



Image Processing in Expts. + Simulations of Plastic Deformation of Polycrystals ICIP 2014, Paris

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+ many colleagues

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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



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

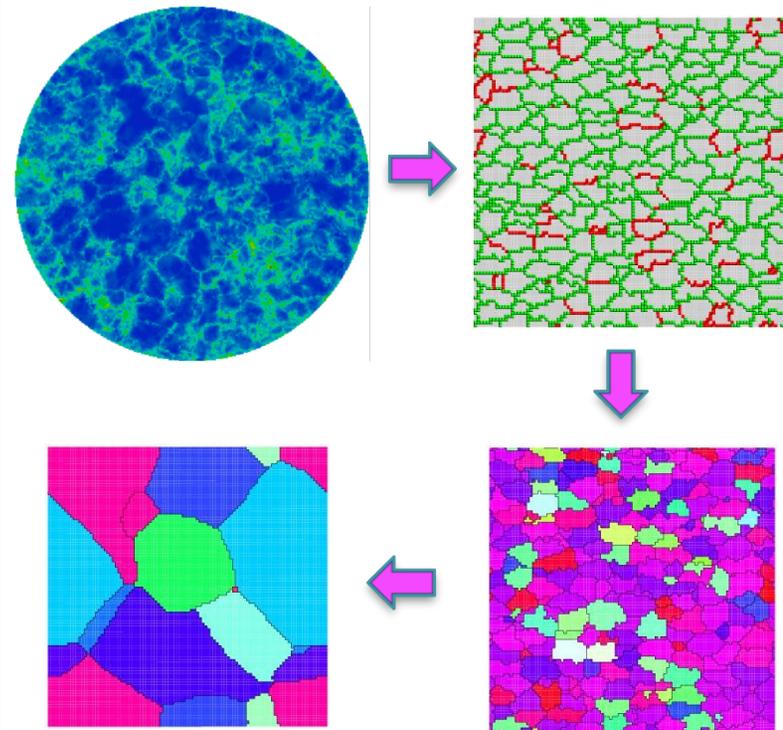


(b)

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



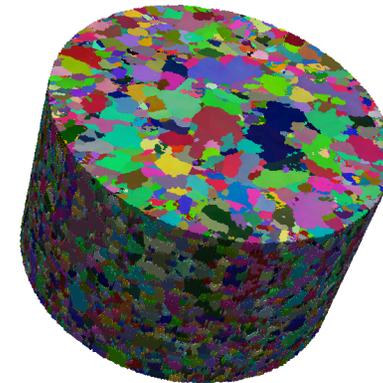
Wang, *Acta mater.* **59** 3872 (2011)

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
- $> 3 \times 10^6$ Bragg peaks
- 10^3 core parallel processing: 2D images to 3D orientation maps

