CARNEGIE MELLON UNIVERSITY

DEPARTMENT OF MATERIALS SCIENCE AND ENGINEERING

DOE-NSF-ONR-AFOSR

Physics Carnegie Mellon

Image Processing in Expts. + Simulations of Plastic Deformation of Polycrystals

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LEM3 LABORATOIRE D'ÉTUDE DES MICROSTRUCTURES ET DE MÉCANIQUE DES MATÉRIAUX

Advanced Photon Source ARGONNE NATIONAL LABORATORY

XSEDE Extreme Science and Engineering Discovery Environment

NERSC

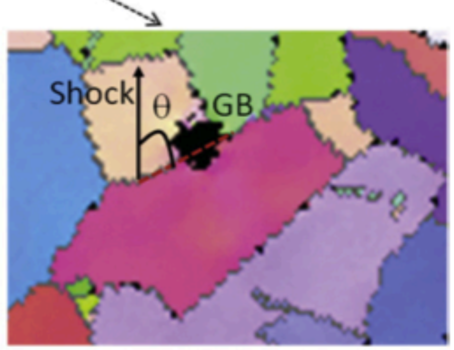
Why understand plastic deformation?

We need to understand plastic deformation down to the scale of individual grains because the extreme values of stress, strain and orientation gradients control many phenomena.

Orientation map of shocked copper

150µm (a)

E.g. Hot spots in normal tractions (plus other components) generate voids:

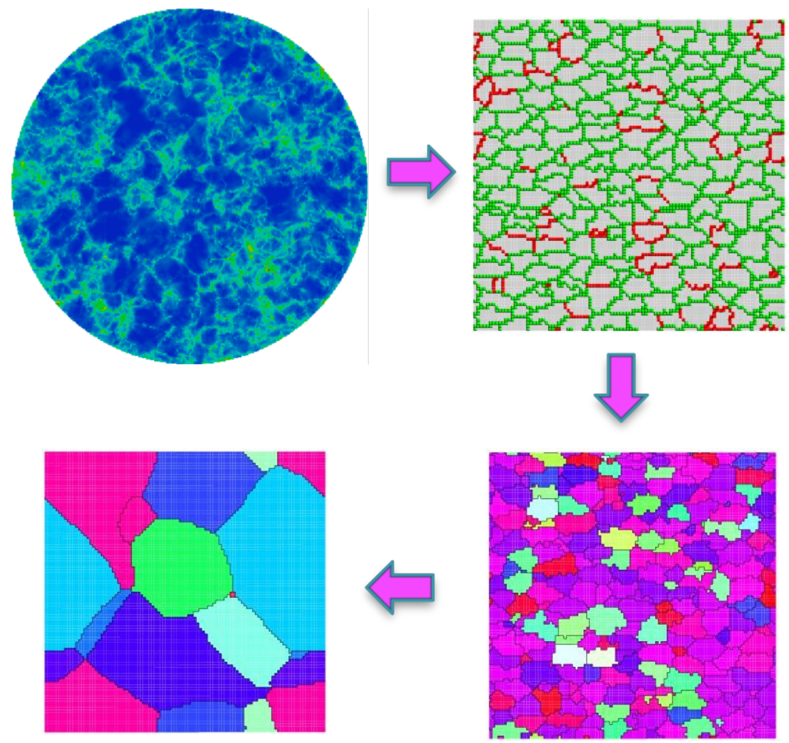


(b)

Voids are easy to find by thresholding a CT image, except when they approach the resolution limit!

Cerreta, Fensin, Lieberman …

E.g. hot spots in orientation gradients nucleate recrystallization



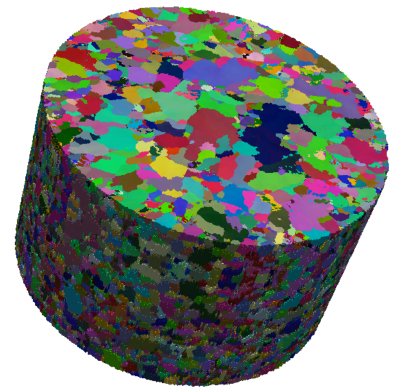
Wang, *Acta mater.* **59** 3872 (2011)

High Energy X-ray Diffraction Microscopy (nf-HEDM)

Advanced Photon Source Measurements

- 1-ID high brilliance, high energy x-rays
- Millimeter samples probed with micron spatial, < 0.1 deg orientation resolution
- Tera-byte data sets
- > 3 x 10^6 Bragg peaks
- 10^3 core parallel processing: 2D images to 3D orientation maps

3D copper microstructure



0.4 mm^3

Stack of layers = 3D microstructure
Colors based on crystal orientations

HEDM measurement schematic

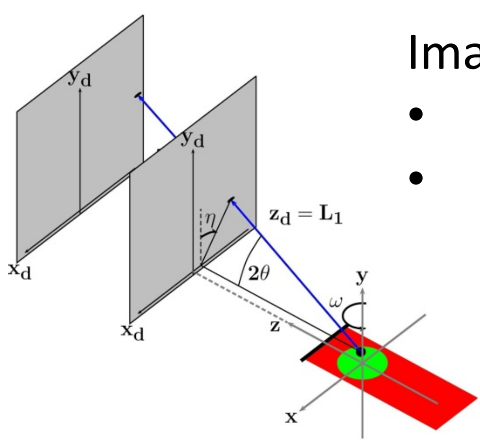
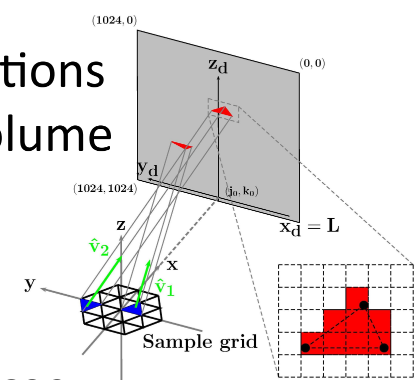


Image diffracted beams

- 360 images/layer
- ~100 successive cross-sections

Reconstruction via Forward Modeling

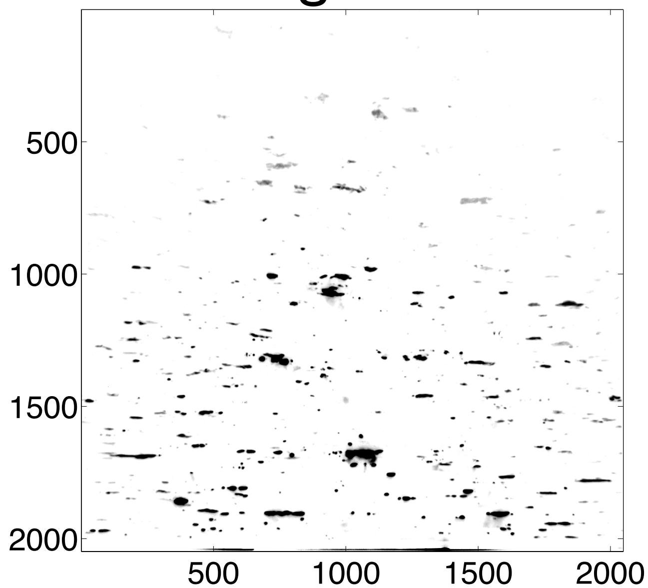
Optimizes orientations in > 10^7 voxels (volume elements)



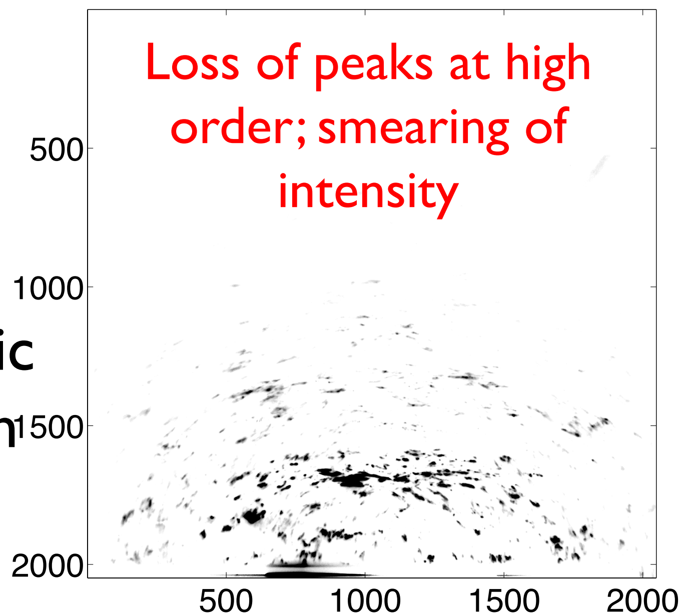
Poulsen, Springer 2004
Suter et al., *Rev. Sci. Instruments*, 2006
Li and Suter, *J Appl. Cryst.* 2013; LLNL-CODE-657639

Detector Images:

