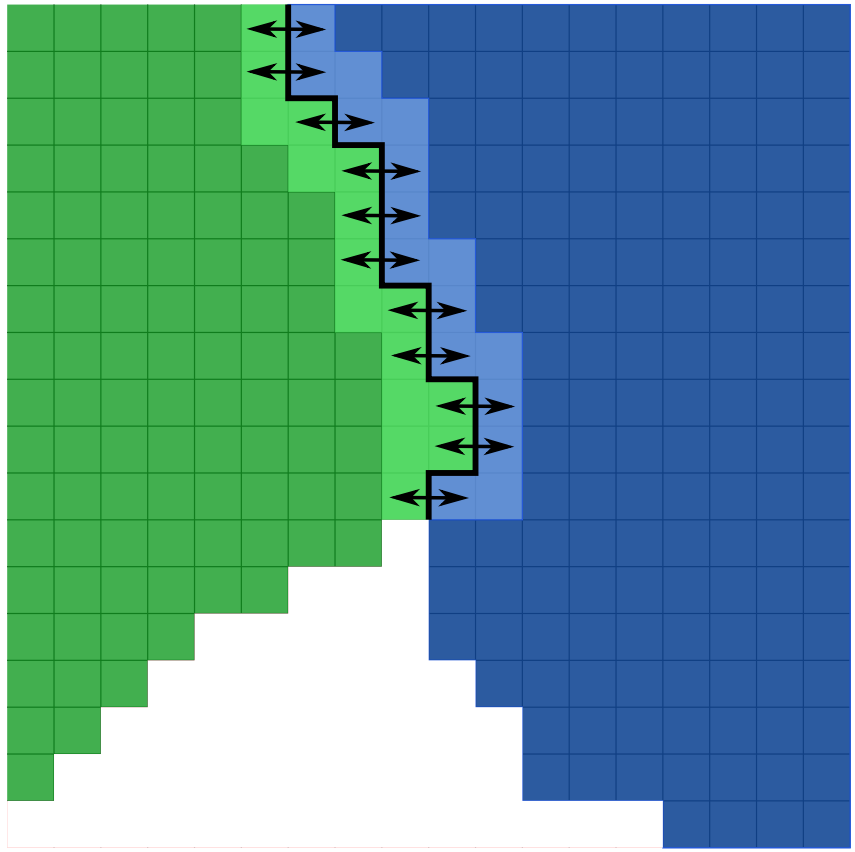


OR region



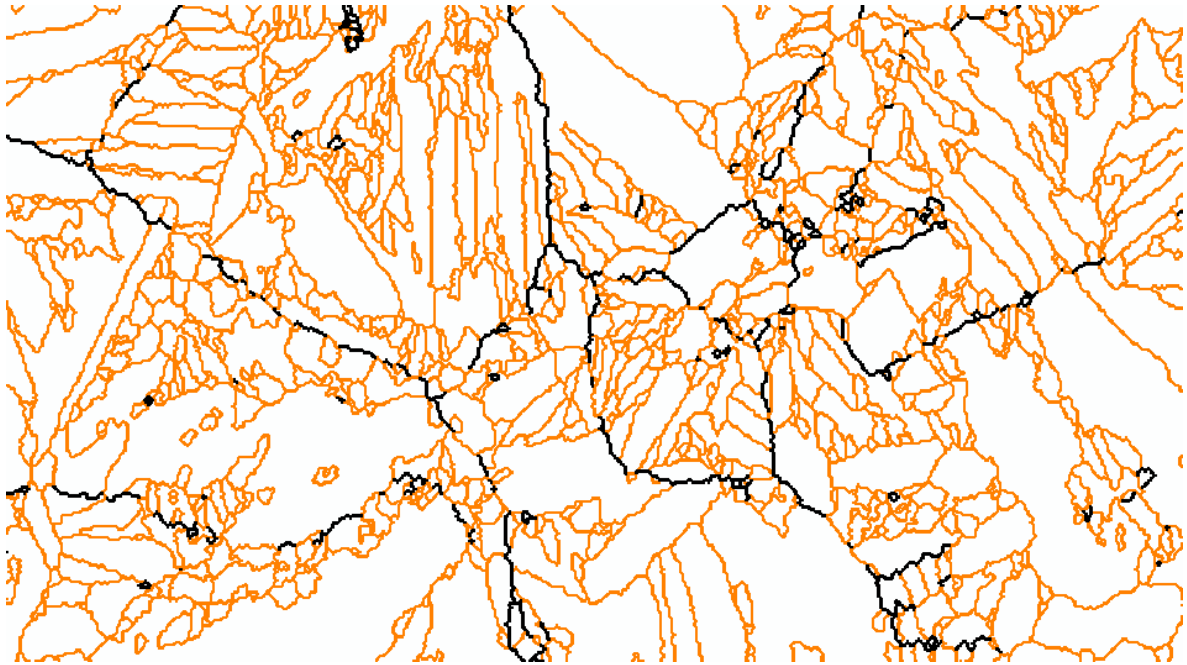
OR region



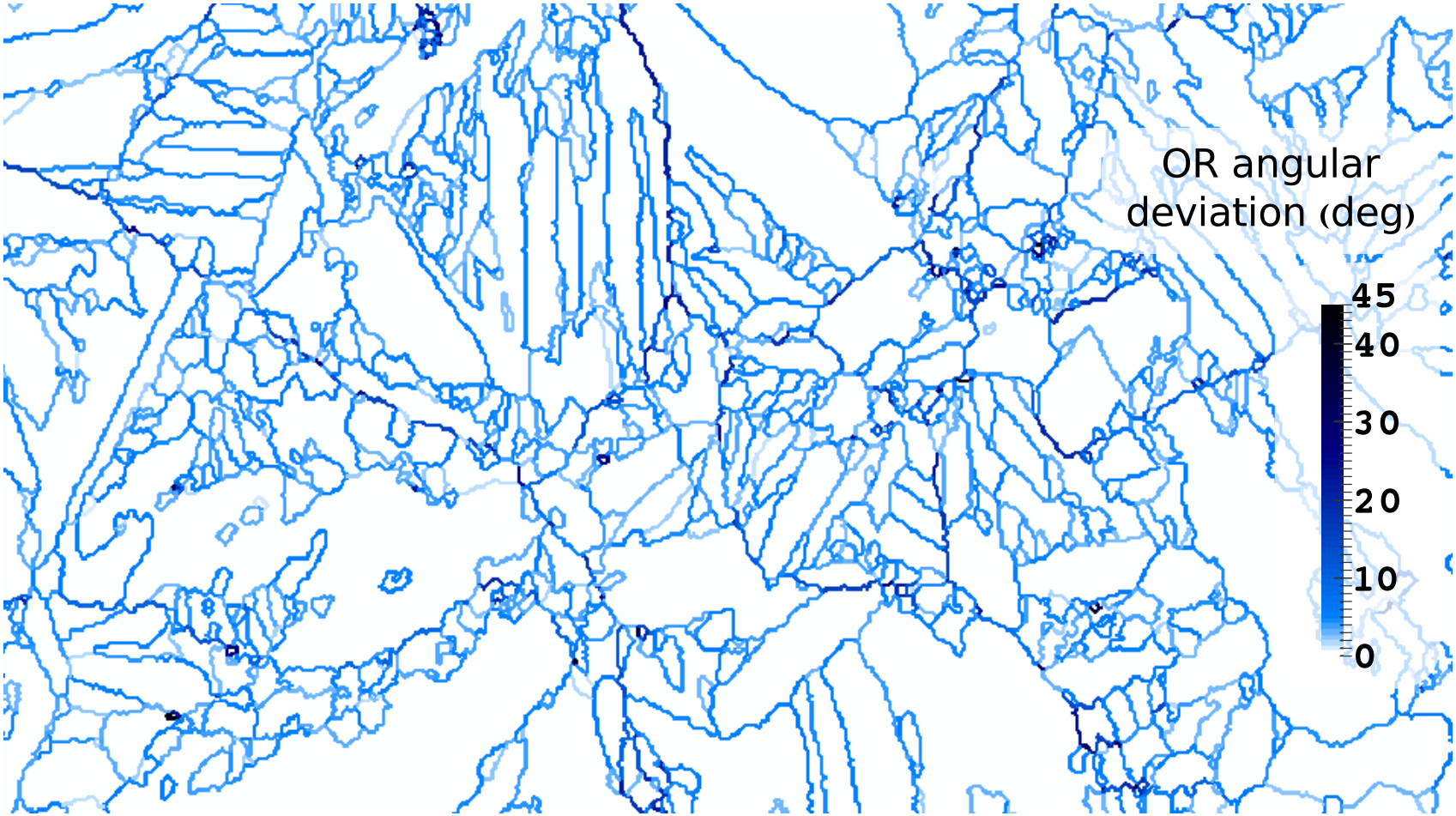


Considerations

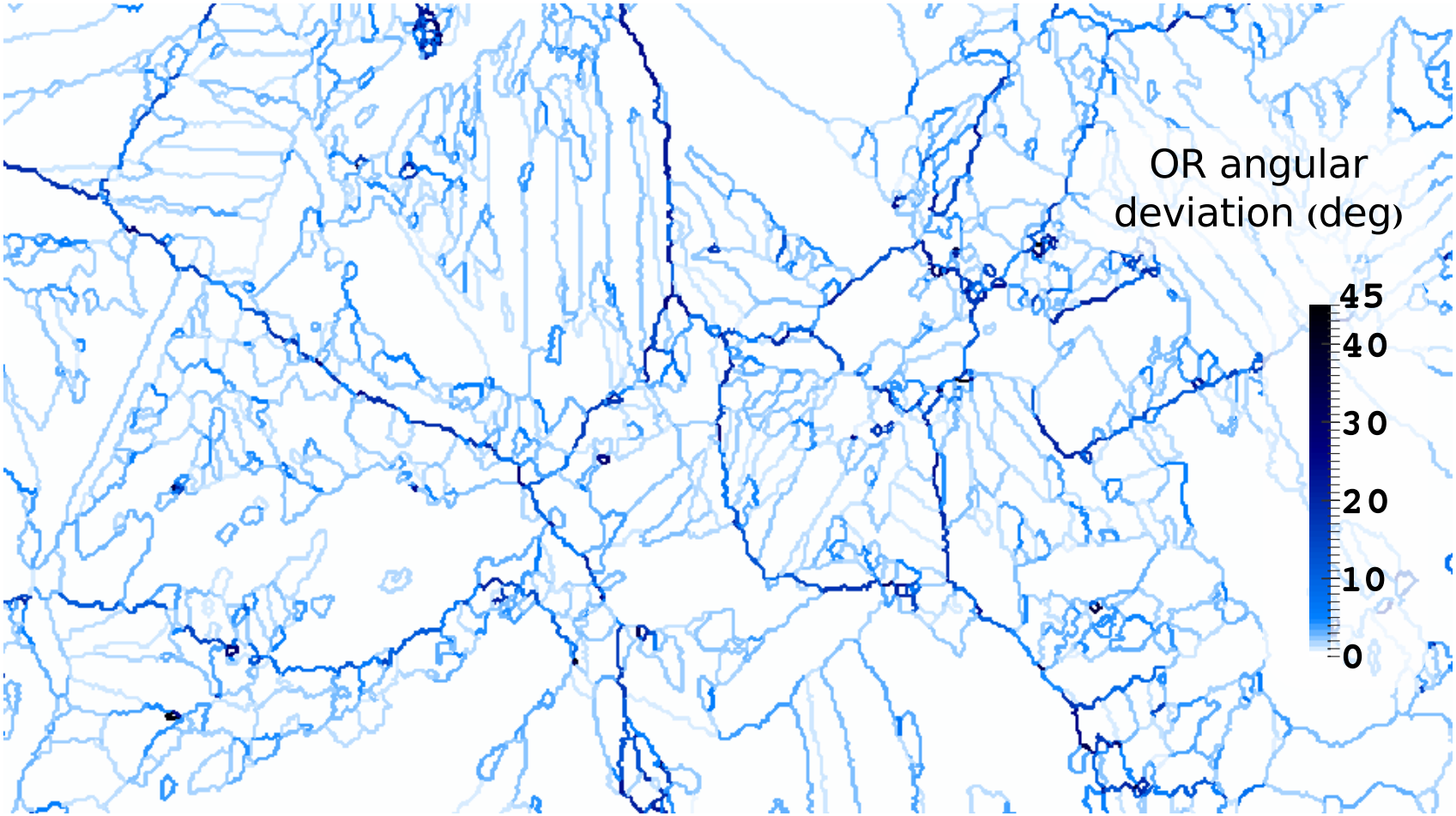
- filter grain boundaries with $\Delta OR \leq 10°$
- randomly sample 1000 grain boundaries
- parent GB $\ll$ product-product GB