3D copper microstructure



0.4 mm³

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

HEDM measurement schematic

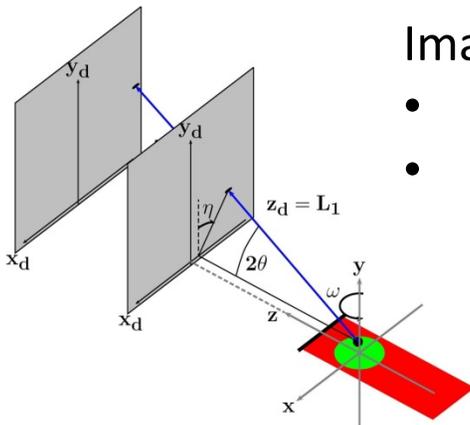


Image diffracted beams

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

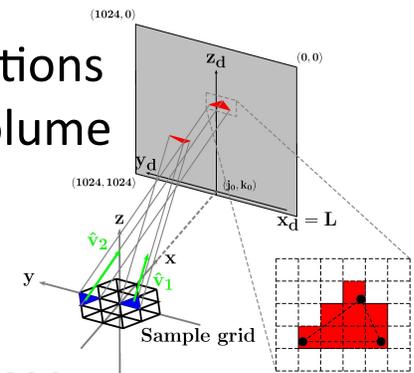
Poulsen, Springer 2004

Suter et al., *Rev. Sci. Instruments*, 2006

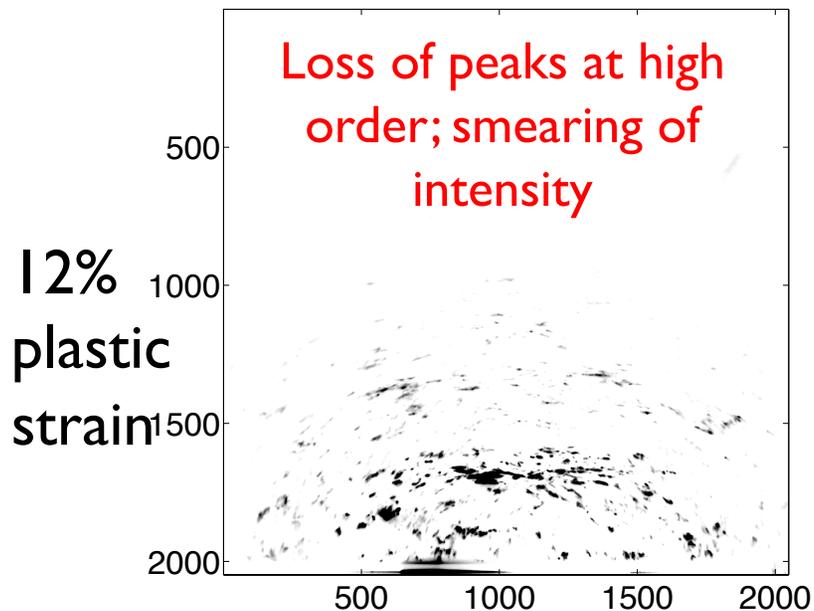
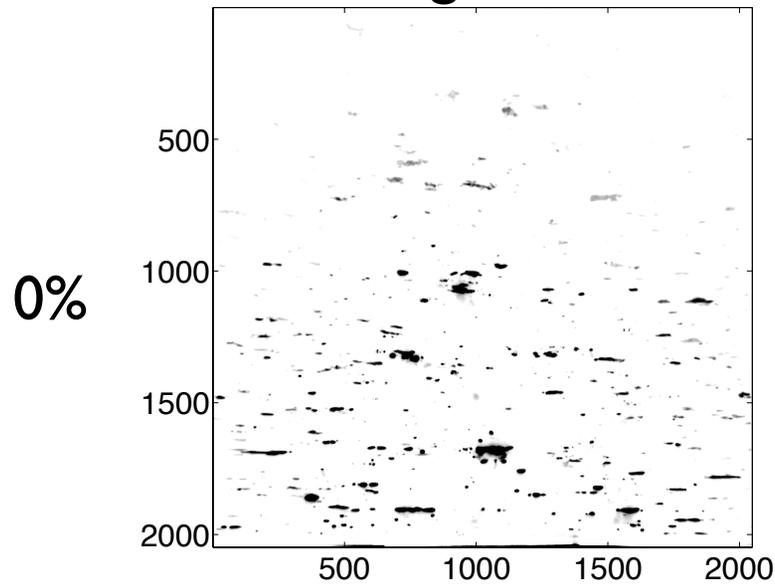
Li and Suter, *J Appl. Cryst.* 2013; LLNL-CODE-657639

Reconstruction via Forward Modeling

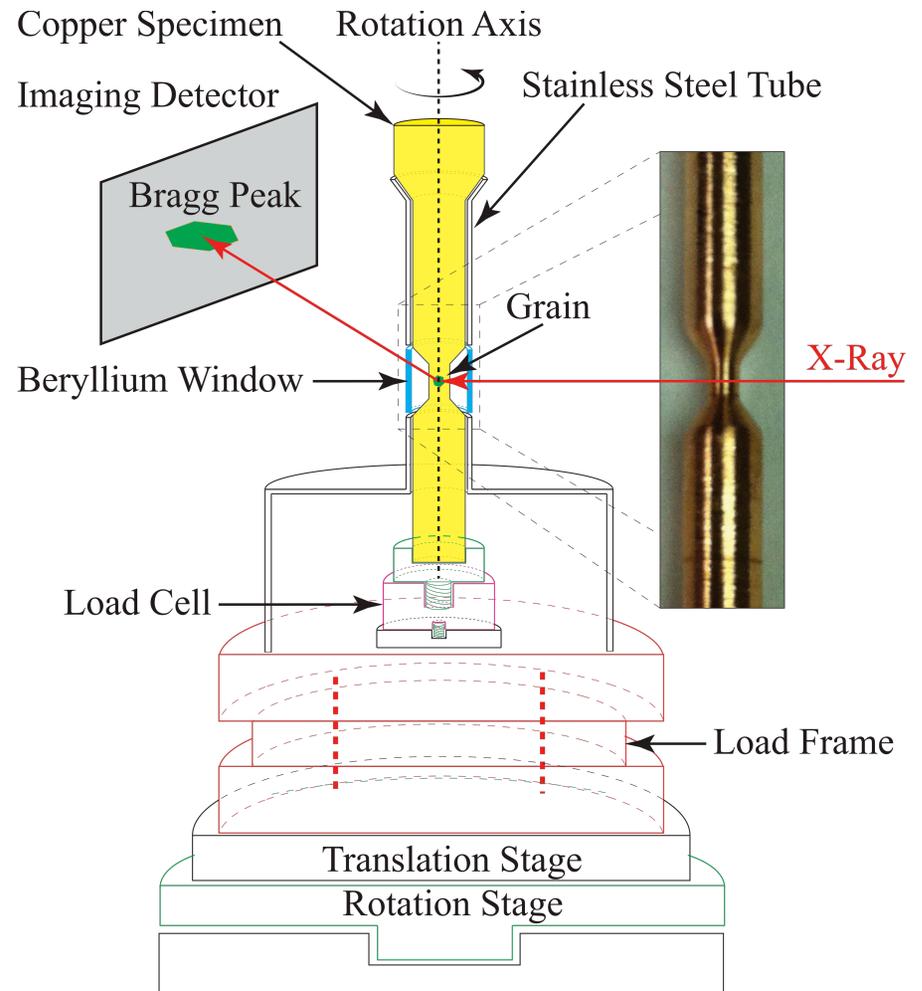
Optimizes orientations
in $> 10^7$ voxels (volume
elements)



