Reconstruction of austenite microstructures in steels by global optimization of misorientation functions

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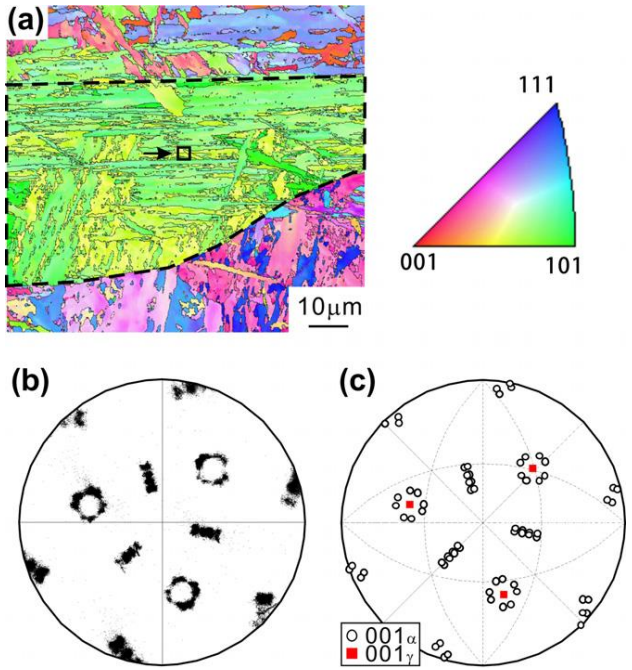
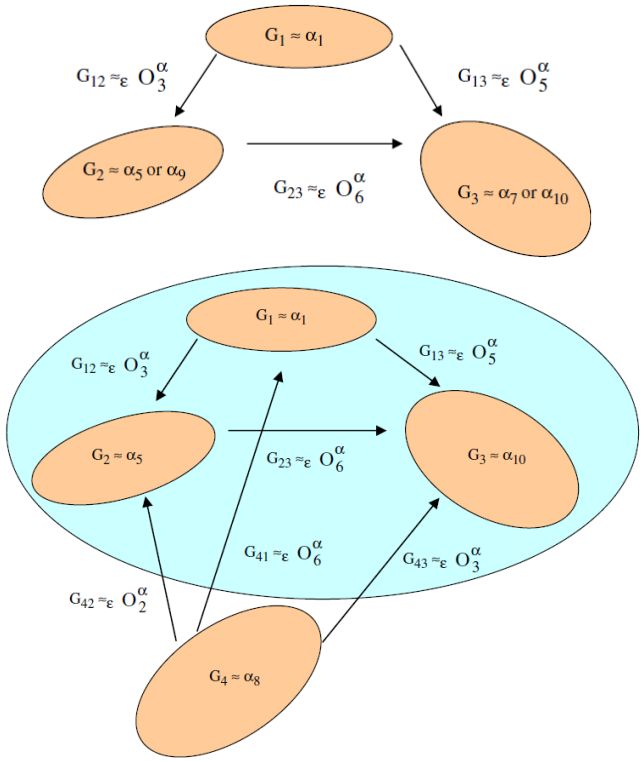
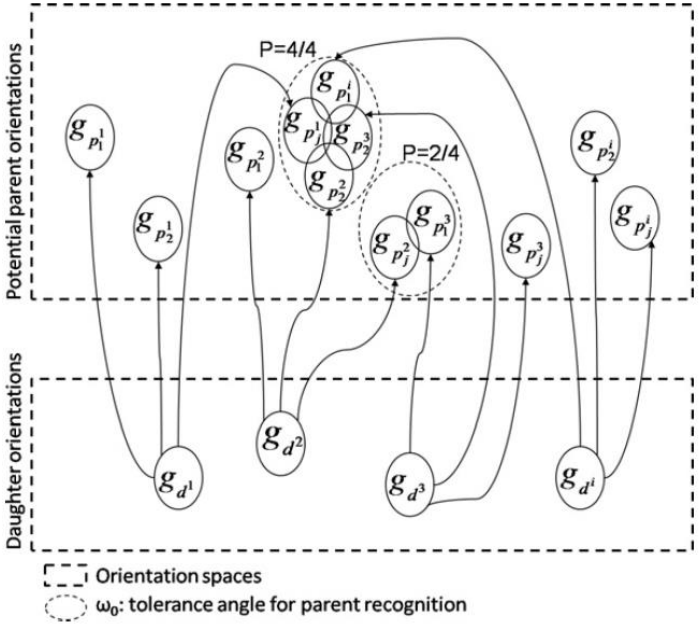
Motivations

- Microstructures and textures of austenite at high temperatures affect properties of steels at room temperature.
- Innovative steel manufacturing processes (i.e. intercritical rolling, Q&P …) demand good control on material states at high temperatures.
- Online microstructure & texture measurements are not usually feasible.
- EBSD measurements provide many interesting information on microstructure and texture of materials.