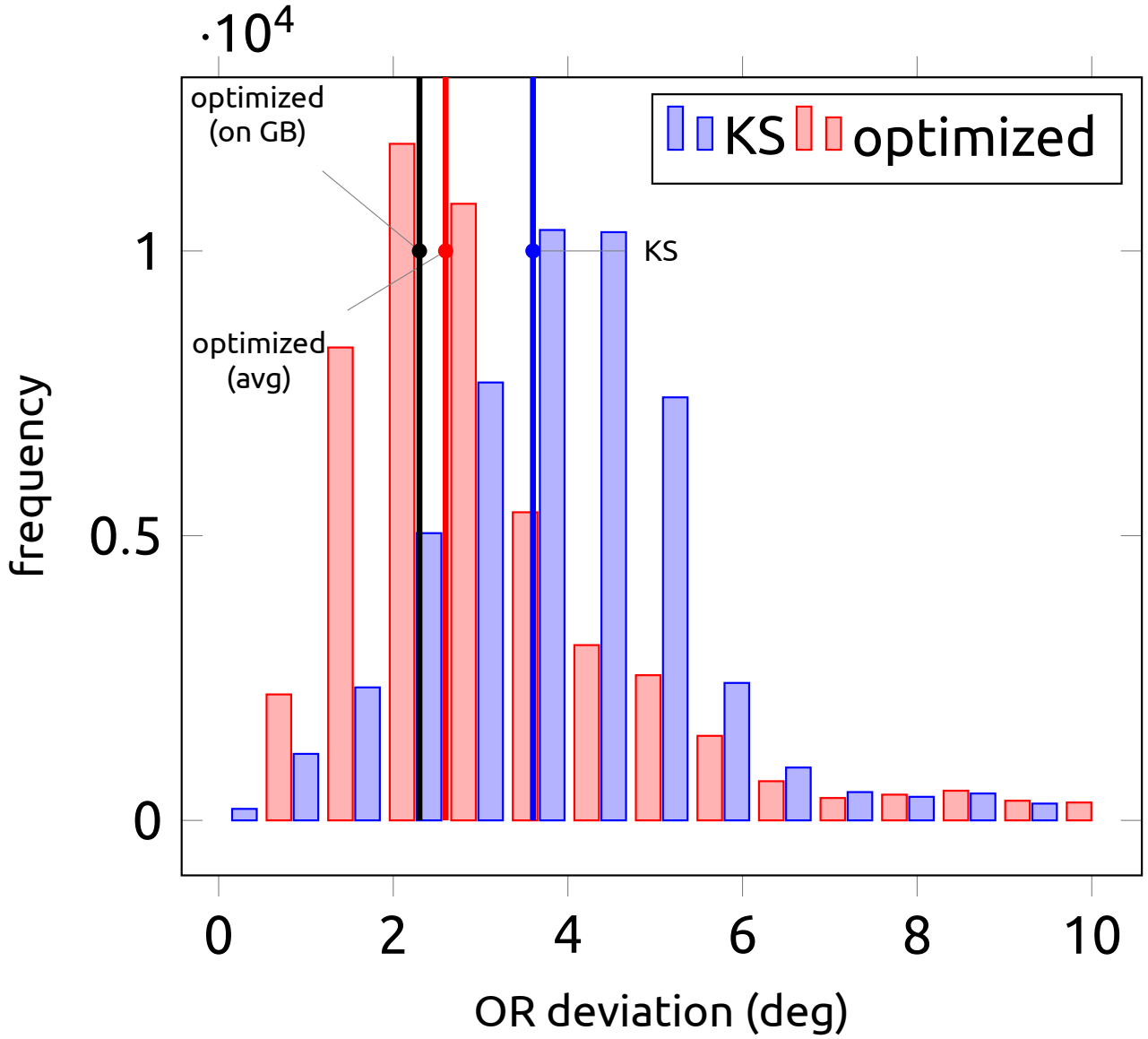
Optimization for FeNi



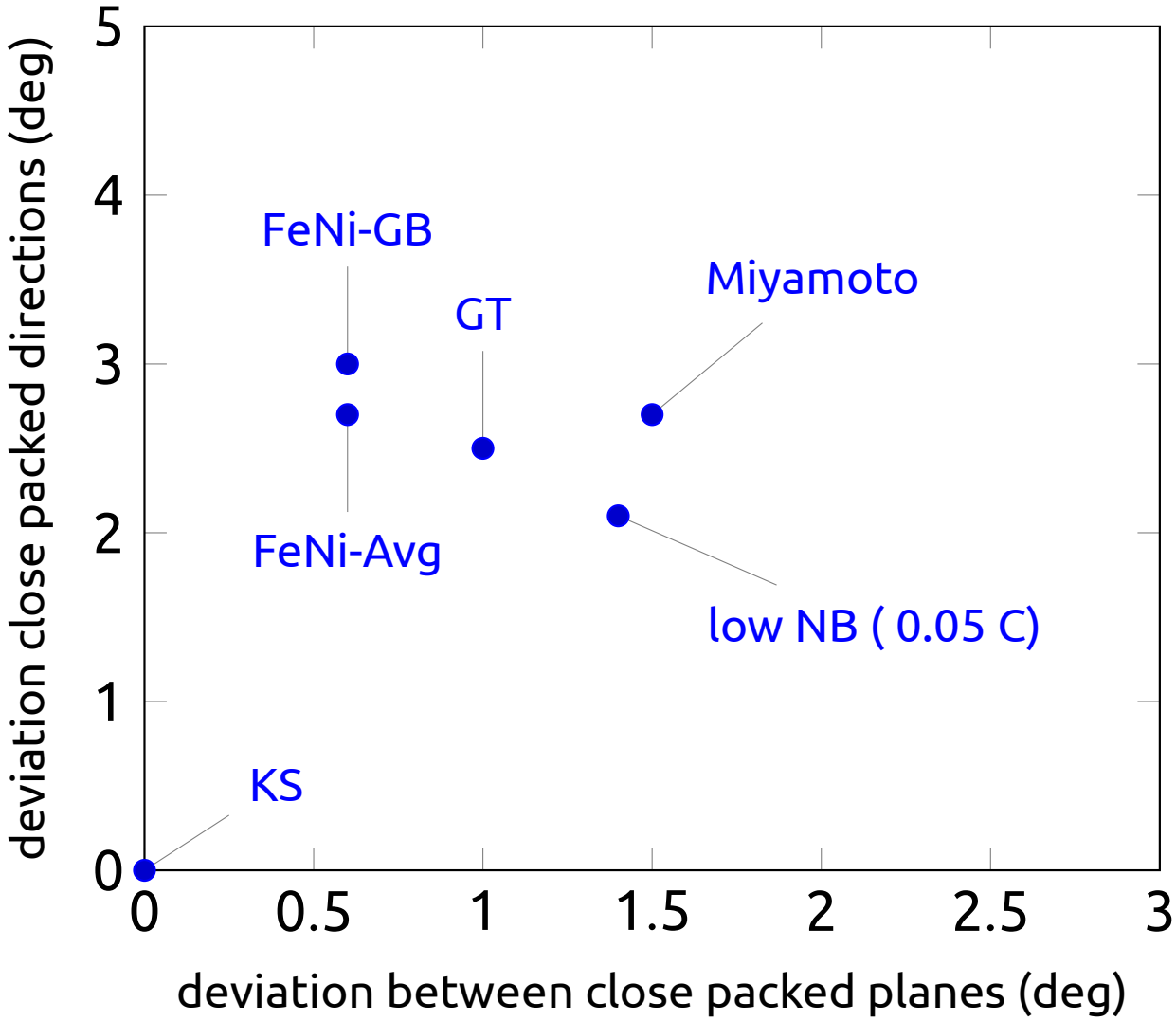
Optimization for FeNi



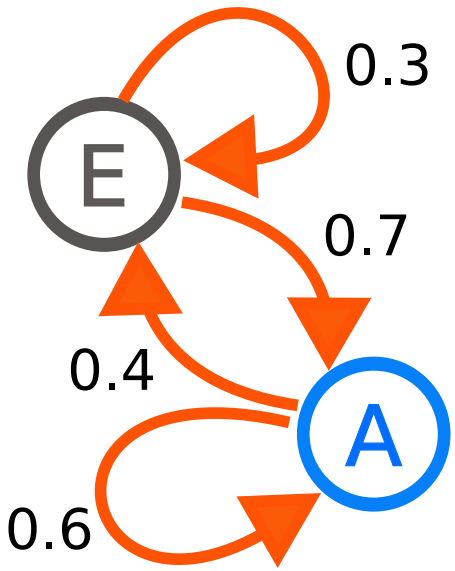
Optimization for FeNi



OR comparison



Markov chain clustering



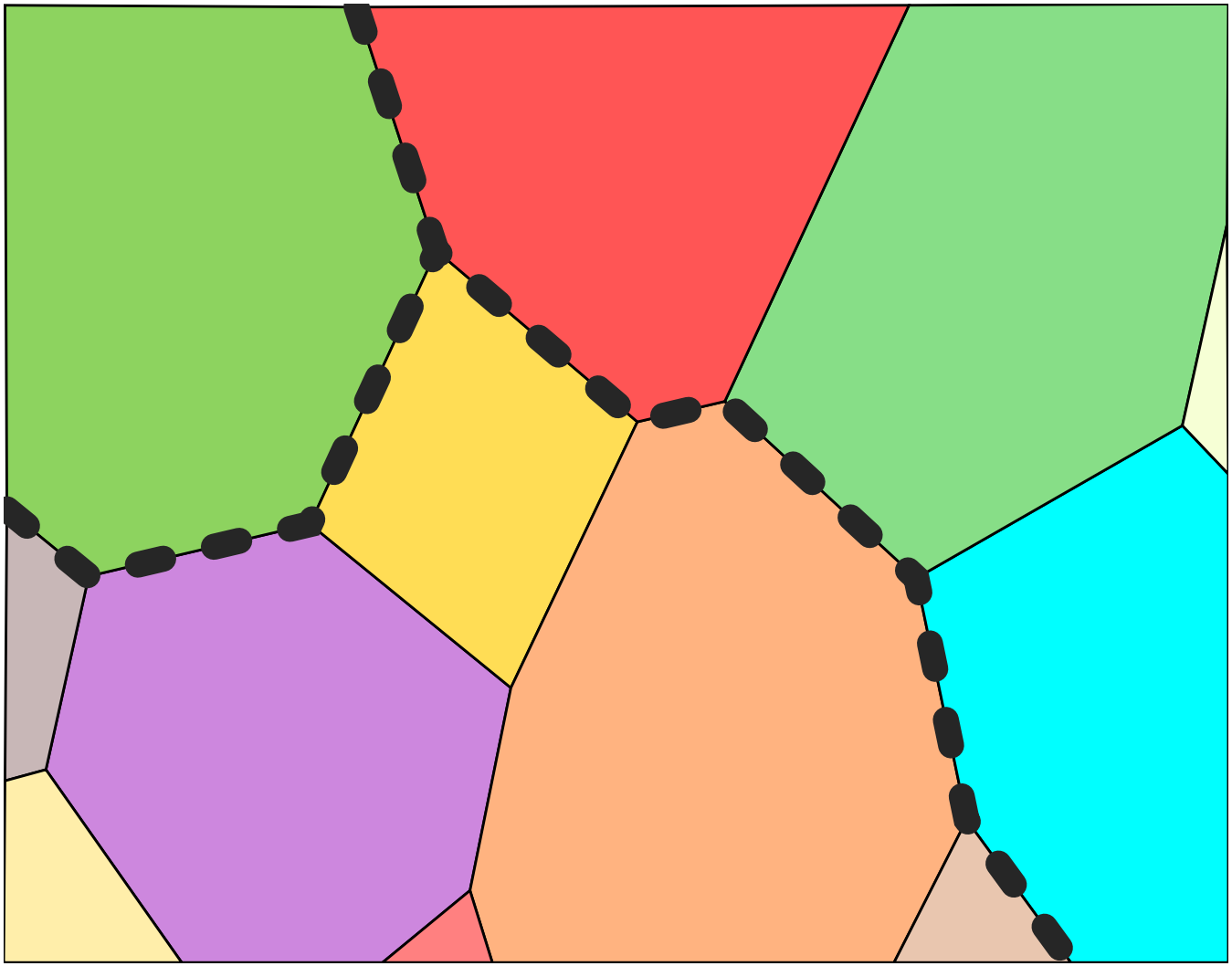
- Random walk
- Based on transition matrix

$$\begin{bmatrix} 0.3 & 0.7 \\ 0.4 & 0.6 \end{bmatrix}$$

- Clustering size control (the only parameter)
- Natural clusters
  - No predefined number of clusters
  - No threshold values