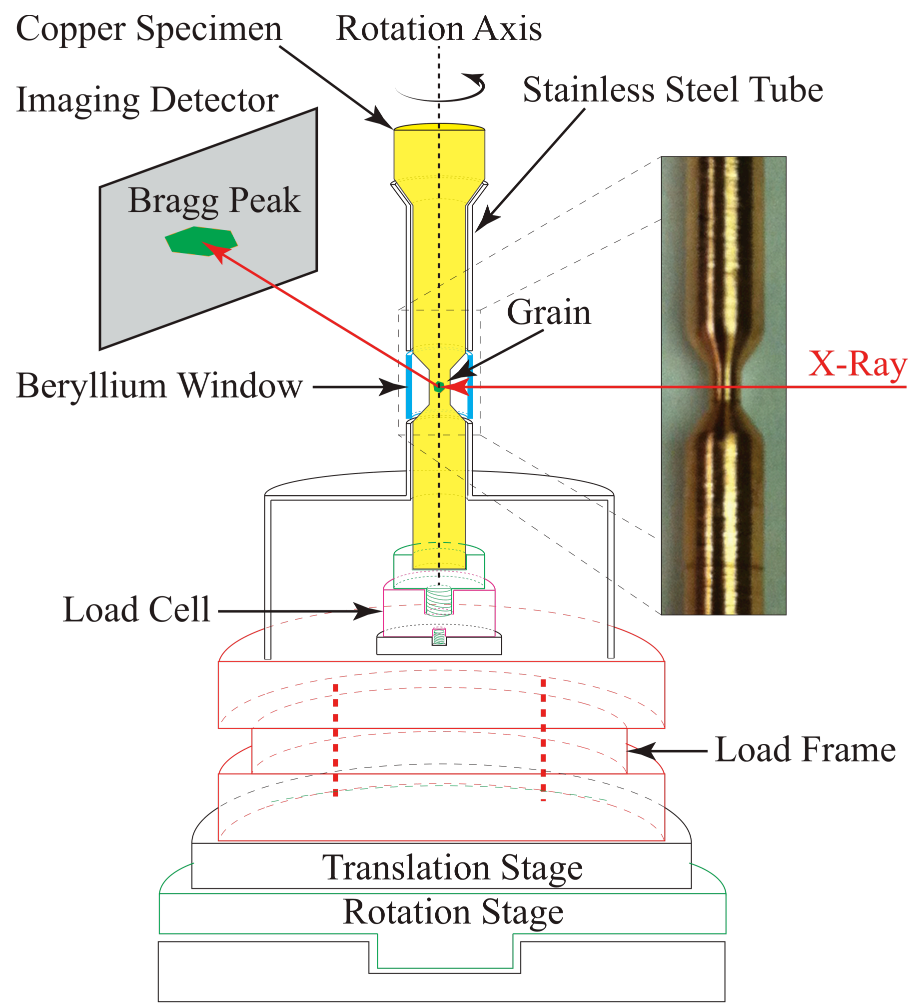
0%



12% plastic strain



Experimental Set-up



Each illuminated layer is reconstructed using the Forward Modeling Method (**FMM**) to a 2D orientation field; layers are then stacked together to obtain a 3D orientation map

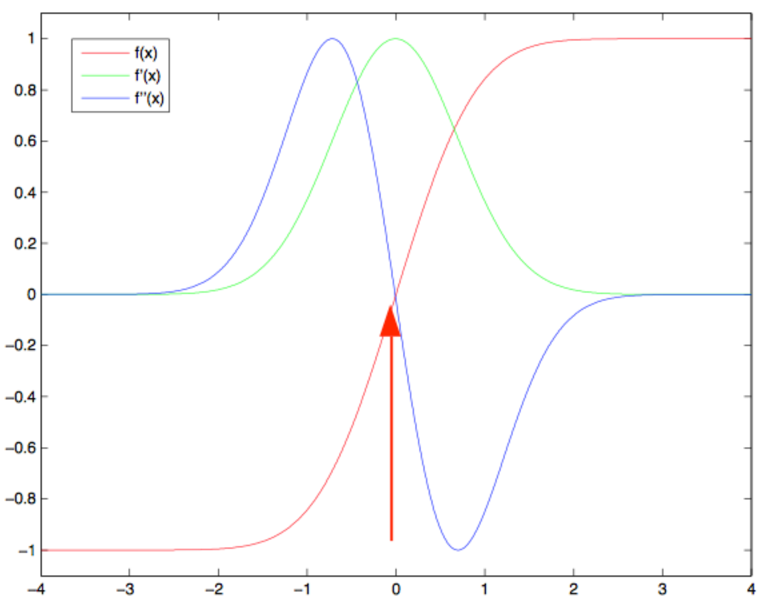
Li & Suter, *J. Appl. Cryst.* **46** 512 (2013)

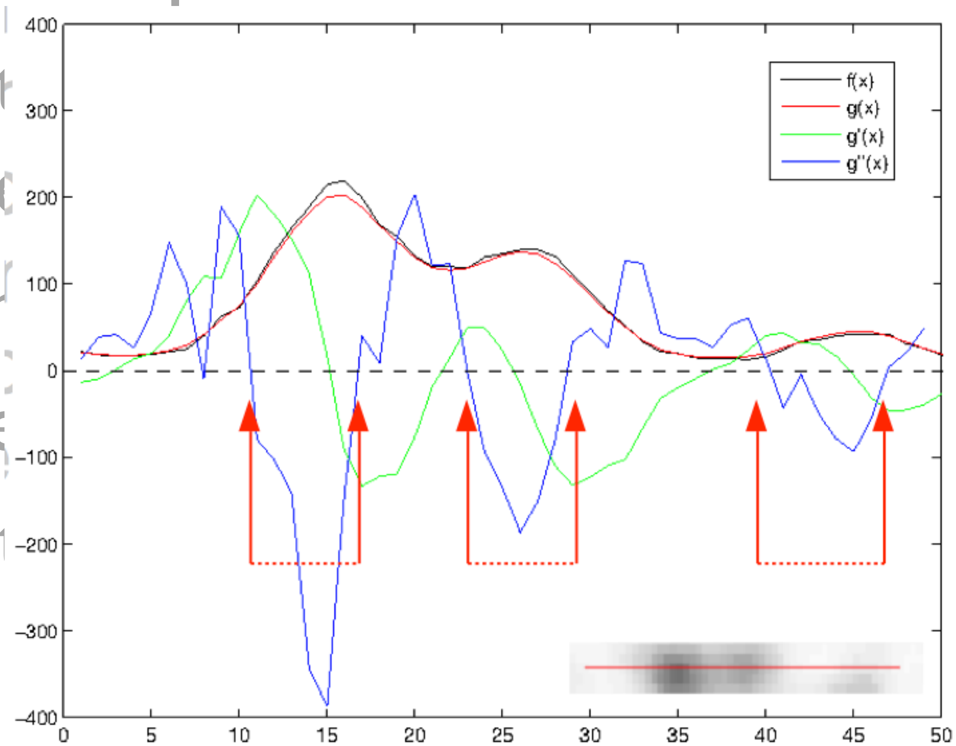
Image Refinement

- Previous : Simple threshold (baseline + ratio)
- Risk of peak overlap, esp. strong adjacent to weak, esp. smeared peaks from plastic strain.
- Added Laplacian of Gaussian (LoG) filter
- Use Δ [Im] == 0 (crossing points) to define peak extent
- Current : Previous with low baseline + local intensity variation edge detection
- Will further segment merged peaks
- Sensitive to internal peak variations (twins)
- *Improved peak segmentation aids Forward Modeling Method because larger fraction of peaks fitted*
- References: Jonathan Lind, PhD thesis in Physics, Carnegie Mellon University (2013); "Tensile twin nucleation events coupled to neighboring slip observed in three dimensions", J. Lind *et al.* Acta mater. (2013) **74** 213-220.