Available reconstruction methods







Among many:

- Least squared fitting method (Miyamoto et al. Acta Mater 2010;58:6393)
- Groupoid structure (Cayron et al. Mater Charact 2006;57:386)
- Probability assessment (Germain et al. Acta Mater 2012;60:4551)
- etc

Hypotheses on phase transformation

- Orientation Relationship (***T***) between parent and product grains

$$\boldsymbol{\gamma} \overset{\boldsymbol{T}}{\leftrightarrow} \boldsymbol{\alpha}$$

- Parent grain orientations are smoothly spread

$$\boldsymbol{\Delta g_{12}^{\gamma\gamma} = g_2^{\gamma} \cdot (g_1^{\gamma})^{-1}}$$

- Product grain orientations are multi-variants

$$\boldsymbol{g_{ij}^{\alpha} = S_j \cdot T \cdot S_i \cdot g^{\gamma}}$$

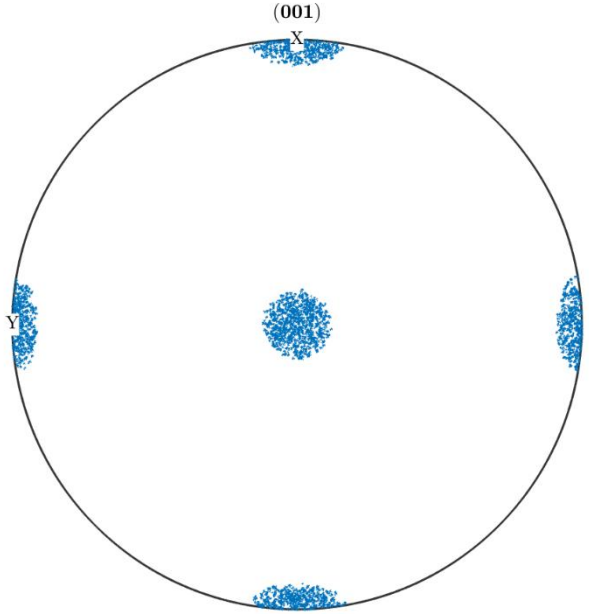
- Boundaries between product variants from the same parent grain

$$\boldsymbol{\Delta g_{12ijkl}^{\alpha\alpha} = (S_l \cdot T \cdot S_k) \cdot \Delta g_{12}^{\gamma\gamma} \cdot (S_j \cdot T \cdot S_i)^T}$$

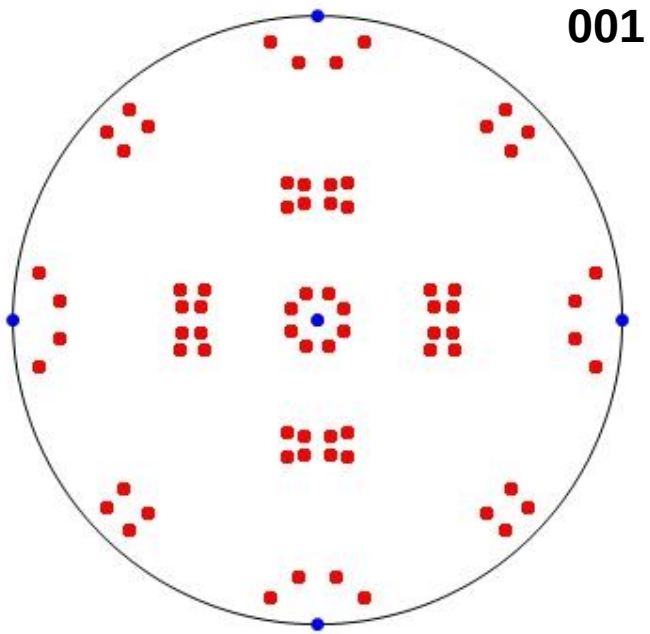
$\gamma \leftrightarrow \alpha$ phase transformation

Conventional orientation relationships (ORs):

- K-S OR: $42.848° < 0.96792 \;\; 0.17767 \;\; 0.17767 >$
- N-W OR: $45.986° < 0.97615 \;\; 0.20058 \;\; 0.08308 >$
- G-T OR: $43.823° < 0.97455 \;\; 0.18746 \;\; 0.12292 >$