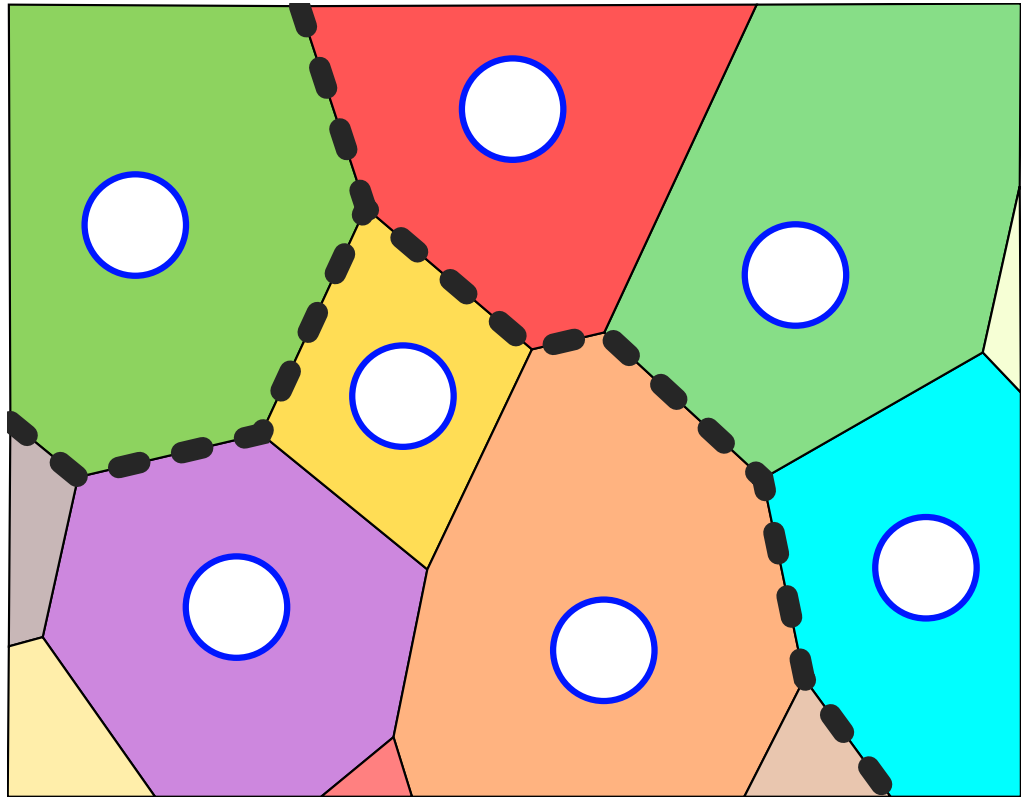
Analogy

Grain clustering



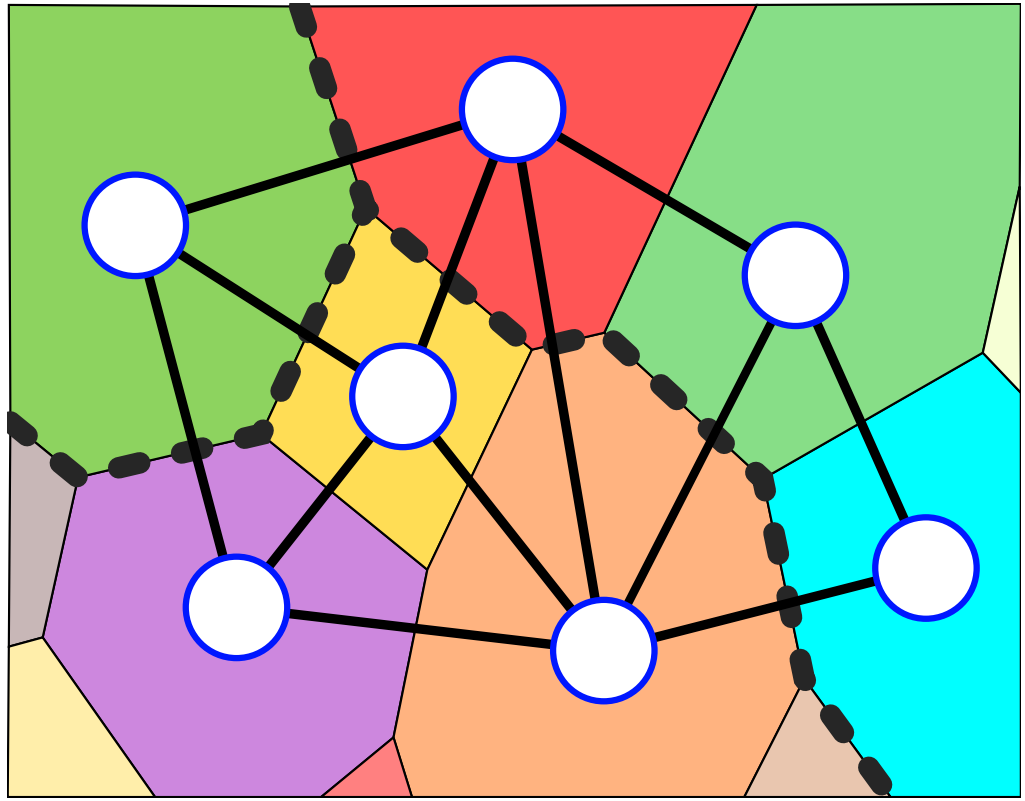
Grain clustering

each grain became a node



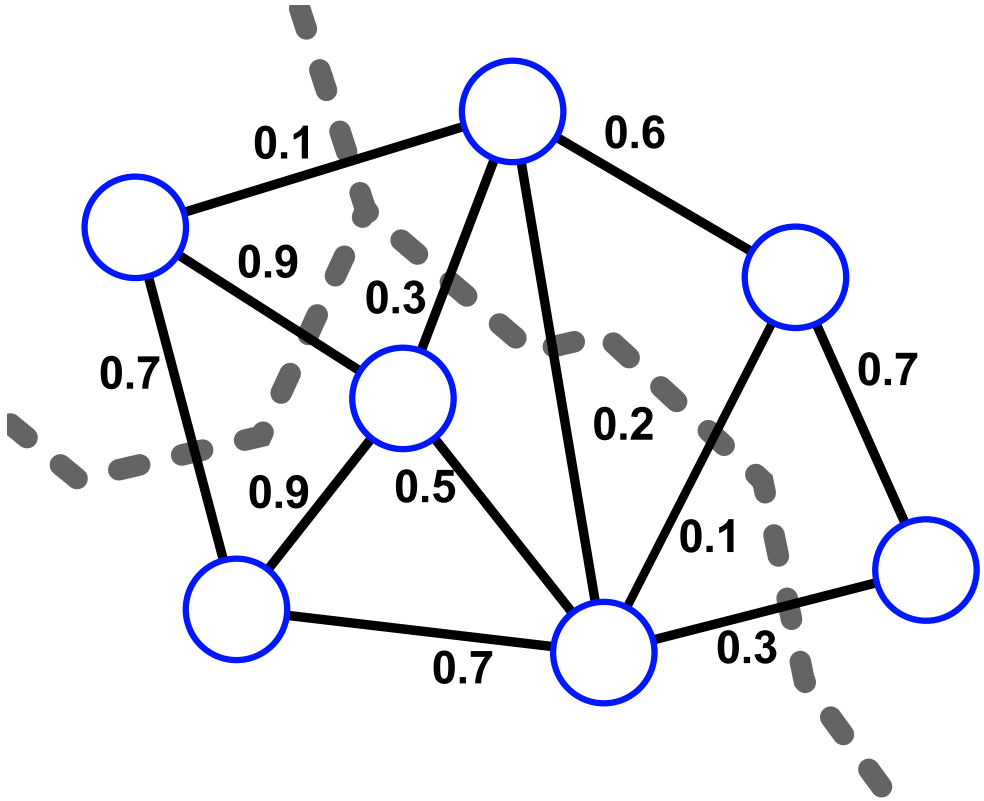
Grain clustering

each GB became a edge