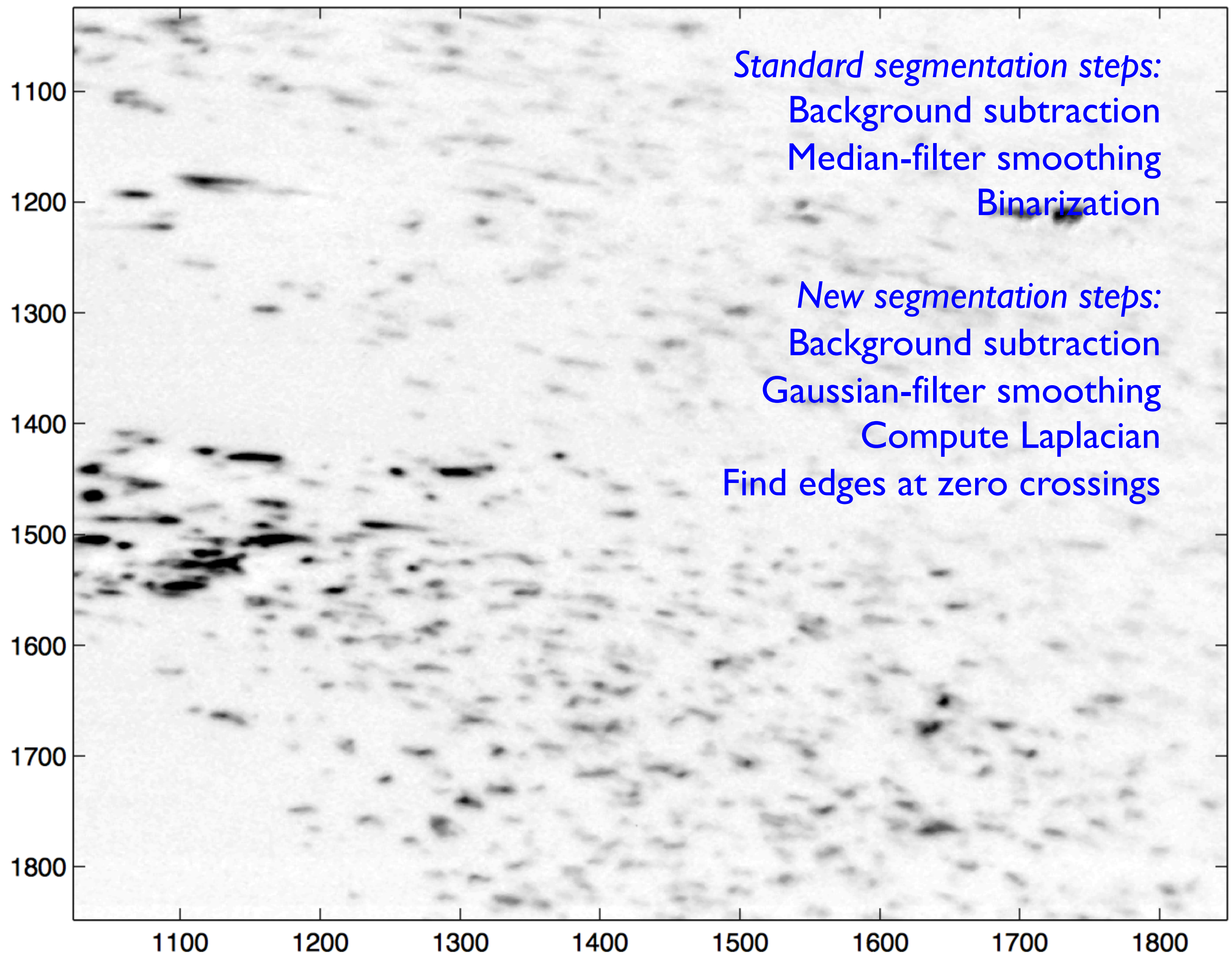
Segmentation of Peaks

- Previous : Simple threshold (baseline + ratio)
- Added Laplacian of Gaussian (LoG) filter
- Use Δ [Im] == 0 to define peak extent





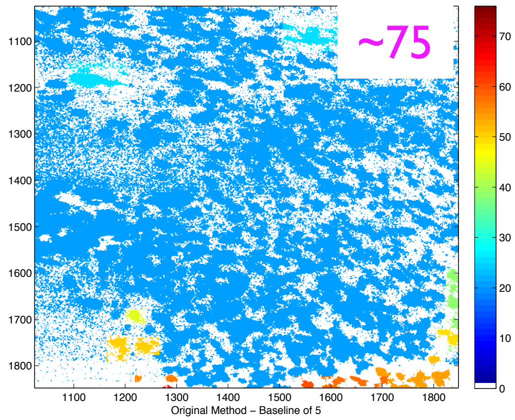
Diffractogram example



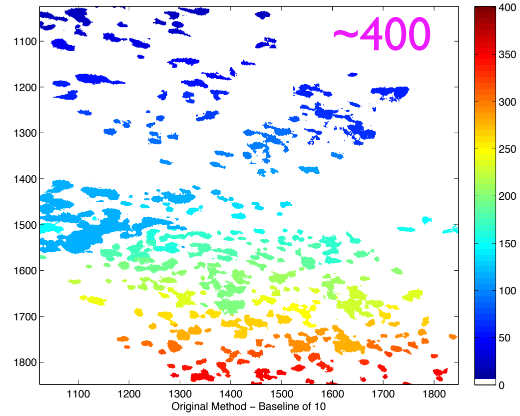
Segmentation: Original vs. LoG

Baseline levels of 5 (left), 10 (center) and 20 (right hand column)
Unique color indicates segmented peak: longer series ⇒ improved segmentation

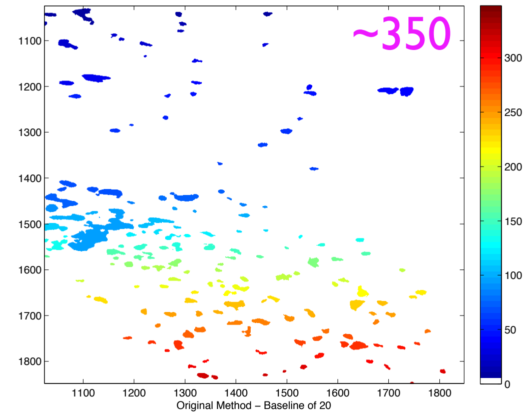
OLD



(a)

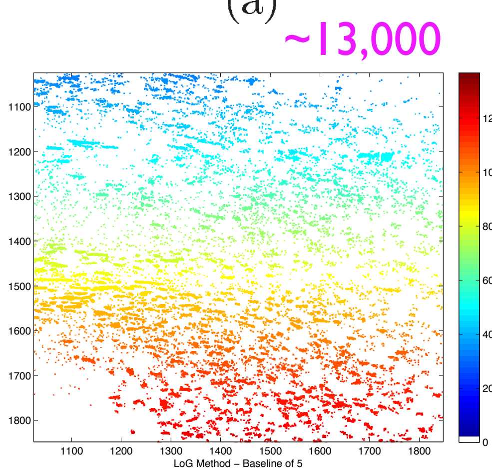


(b)

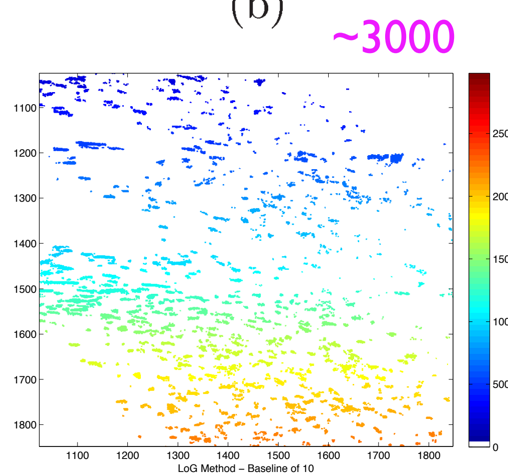


(c)

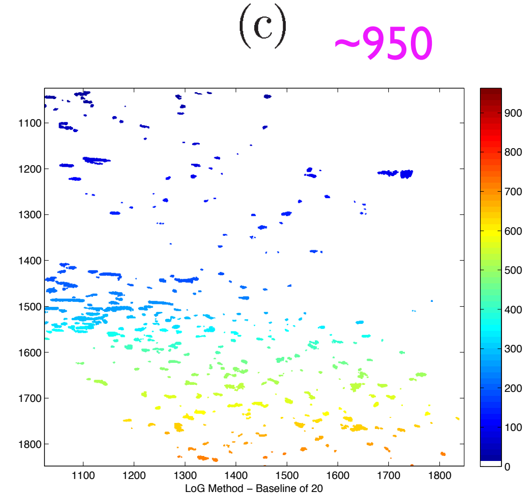
LoG



(d)