Orientation transformation



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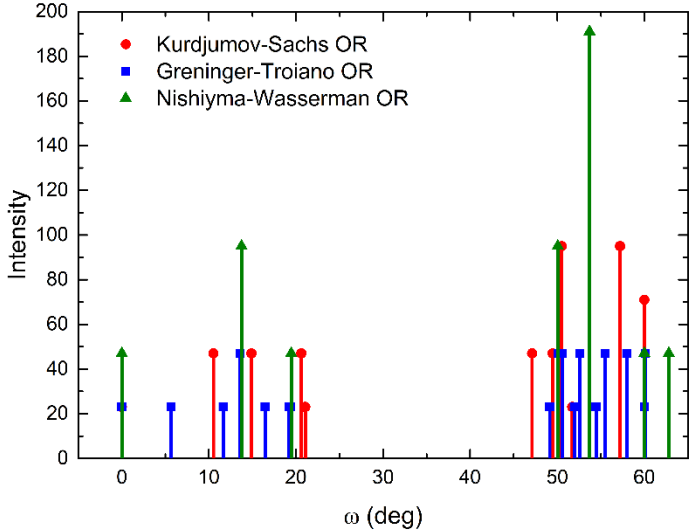
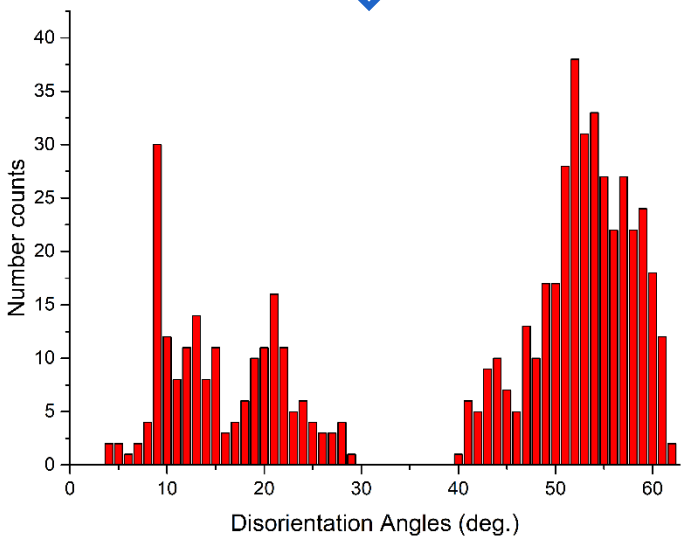


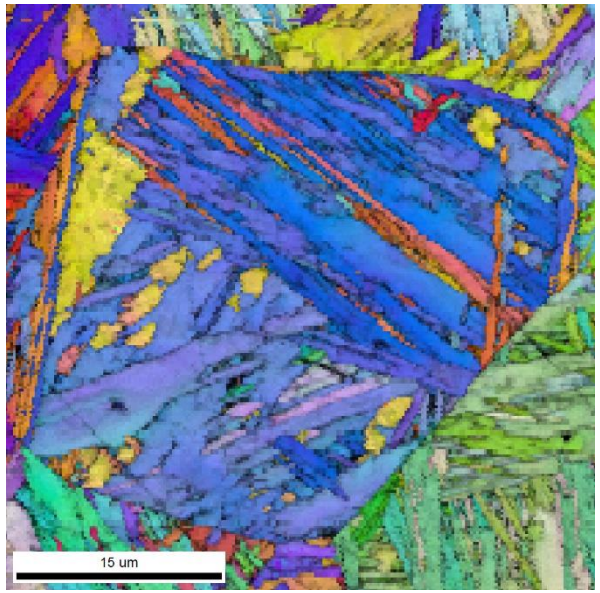


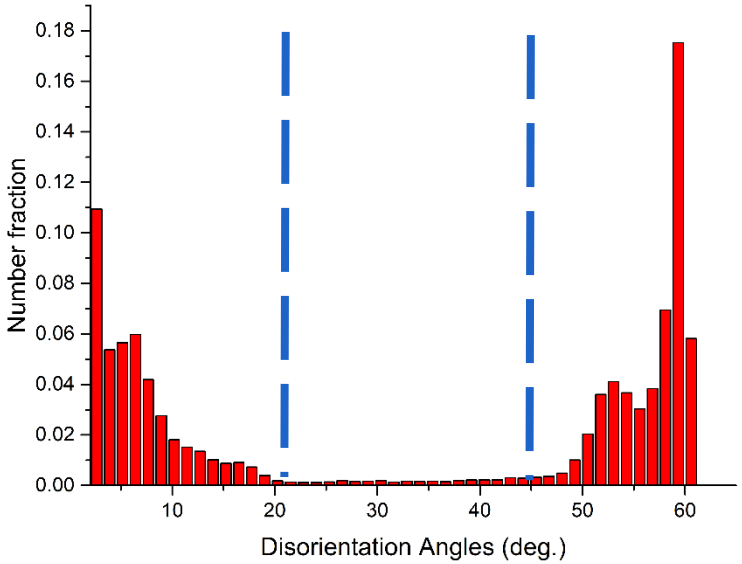
Reconstruction Procedure

Parent grain is able to be reconstructed if the OR and several product variants are known