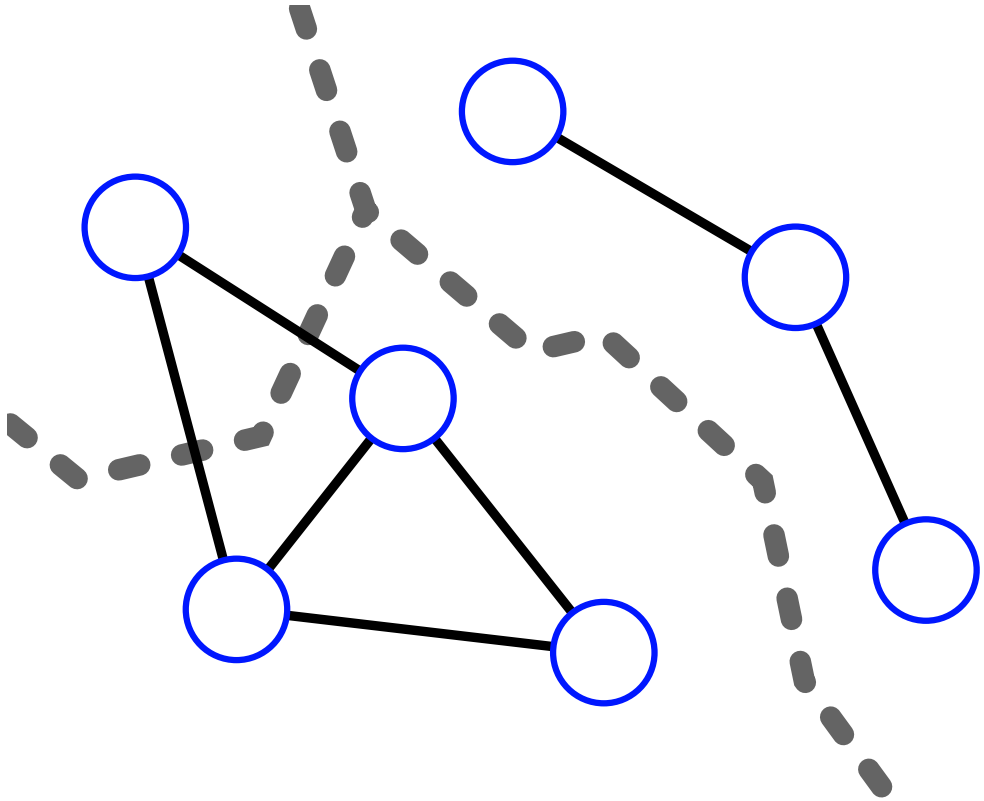
Grain clustering

the value of the edge is given by the value of OR deviation



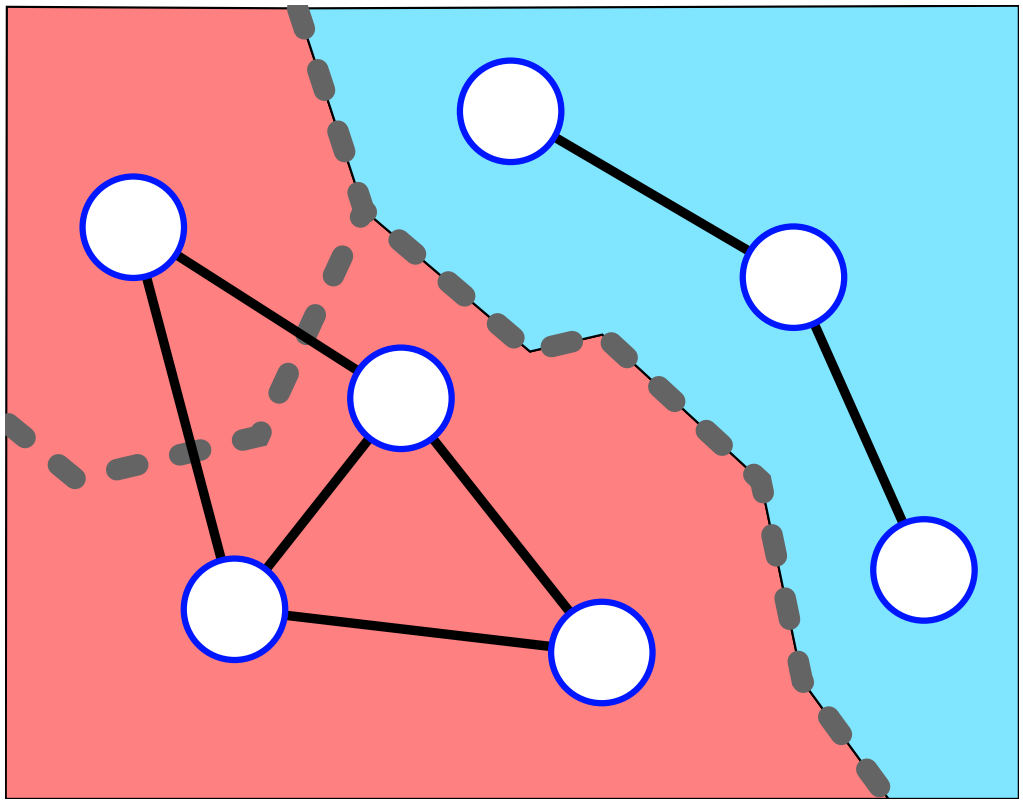
Grain clustering

run the clustering algorithm with coarse clustering