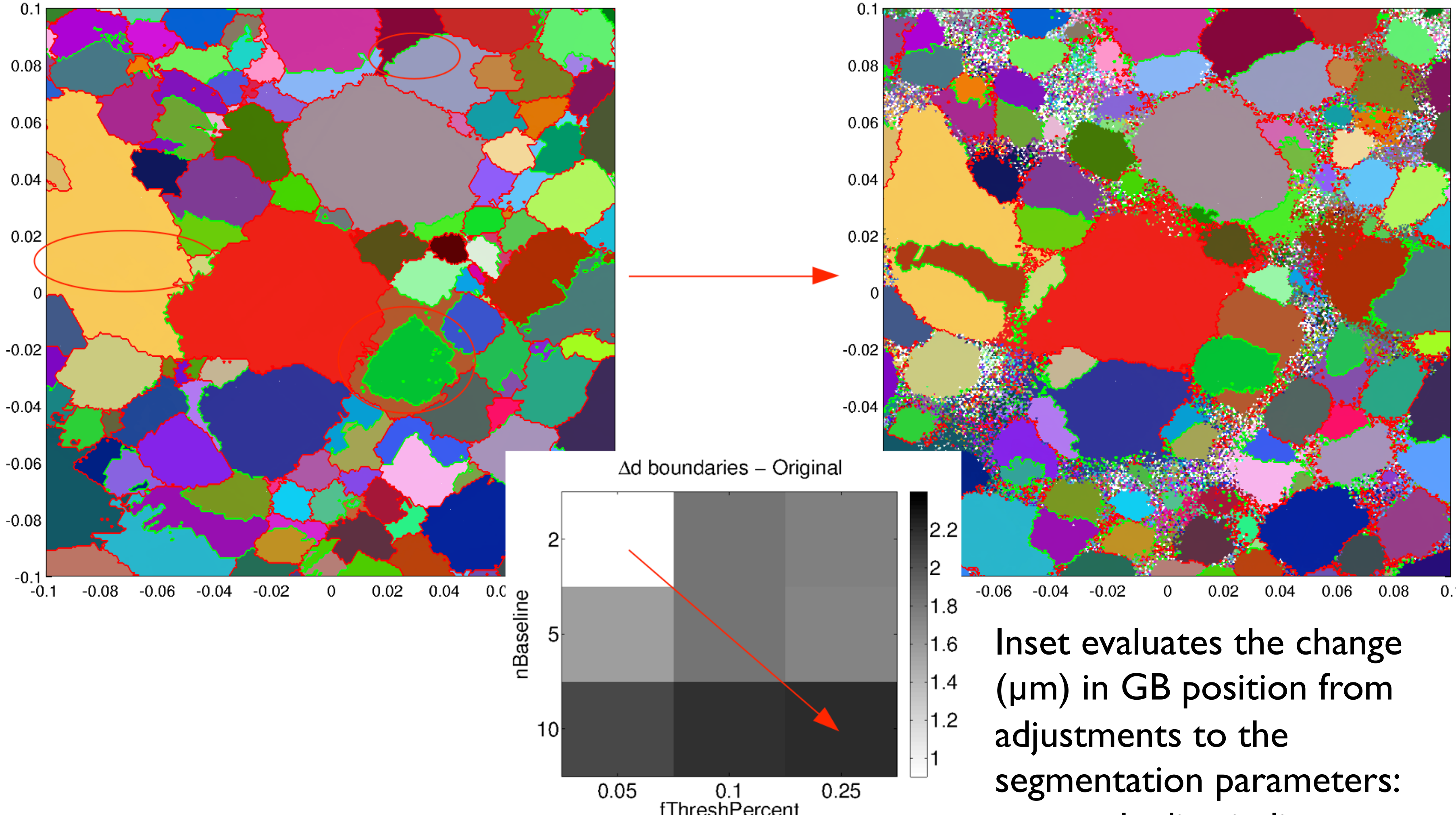


(e)



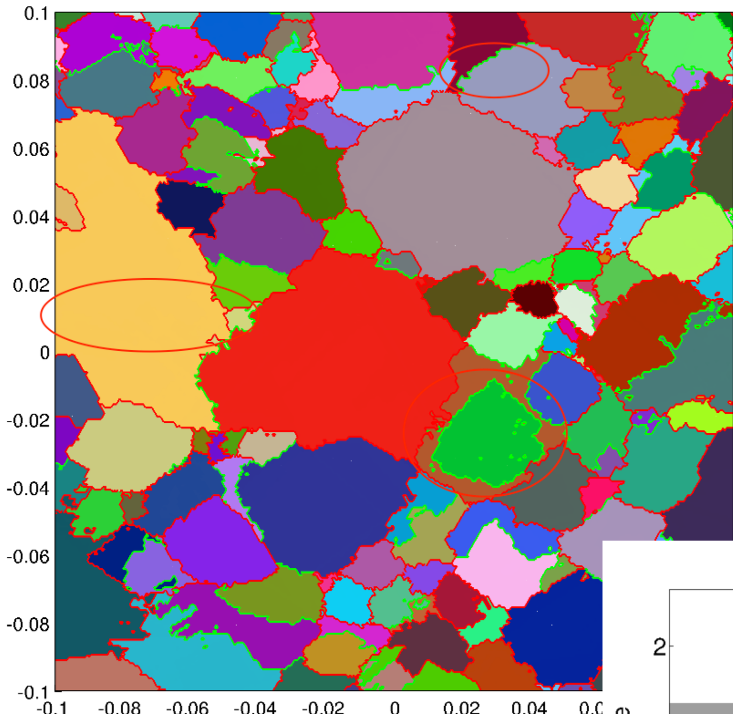
(f)

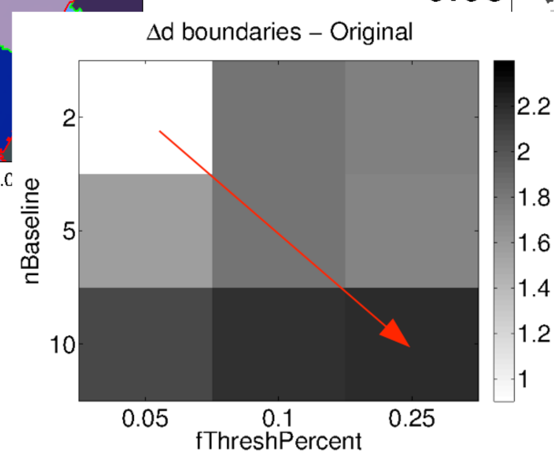
Old method (threshold)

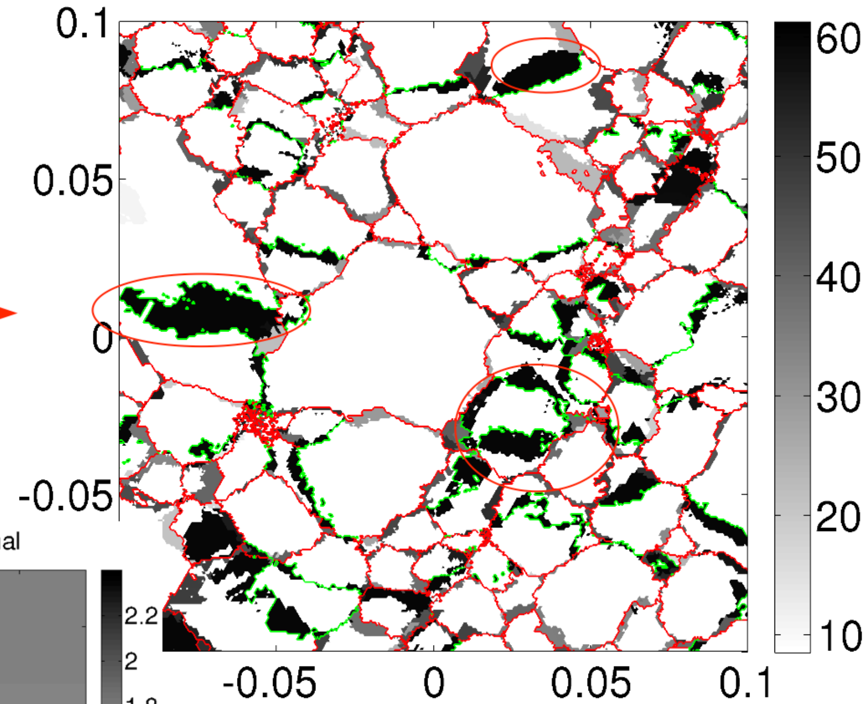


Inset evaluates the change (μm) in GB position from adjustments to the segmentation parameters: strong shading indicates sensitivity

Old method (threshold)