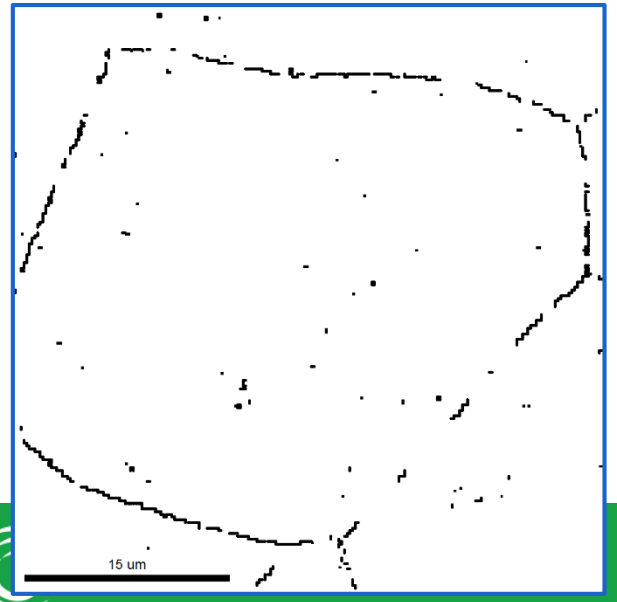
- Import EBSD data
- Calculate martensite boundary network
- Identify orientation relationship
  - Classify martensite boundary segments
  - Minimize disorientation angles between martensite variants
- Austenite grain reconstruction
  - Find the mean orientations for each austenite grains
  - Apply transformation operation to each martensite pixels
- Export results

Martensite Boundary classification

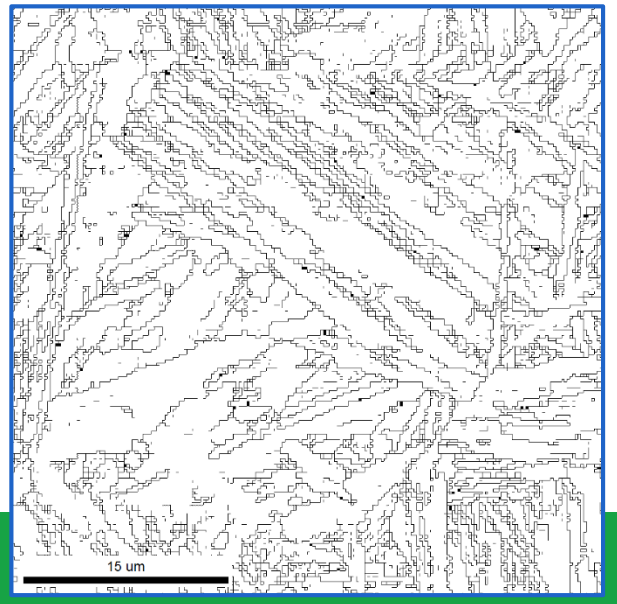




- $2.0° \leq \omega^{\alpha\alpha} < 21.0°$
  $45.0° < \omega^{\alpha\alpha} \leq 62.8°$
- Number fraction: 96.2%
- Include martensite variant boundaries + small fraction of austenite boundaries
- Will be used for OR optimization



- $21.0° \leq \omega^{\alpha\alpha} \leq 45.0°$
- Number fraction: 3.8%
- Mainly contain prior austenite grain boundaries
- Will be used for austenite grain reconstruction



Orientation relationship identification

Objective function: **Average disorientation angle of γ- γ boundaries**

$$\bar{\omega} = \frac{\sum_{m=1}^{n_{seg}} \omega_m}{n_{seg}}$$

Minimize

$$\Delta g_m^{\gamma\gamma}(\omega_m, \vec{d}) = (S_l T S_k) \cdot \Delta g_m^{\alpha\alpha} \cdot (S_j T S_i)^{-1}$$

Optimization parameter

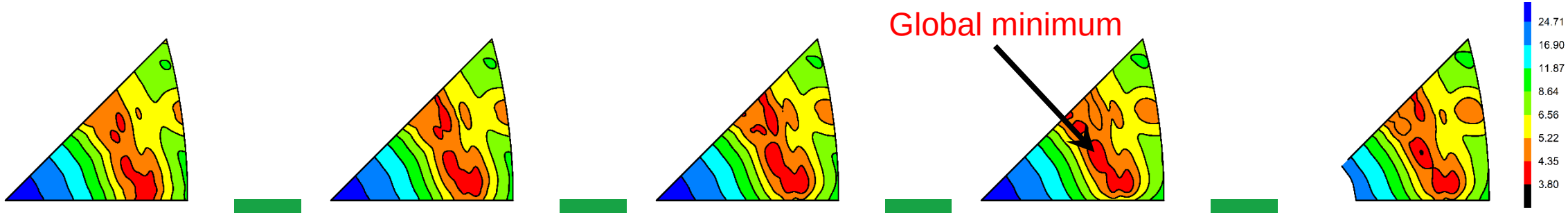
From EBSD measurements

Idea conditions:

- Orientation distributions of parent grains are sharp
- OR between parent and product grains is unique

$$Min(\bar{\omega}) = 0.0$$

Global optimization by **Simulated Annealing algorithm**



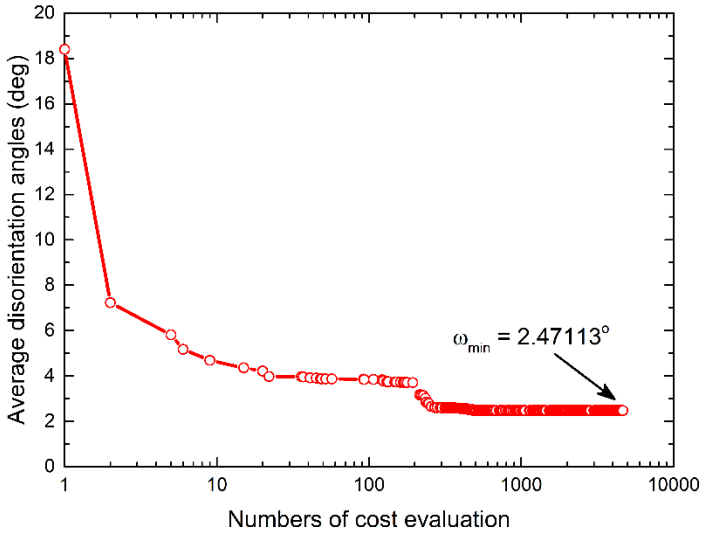
ω = 42° ω = 43° ω = 44° ω = 45° ω = 46°

Orientation relationship identification

Input

- Initial OR: $\mathbf{0.00° < 1\ 0\ 0 >}$
- $\{\boldsymbol{\Delta g_m^{\alpha\alpha}}\}$

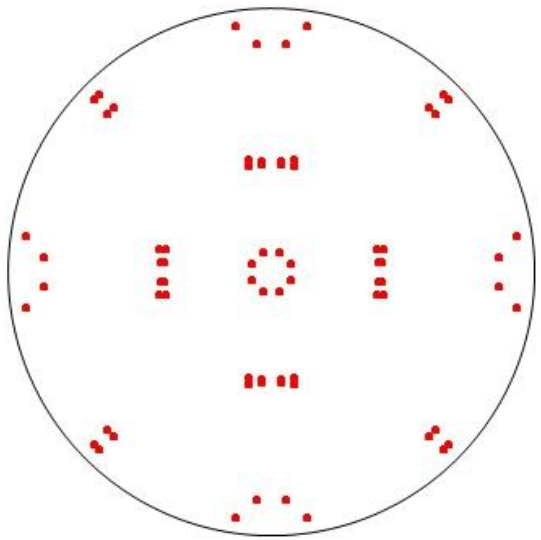
Mimimize $\bar{\omega}$

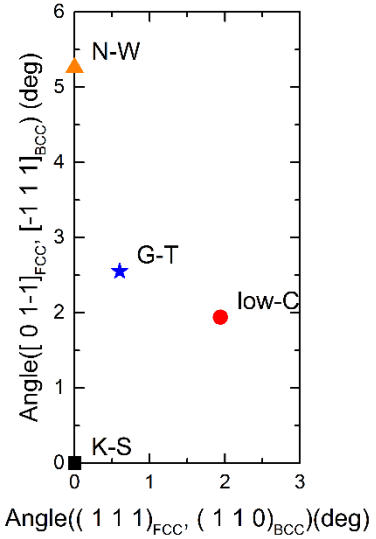


Output

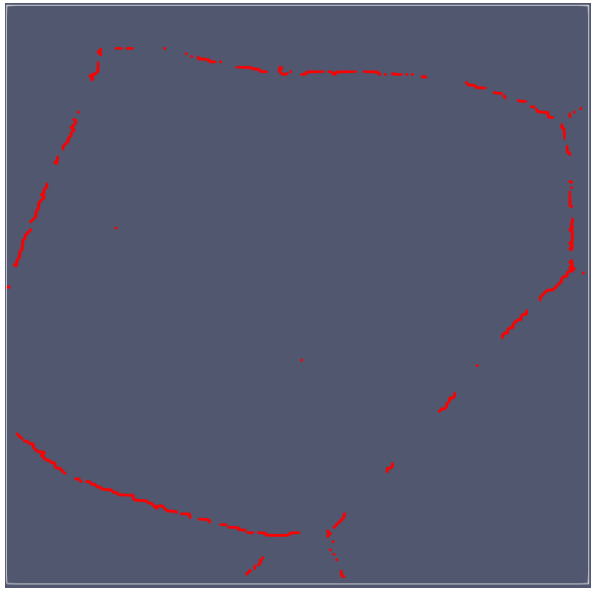
Optimize OR:

$\mathbf{44.853° < 0.97831\ \ 0.14647\ \ 0.14647 >}$



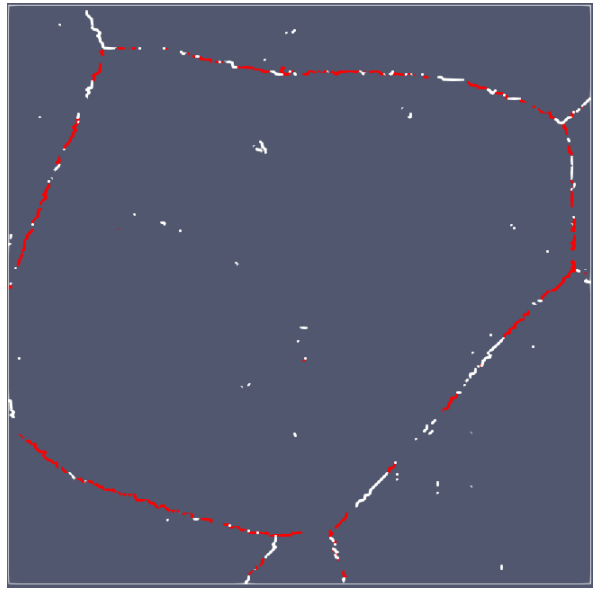


Identify parent grain boundaries

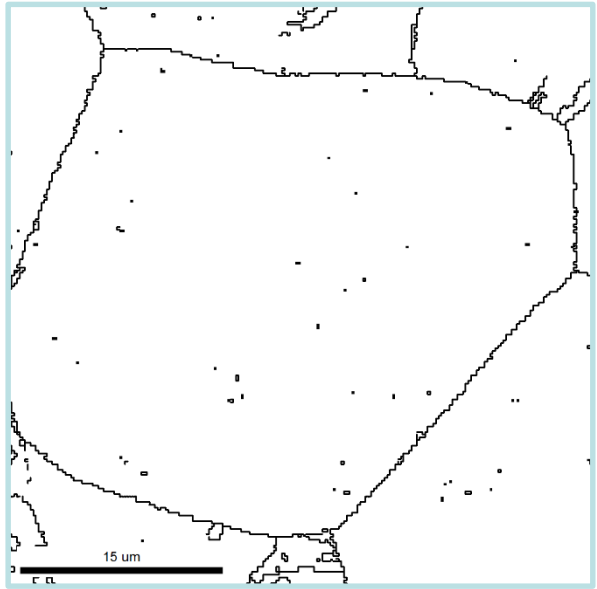


Martensite boundaries

$21° \leq \omega^{\alpha\alpha} \leq 45°$



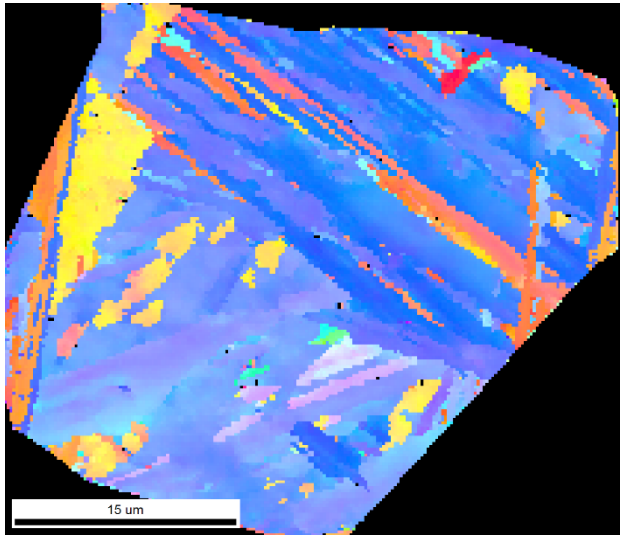
Transform martensite boundaries using the optimized OR, then threshold boundaries having $\omega^{\gamma\gamma} \geq 5°$