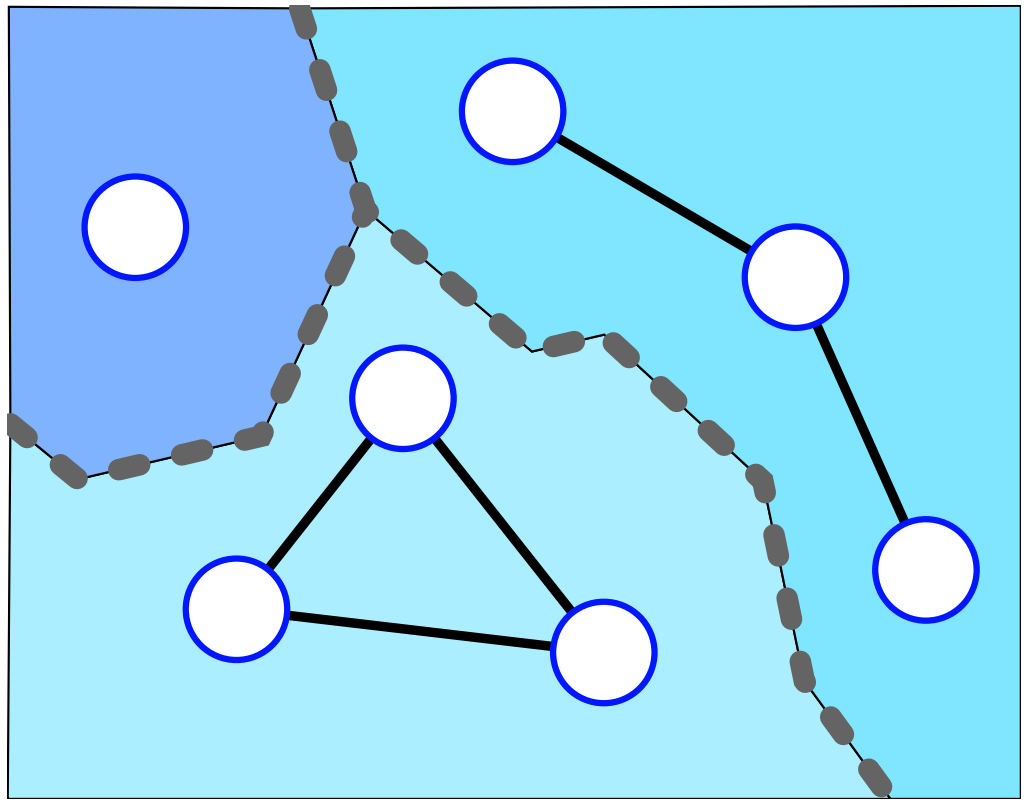
Grain clustering

evaluate the error on each reconstructed grain

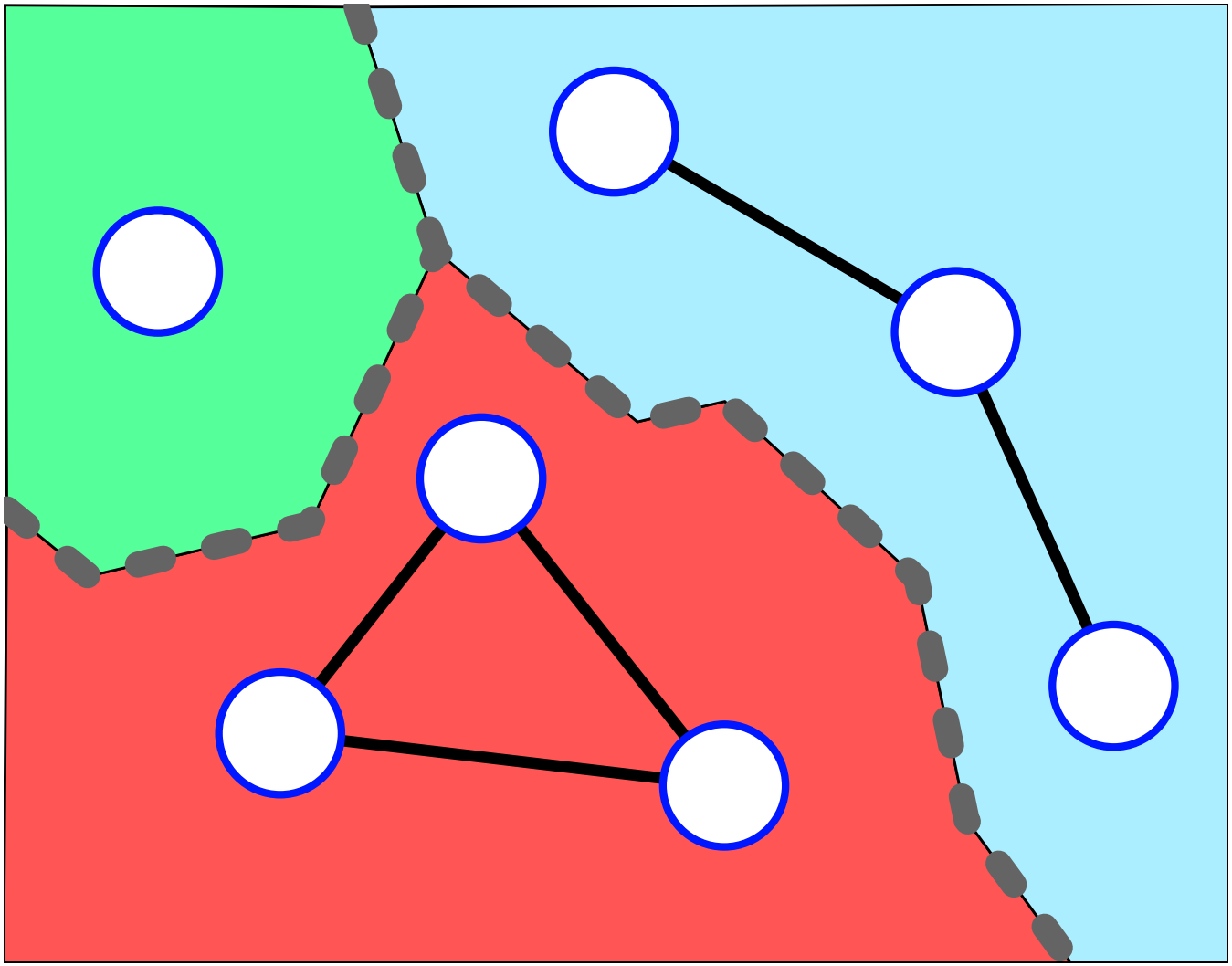


Grain clustering

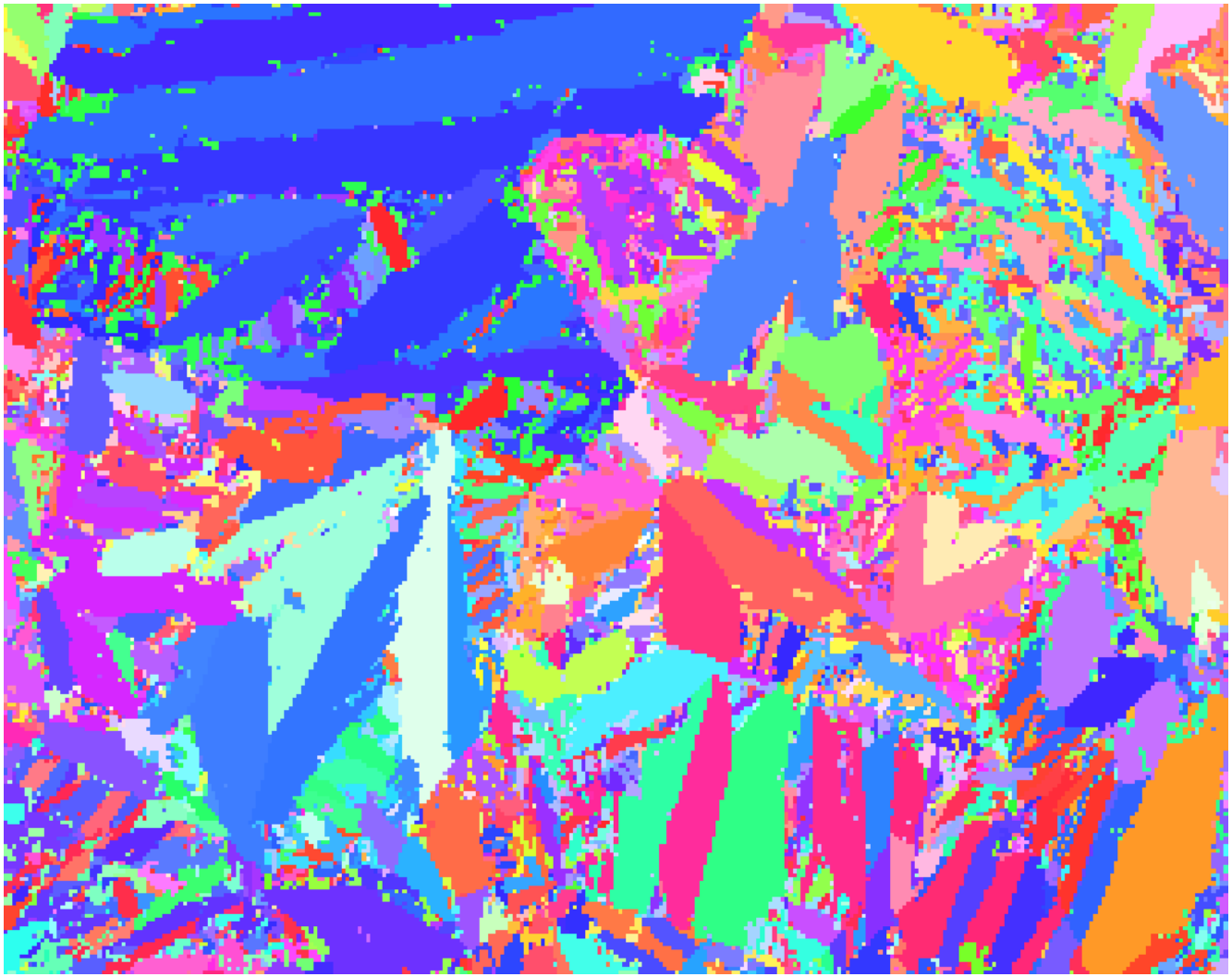
reapete the procedure
with finer clustering