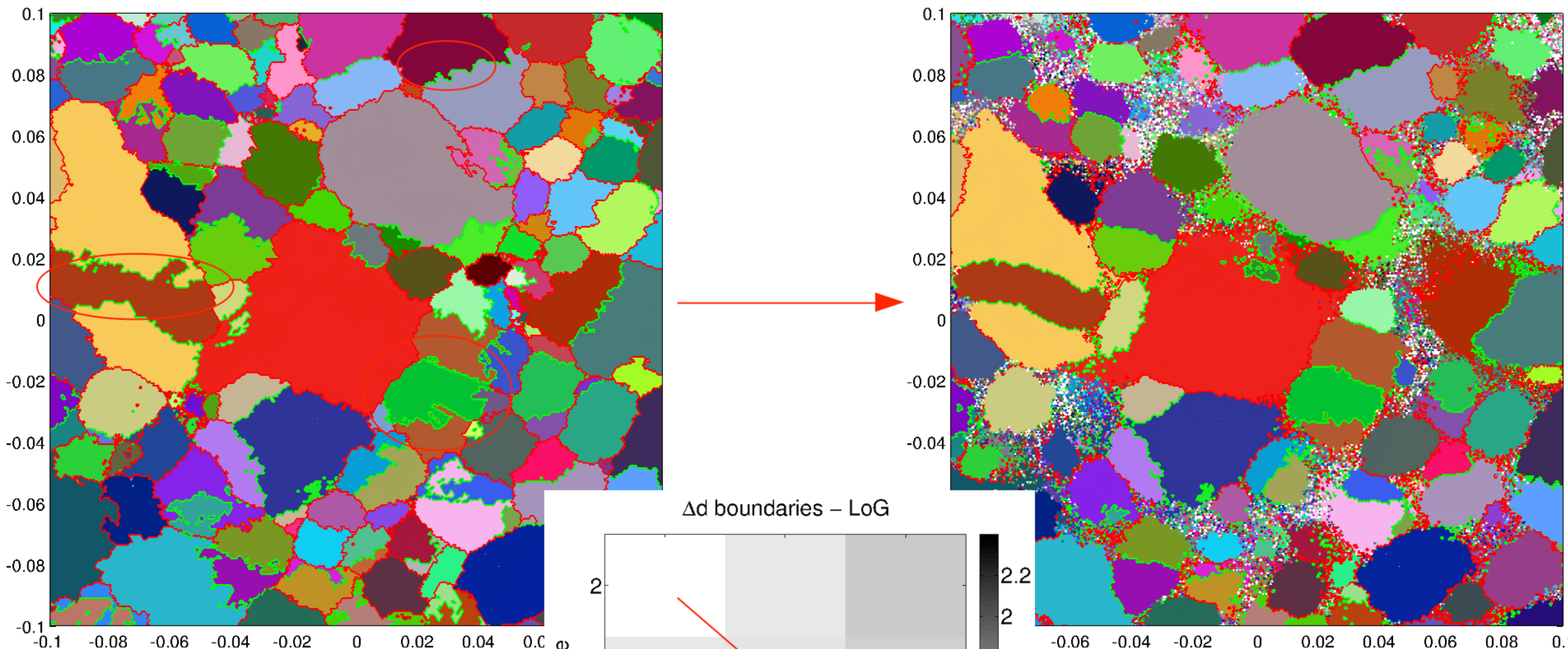


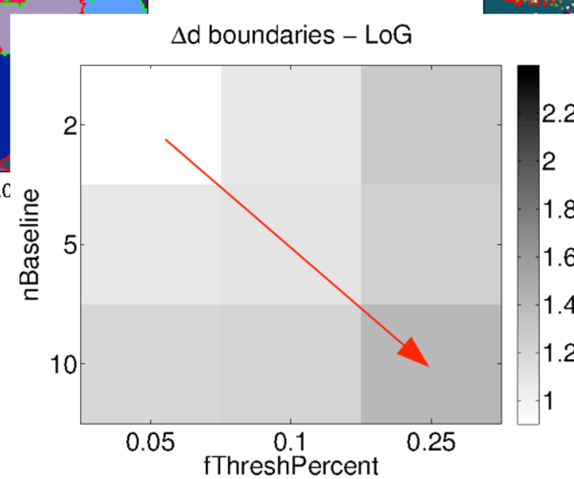




Map on right indicates the extent of changes in boundary position (significant) from parameter changes

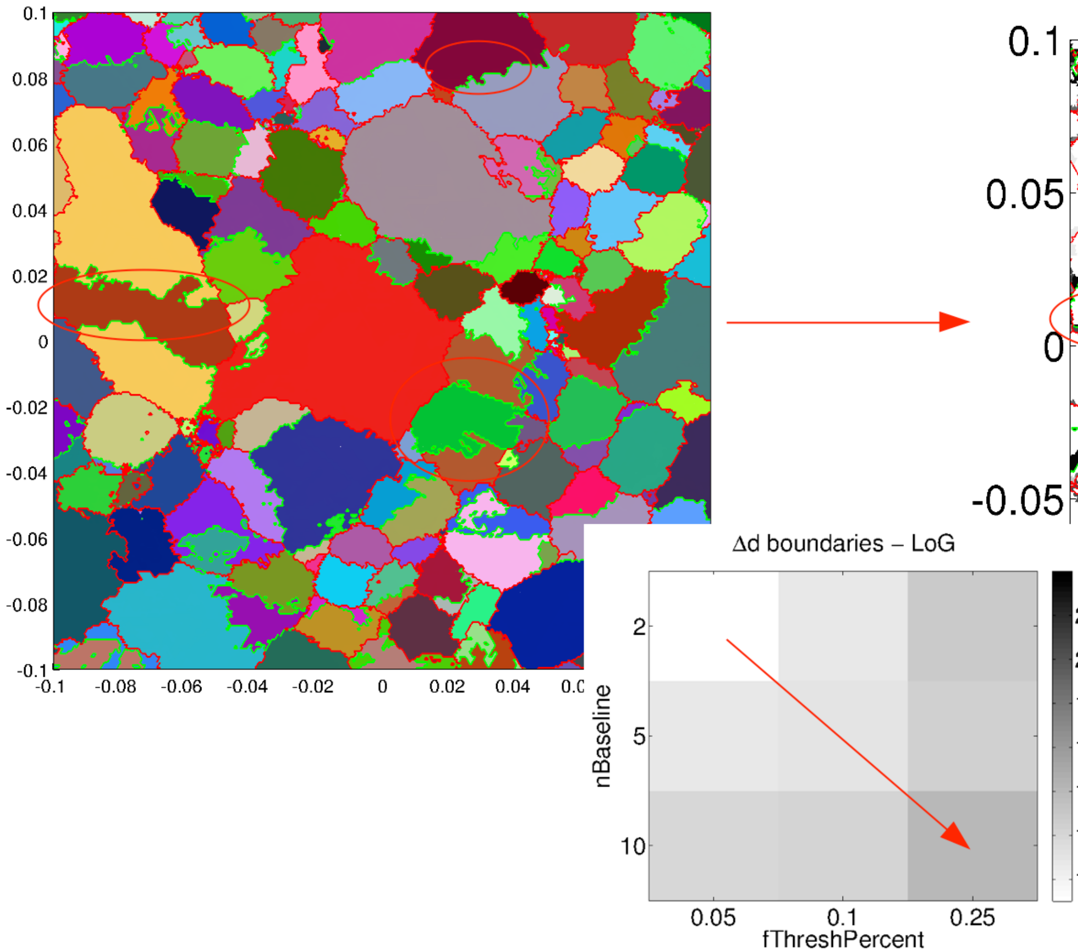
New Method (LoG)

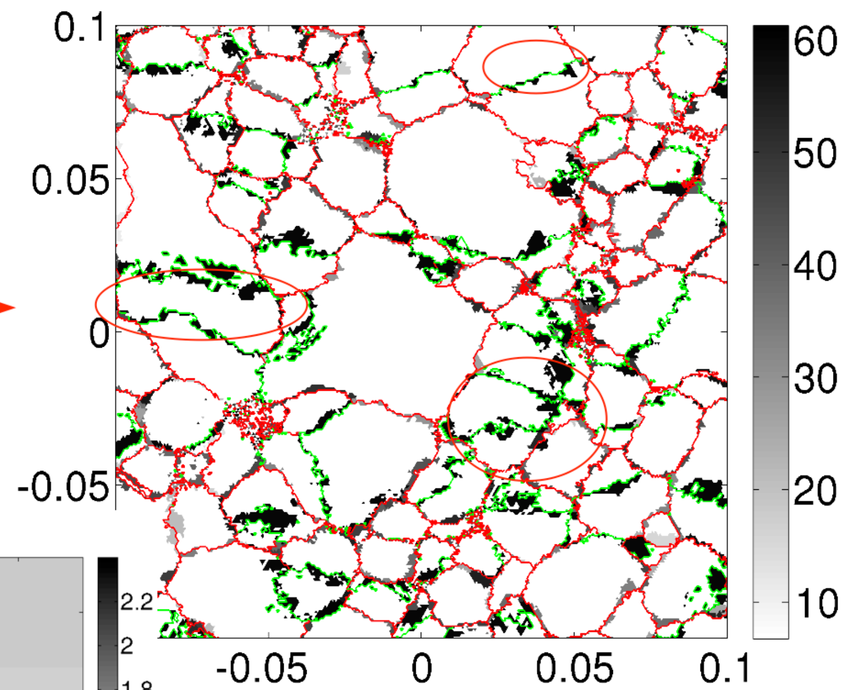




Inset evaluates the change (μm) in the result from adjustments to the segmentation parameters: light shading indicates lesser sensitivity