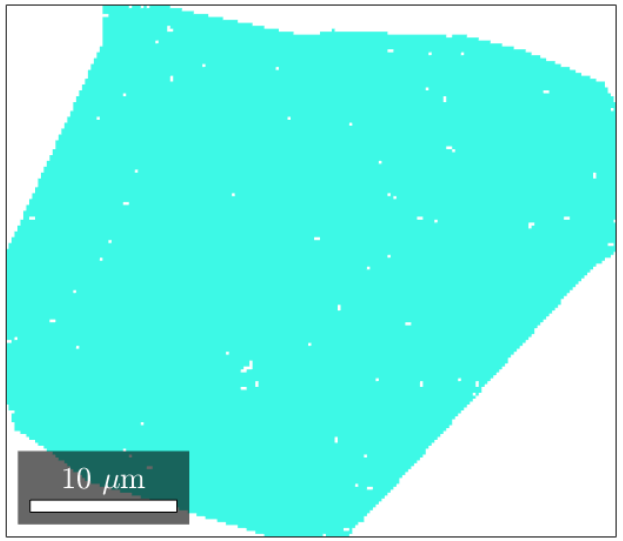
Completely identify austenite boundary network by Markov chain clustering (MCL) [1]

[1] Stijn van Dongen, *Graph Clustering by Flow Simulation*. PhD thesis, University of Utrecht, May 2000