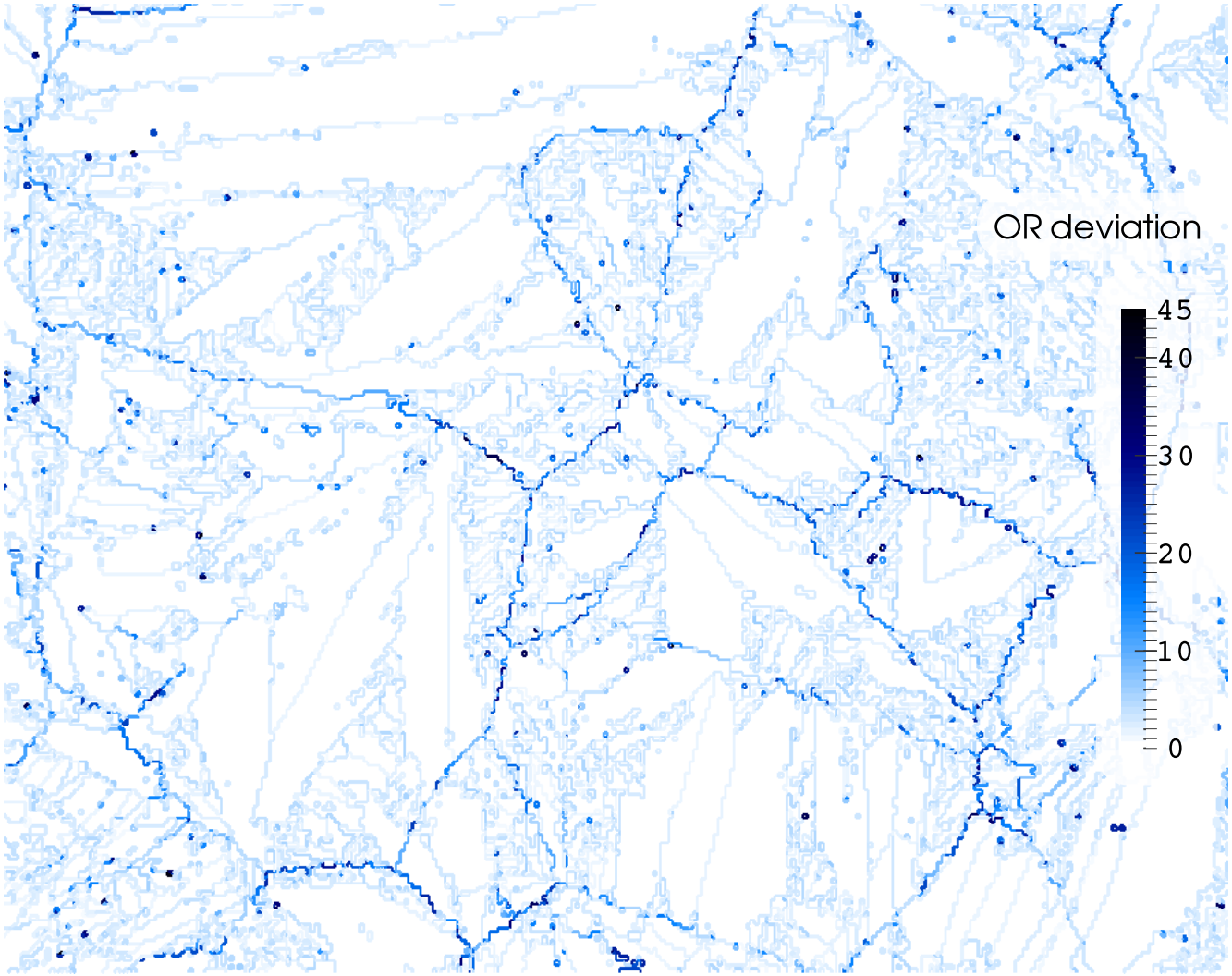
Grain clustering



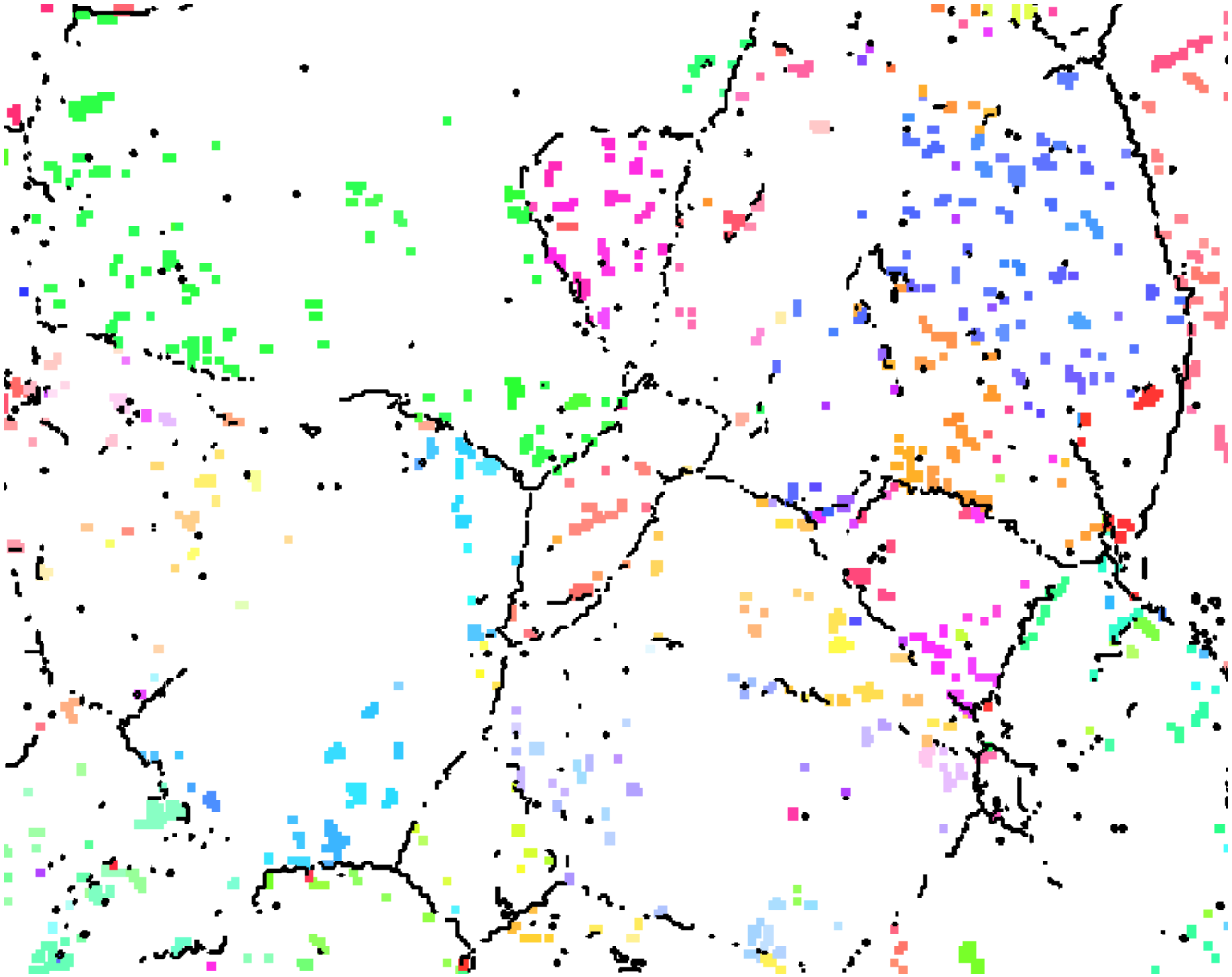
FeNi after phase transformation



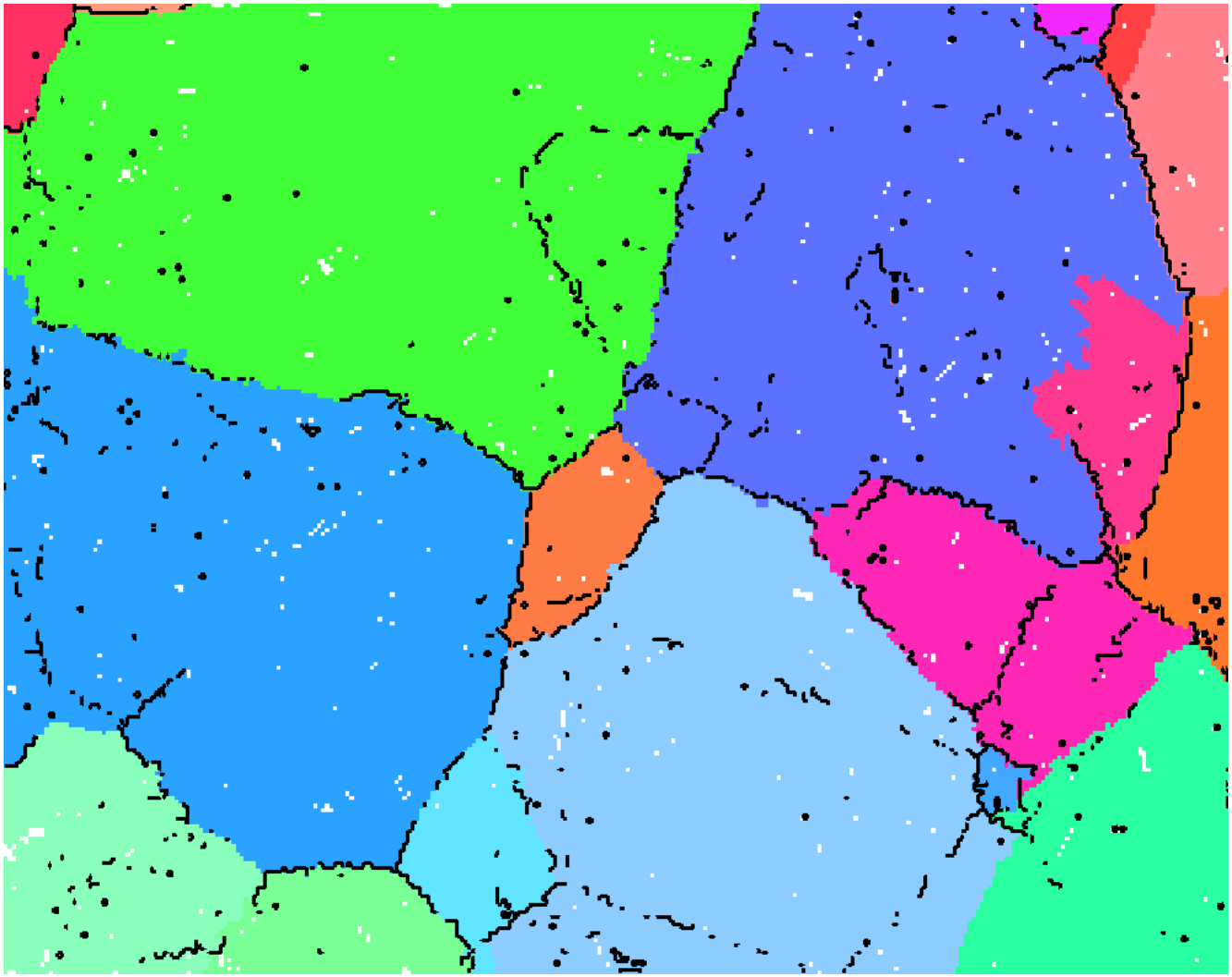
Grain Boundary OR deviation



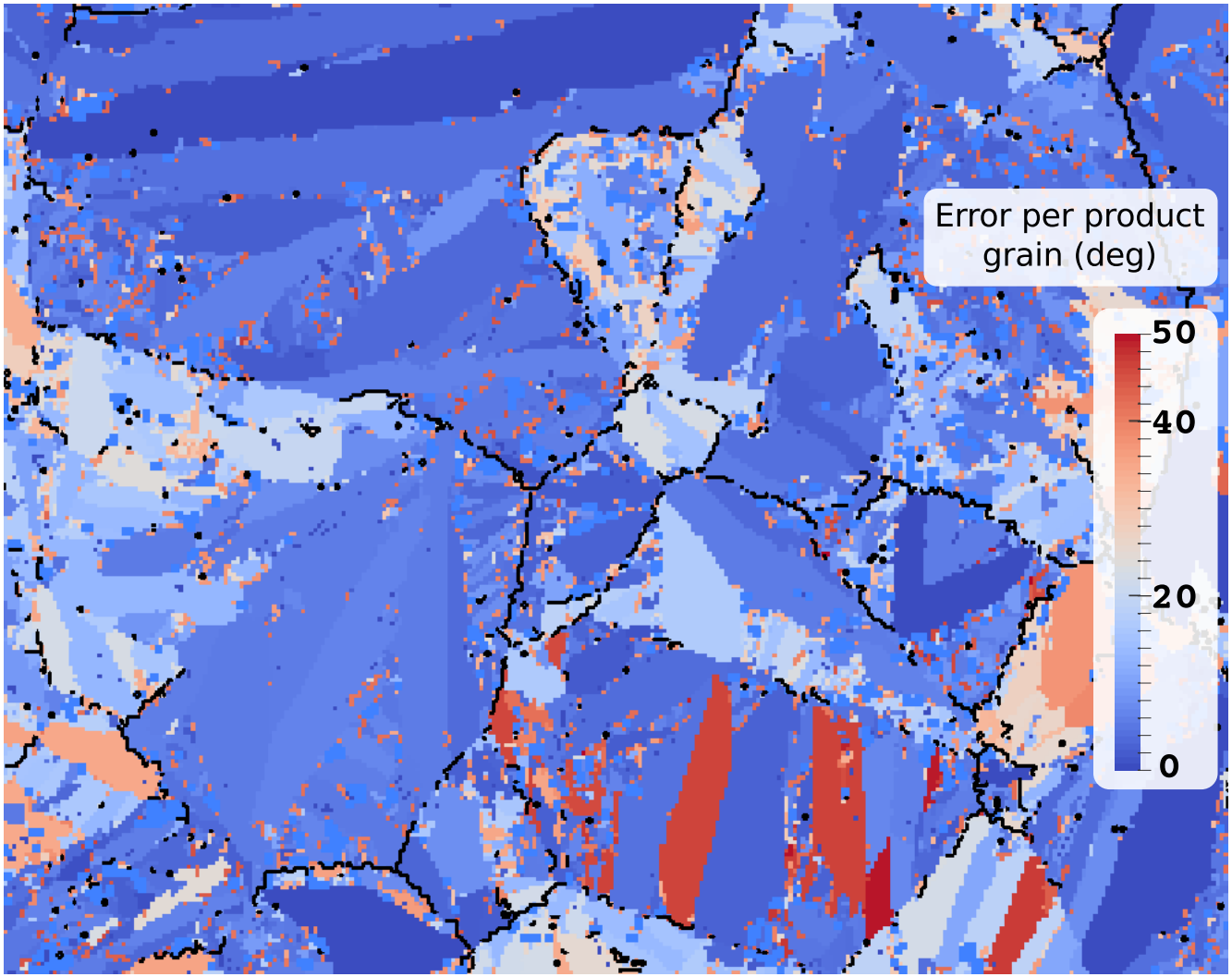
Retained Austenite



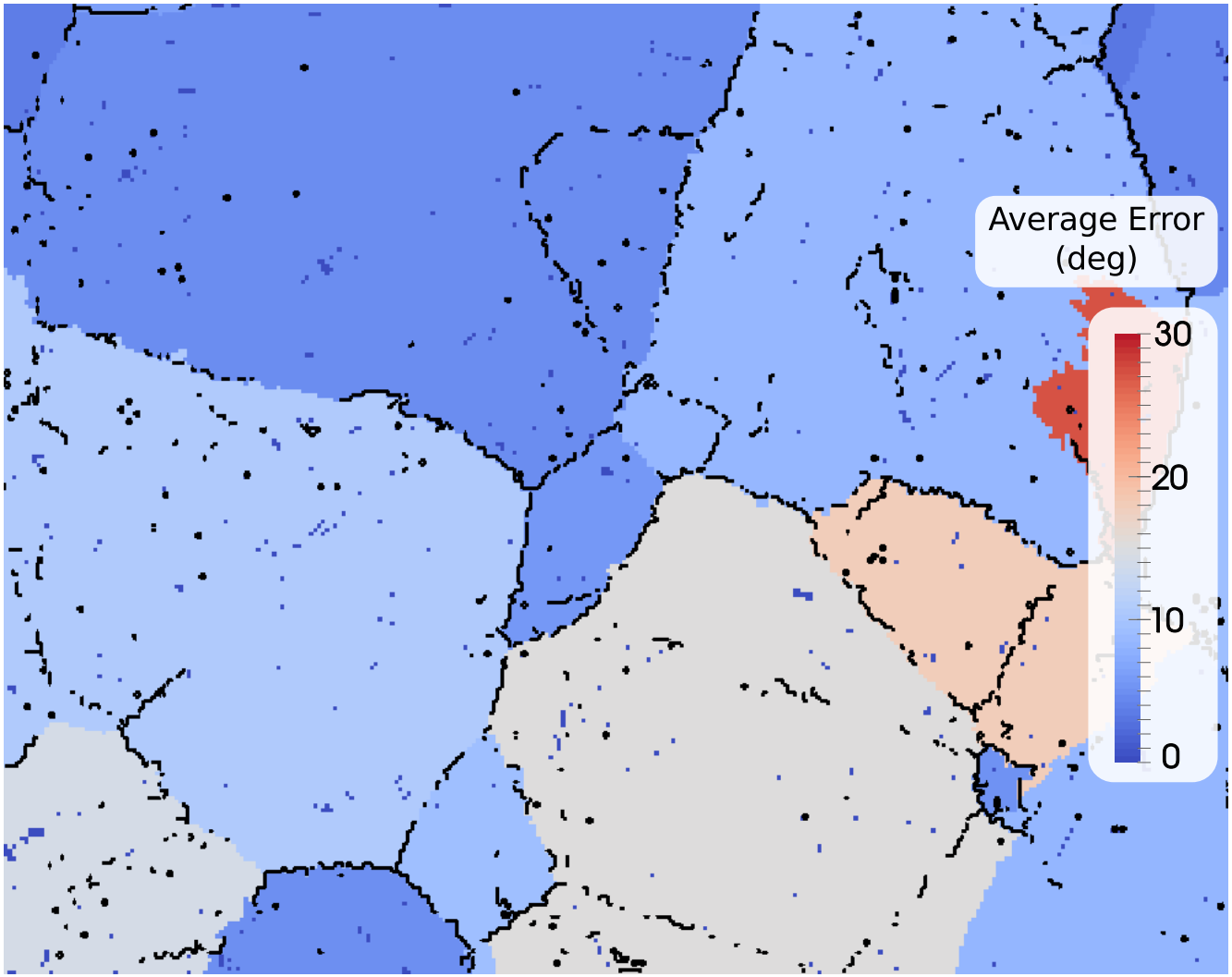
Reconstruction - 1st step



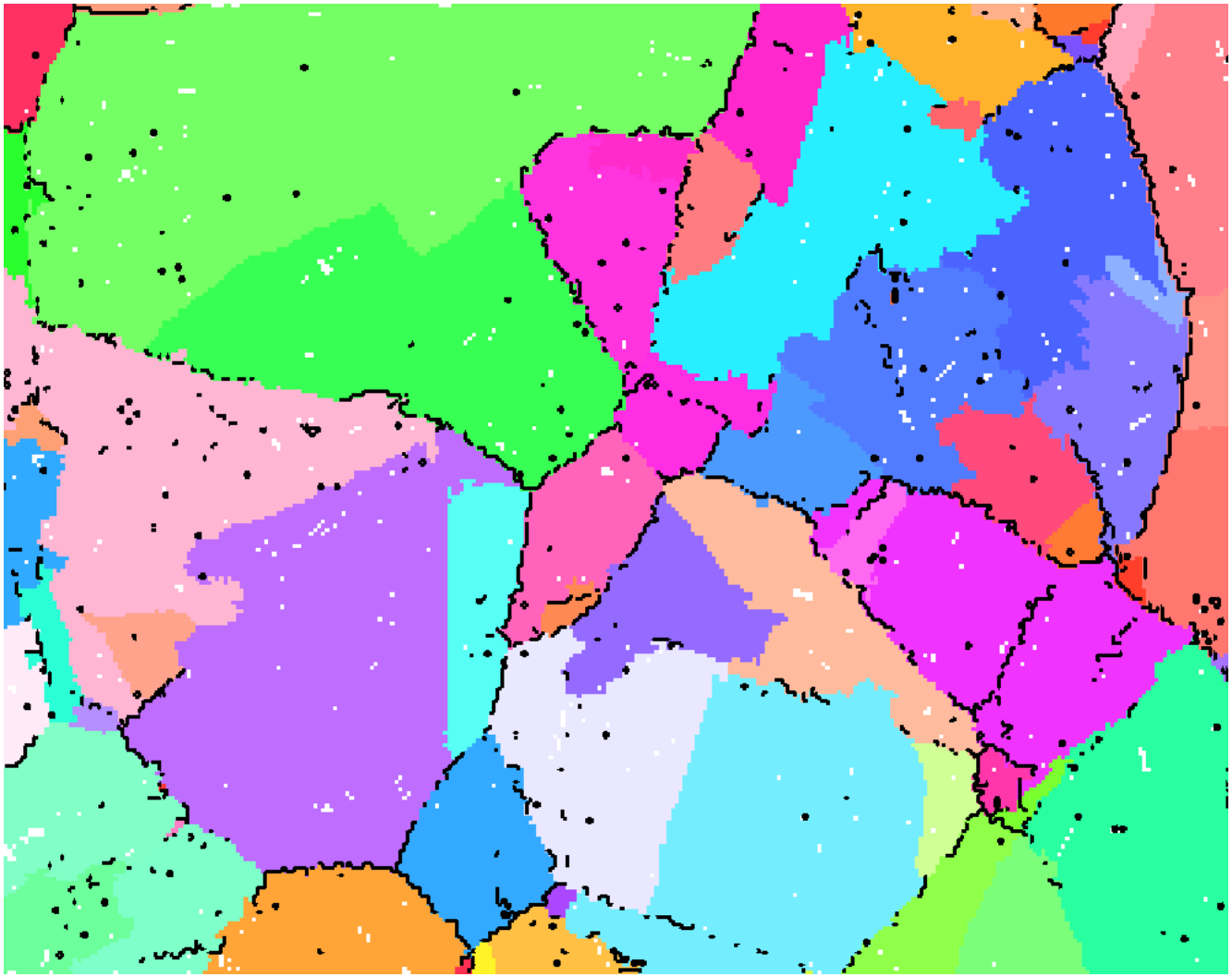
Error per product grain



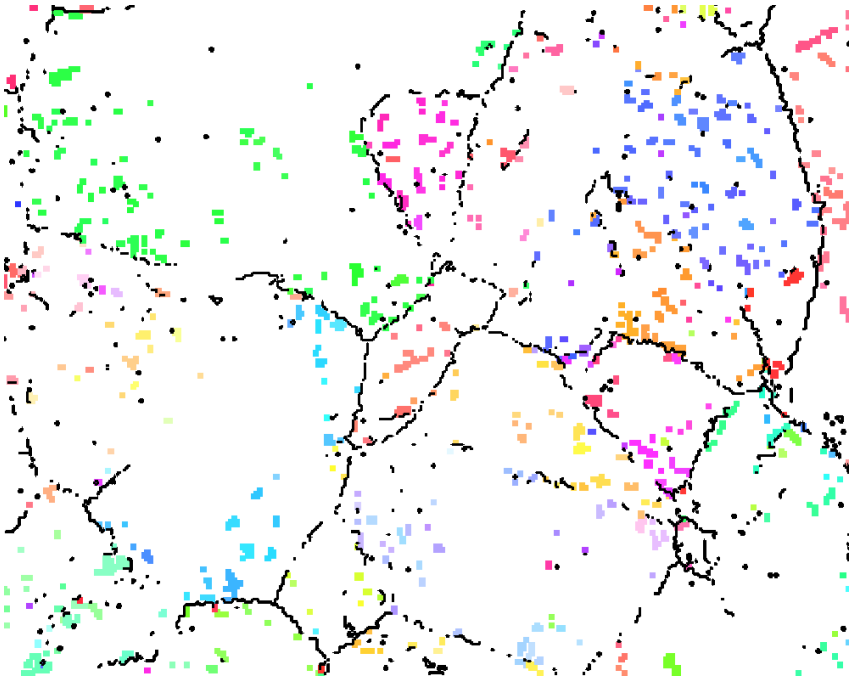
Average error