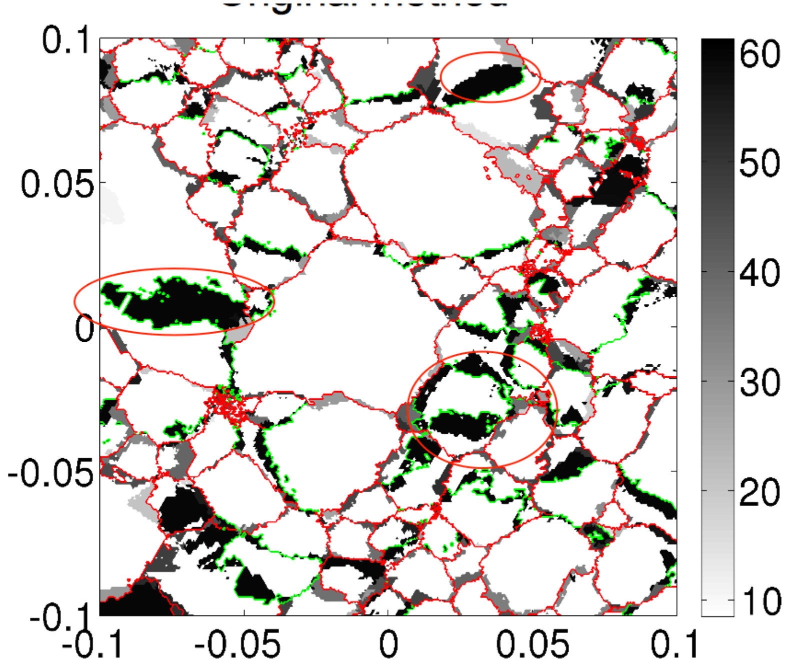
LoG – Quality map

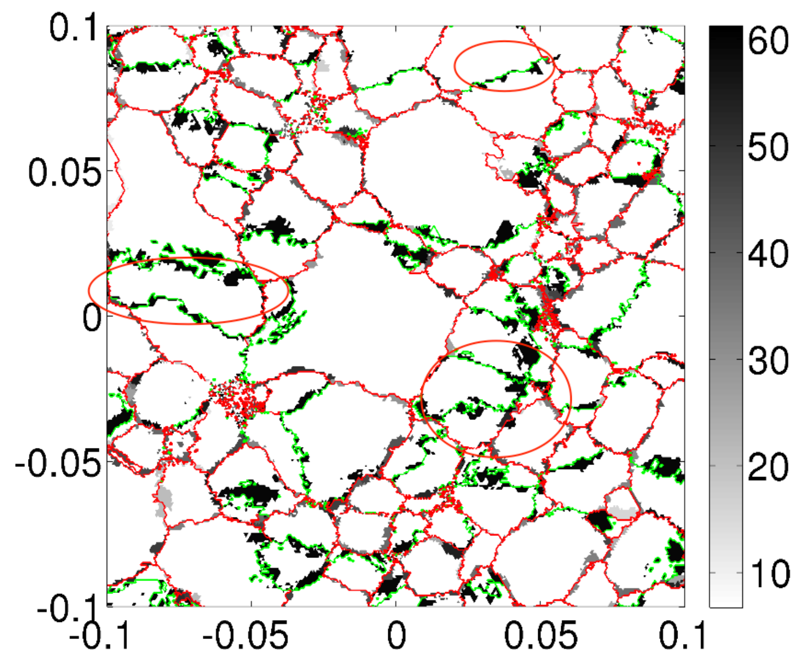


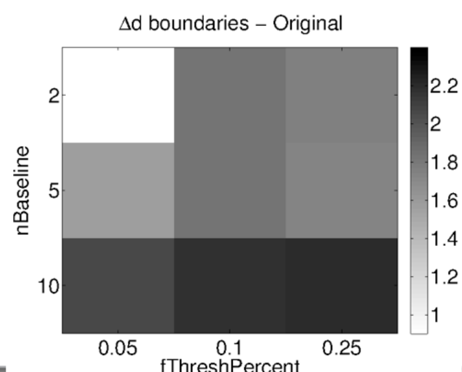


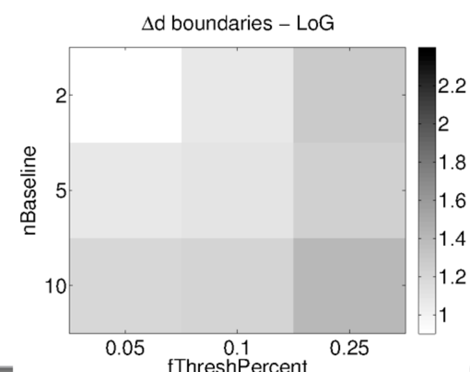
Map on right indicates the extent of changes (μm) in boundary position (minor) from parameter changes