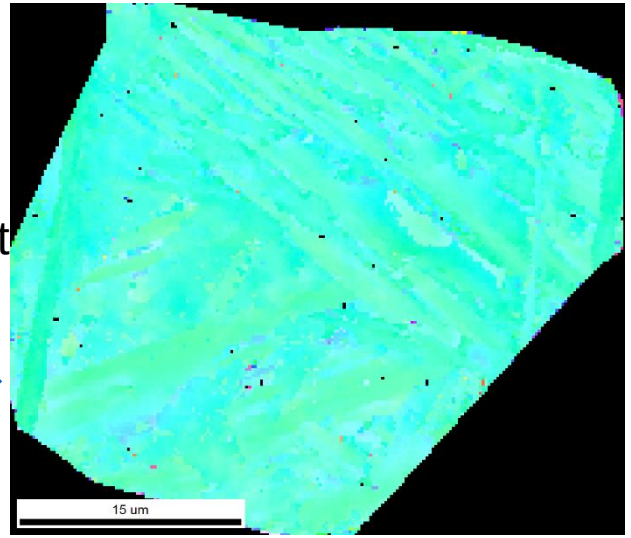
Parent austenite reconstruction

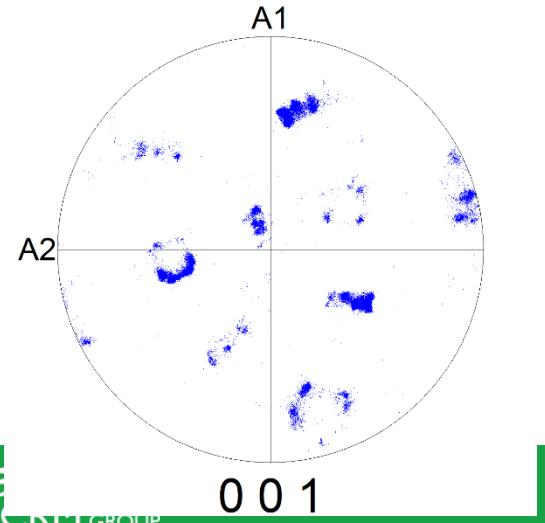


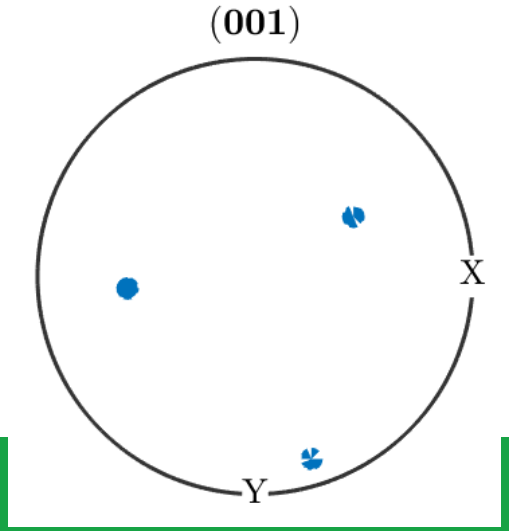
Find mean orientation

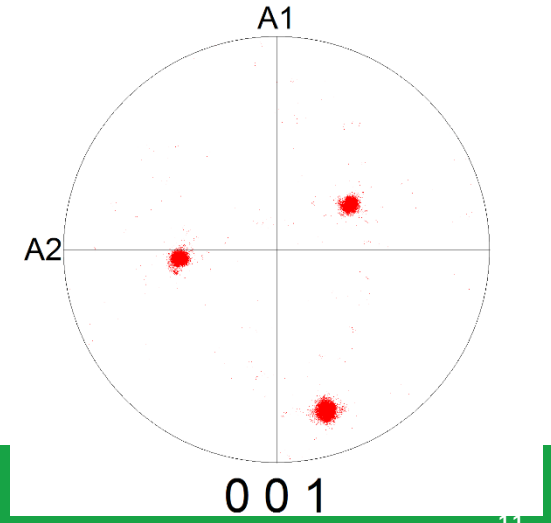


Reconstruct each pixels





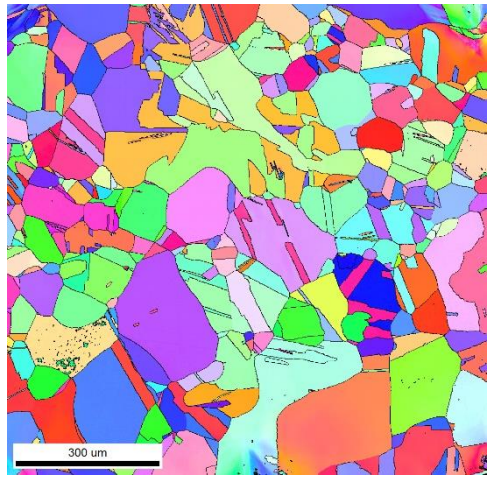




Validation

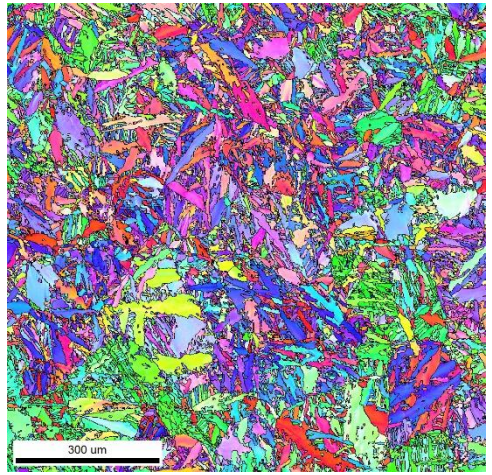
Material: Fe – 29 wt.% Ni alloy

Austenite @ RT



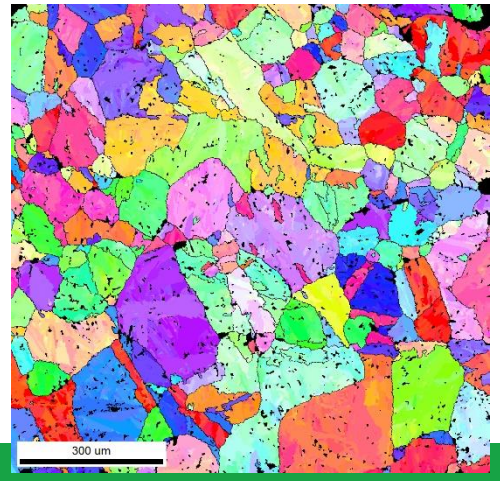
Liquid N_2 quench

Martensite @ RT



Reconstruct

Reconstructed Austenite



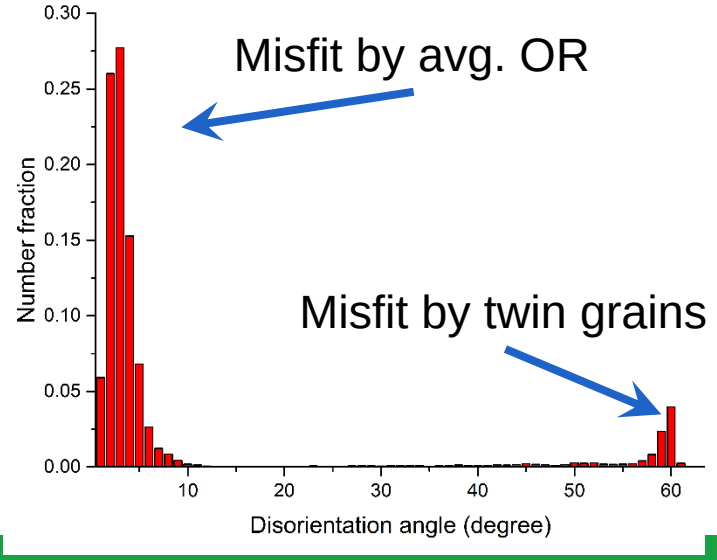
Cross correlation

Cross correlation

Find the optimized position (x, y, θ_Z…) between measured and reconstructed austenite microstructures

Calculate disorientation angles between corresponding points from the two microstructures

$$\Delta g_{12}^{\gamma\gamma} = g_2^{\gamma} \cdot (g_1^{\gamma})^{-1}$$



Courtesy Dr. Pirgazi (UGent)

Summary & conclusion

- Austenite microstructure is reconstruct-able if the OR between parent-product and the variant indices of products are known.
- The OR between parent and product grains is able to recover from product-product boundaries.
- Parent grain reconstruction requires criteria to include/exclude product variants on the calculation.
- Shape strain which is not considered by current model may produce errors on local parent grain orientations.
- Reconstruction could be fail if parent grains have twinned variants (required special treatment)

Thank you for your kind attention!