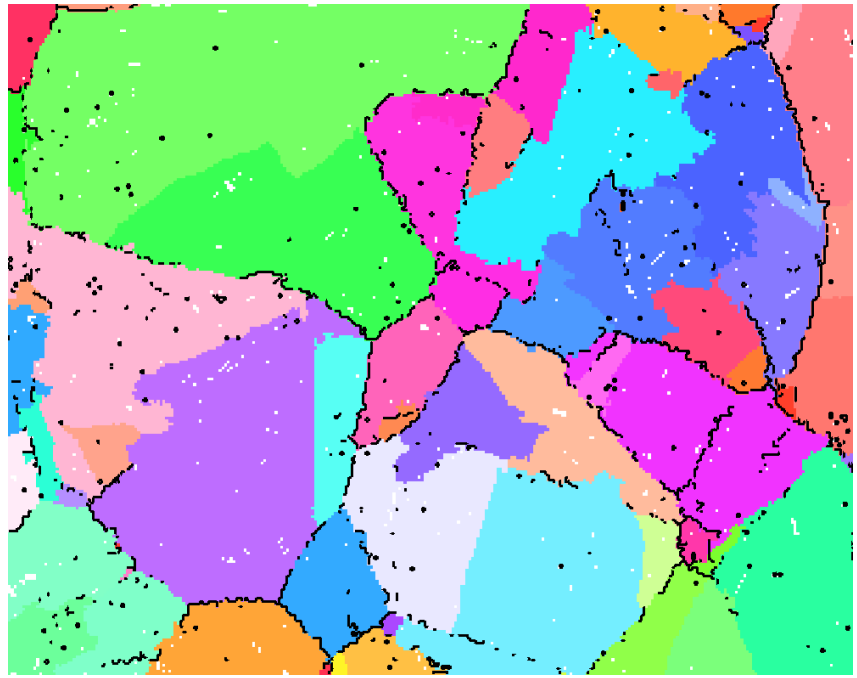
Reconstruction - 2^{nd} step



Comparison

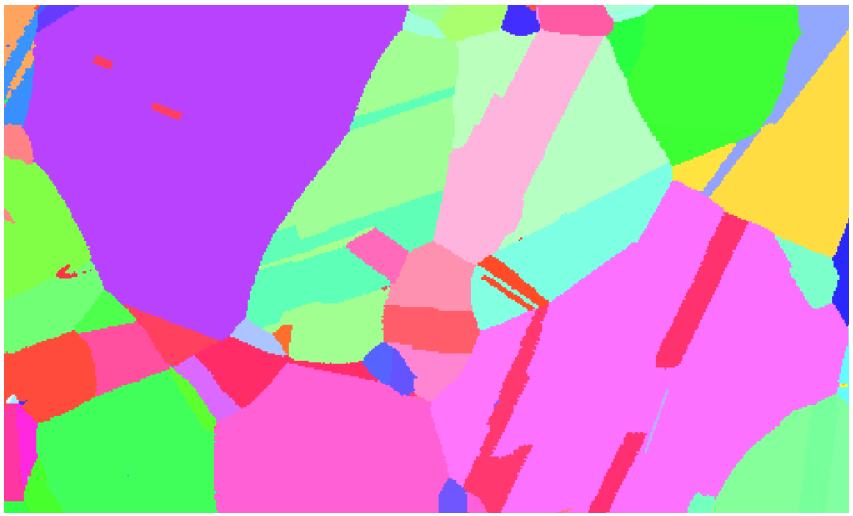


Retained austenite

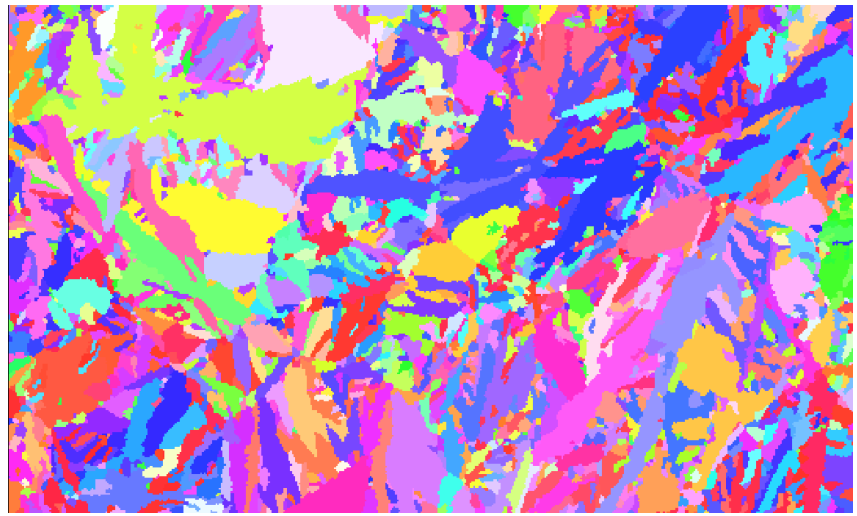


Reconstructed austenite

FeNi29 quenched on liquid Ni

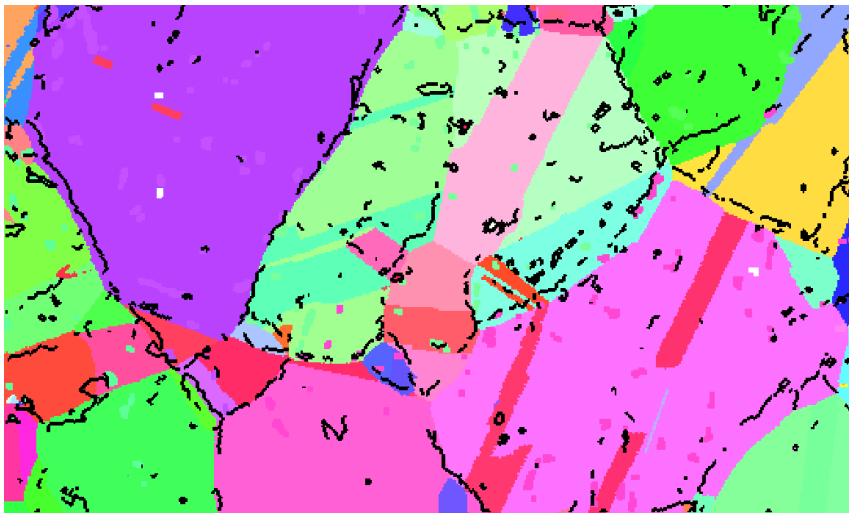


Before phase transformation

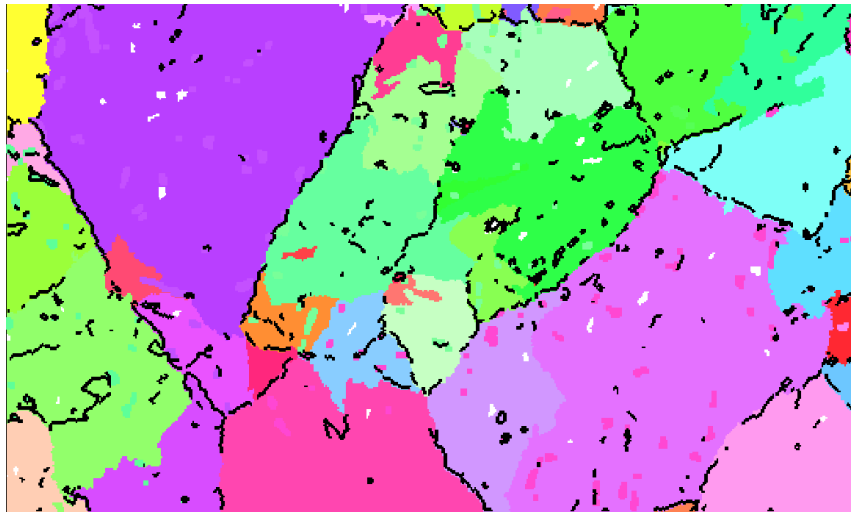


After phase transformation

Comparison



Before phase transformation



After reconstruction

Conclusions

1. Using grain boundary misorientation allows to calculate the real OR in a fully automated manner.
2. Markov chain clustering was successfully used for reconstruction of prior austenite phase
3. Further work has be done on:
    1. the analyze of the accuracy of the OR calculation.
    2. the improvement of the cluster refinement
    3. the parent orientation calculation

Thank you for your attention !

Questions ?

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