Compare Old vs LoG methods

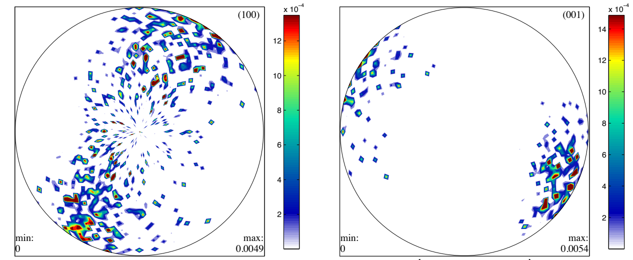




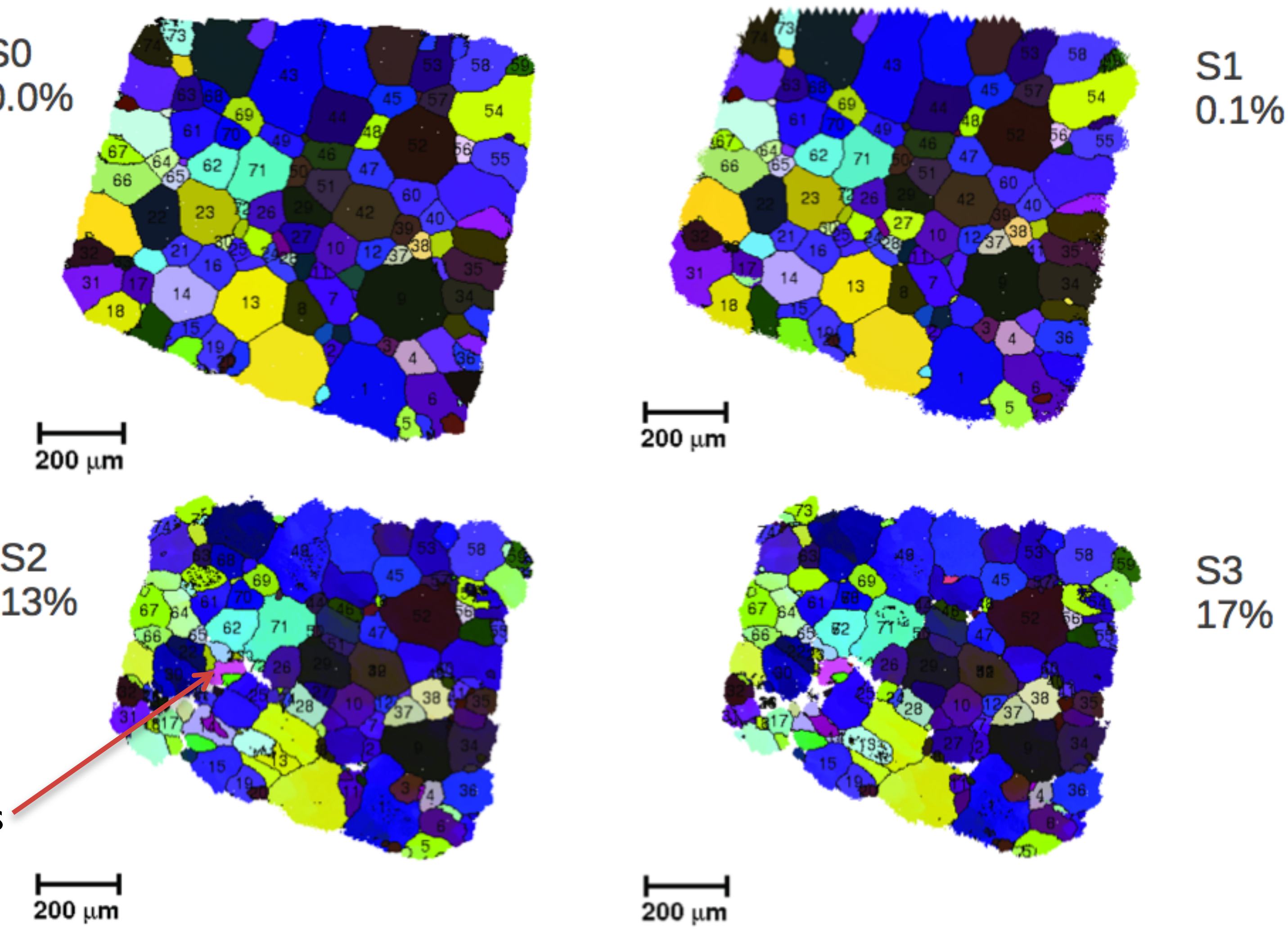




HEDM of Tensile Test on Zr



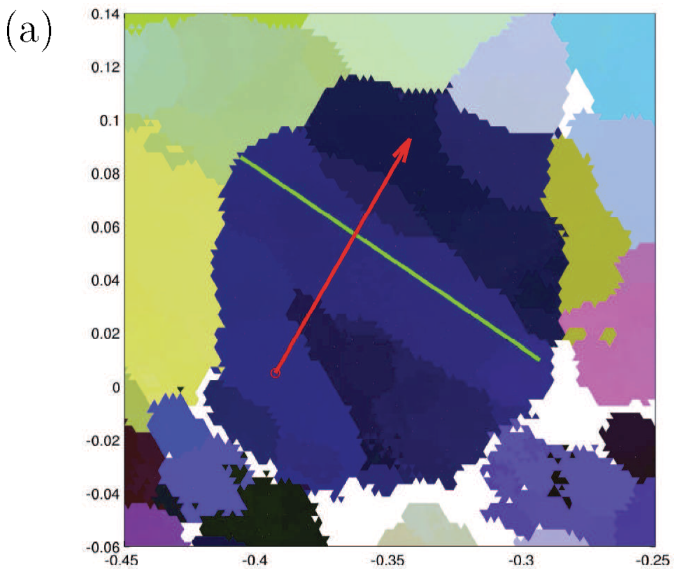
- Initial goal was to correlate void formation with microstructural features
  - Dogbone design but with rectangular cross-section
  - HEDM snapshots at: 0%, 0.1%, 13% and 17%
  - Note near-plane strain

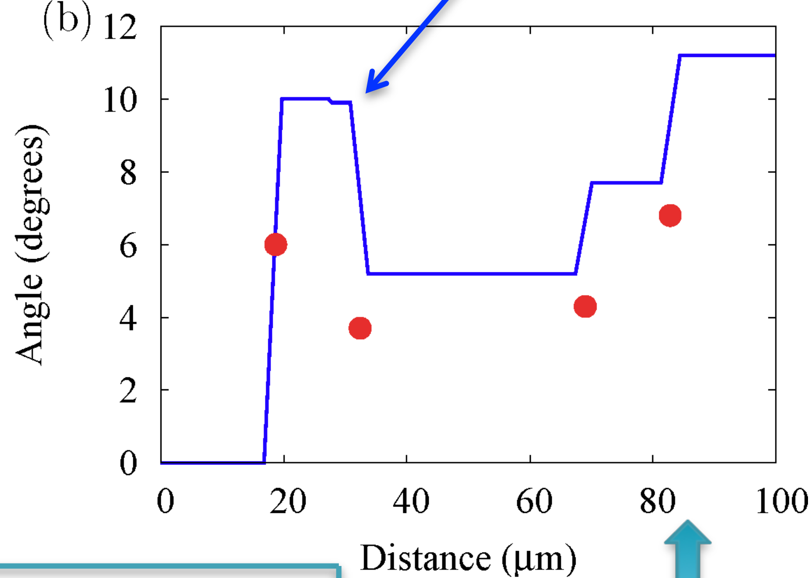


“Tensile twin nucleation events coupled to neighboring slip observed in 3D”, Lind et al., *Acta mater.,* 74 213-220 (2014)

Zr: Rotation axes, twinning

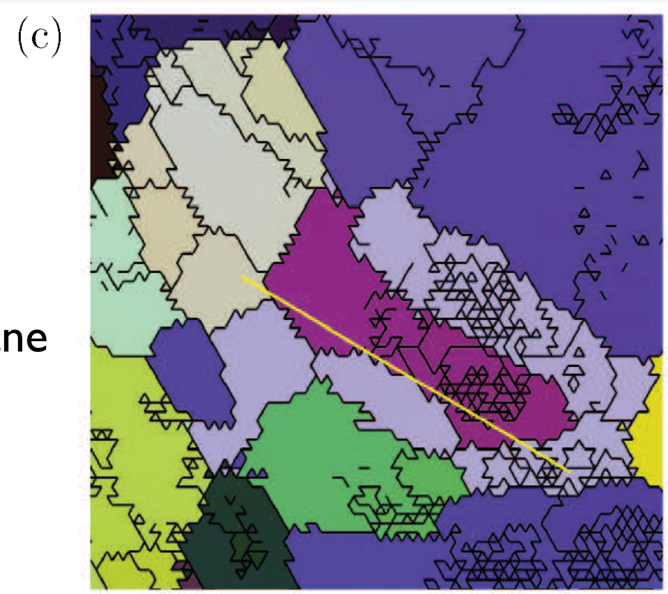
Misorientation from origin



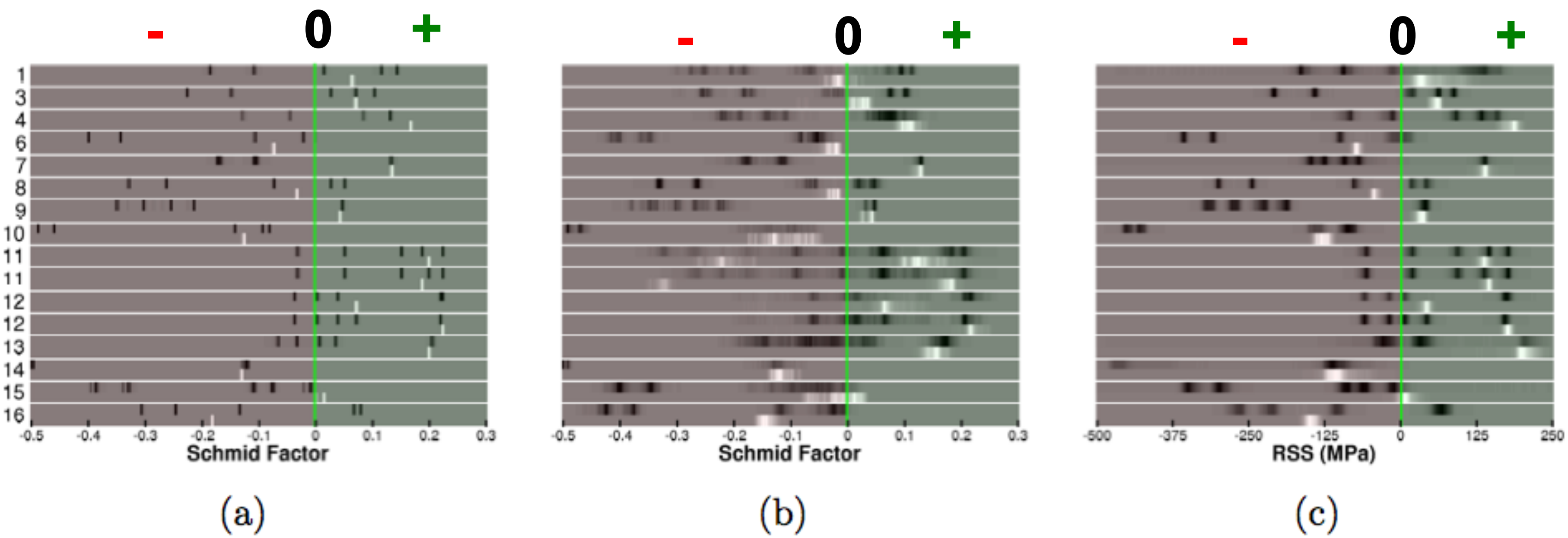


Edges of deformation bands (jumps in orientation) = local misorientation axis is // 0001, consistent with prismatic slip.

Magenta: twin
Yellow line:
{1012} twin plane



Schmid factors, Resolved Shear Stress

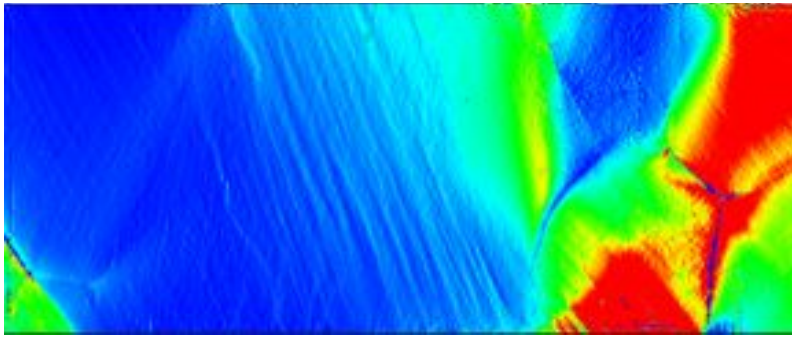


Schmid factors at 0 % - Schmid factors at 13 % – Resolved Shear Stress

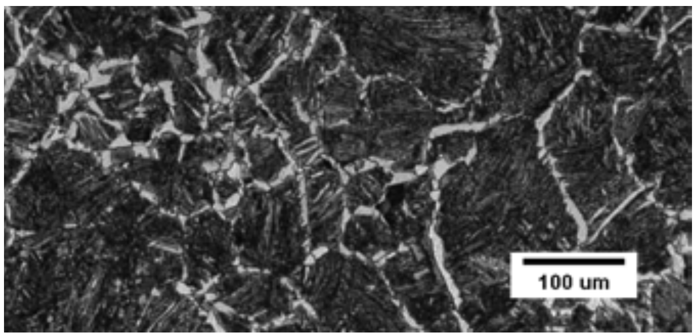
- Each line = an observed twin
- Green zone: positive Schmid factors
- Red zone: negative Schmid factors
- Set of 6 marks indicates the variants; white mark = observed twin variant
- Full field elastic stress calculation provides resolved shear stresses; little change compared to simple Schmid factors
- Several variants occur with *negative Schmid factors* ⇒ Plasticity influences twinning

(Anisotropic) elastic stress-strain fields computed with FFT method

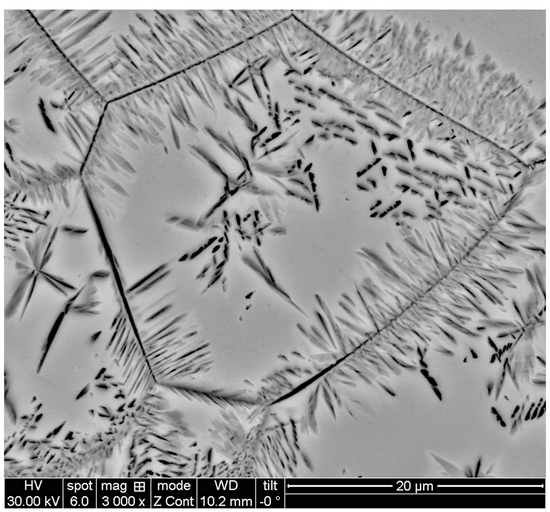
Other Image Challenges



The striations are "**slip bands**" i.e. concentrated surface displacement from dislocation motion: how best to quantify such features?



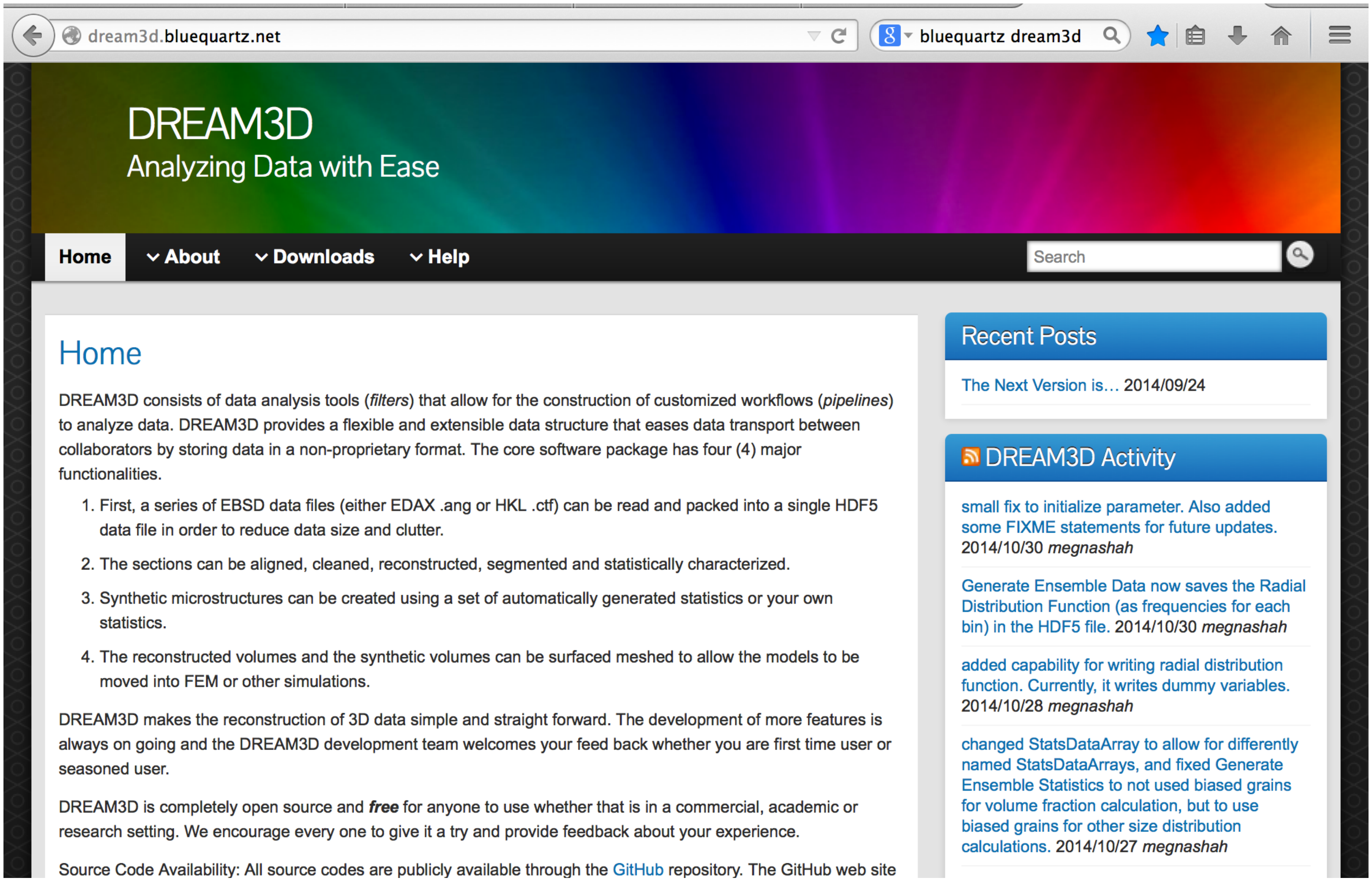
Deformed metal reveals a grain structure but the **boundaries** (white lines) are incomplete: how to complete the network?



One complete crystallite (grain) visible. Many platy (anisotropic) precipitates (2nd phase **particles**) visible. How to segment and measure the particles?

Software …

Many of the algorithms that we use to analyze 3D microstructures are available in Dream3D (open source, Mac/PC/Linux); also ITK.

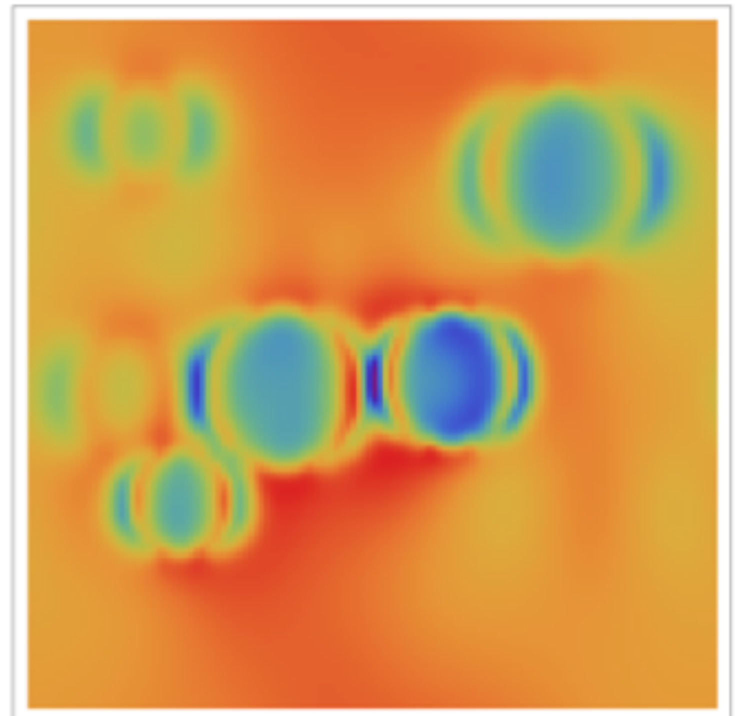


Summary

- The Forward Modeling Method for indexing diffractograms from x-ray diffraction experiments at synchrotrons depends on identifying peaks. Simple thresholding works for well annealed samples and isotropic intensity peaks. For smeared anisotropic peaks from plastically deformed materials, the Laplacian-of-Gaussians works significantly better.
- Comparisons do not show good agreement between experiment and simulation; statistical comparisons look reasonable (e.g. texture development, orientation gradients).
- A tensile test on Zr showed several twinning events, despite unfavorable texture. Some twins appeared in grains with negative Schmid factor. Links to slip activity also evident.
- Recent review of literature suggests that lack of agreement is the general result (with no known exceptions).
- Orientations and orientation gradients evaluated in a Cu specimen; compared with vpFFT simulation.
- KAM is higher near to grain boundaries; correlated with gradients in stress.

Prospects

- Direct comparison with diffraction data sets
- We need maps of the elastic strain tensor
- Simulations that include finite strain
- Test various concepts such as latent hardening, strain gradient etc.
- Model polycrystal problems with dislocation dynamics
- Use better constitutive descriptions



Stress from dislocation loops, calculated with FFT method.