Detector Images:



Experimental Set-up



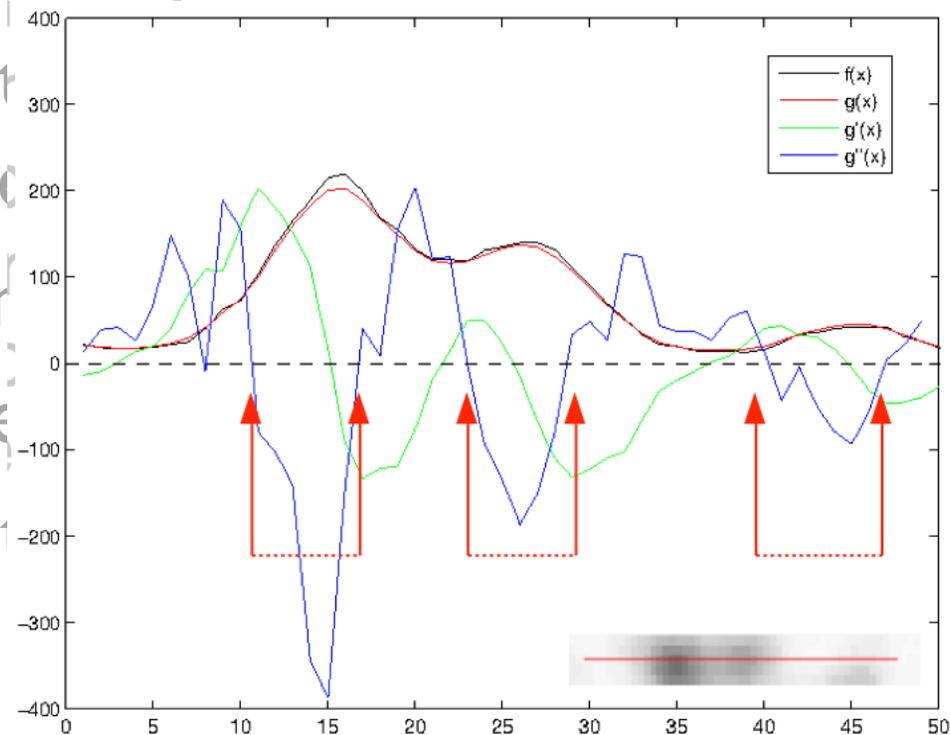
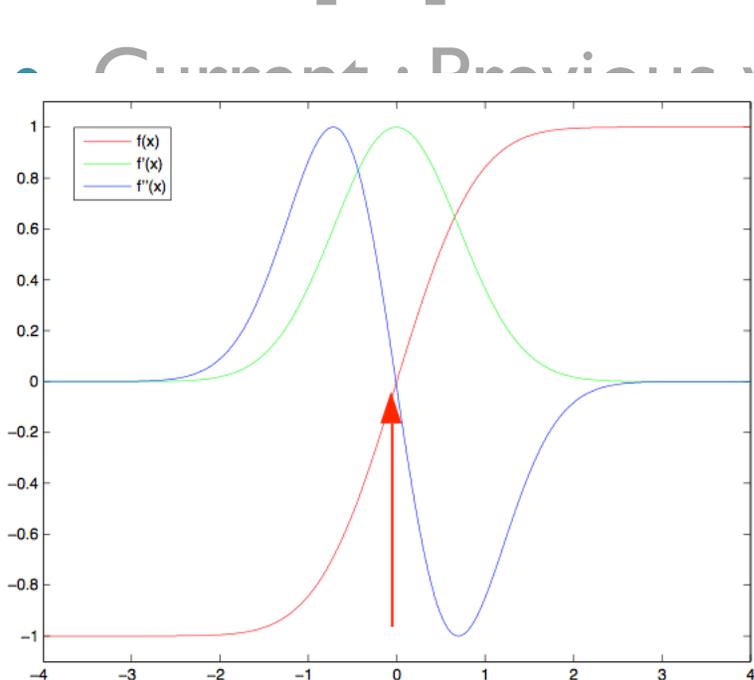
Each illuminated layer is reconstructed using the Forward Modeling Method (**FMM**) to a 2D orientation field; layers are then stacked together to obtain a 3D orientation map

Image Refinement

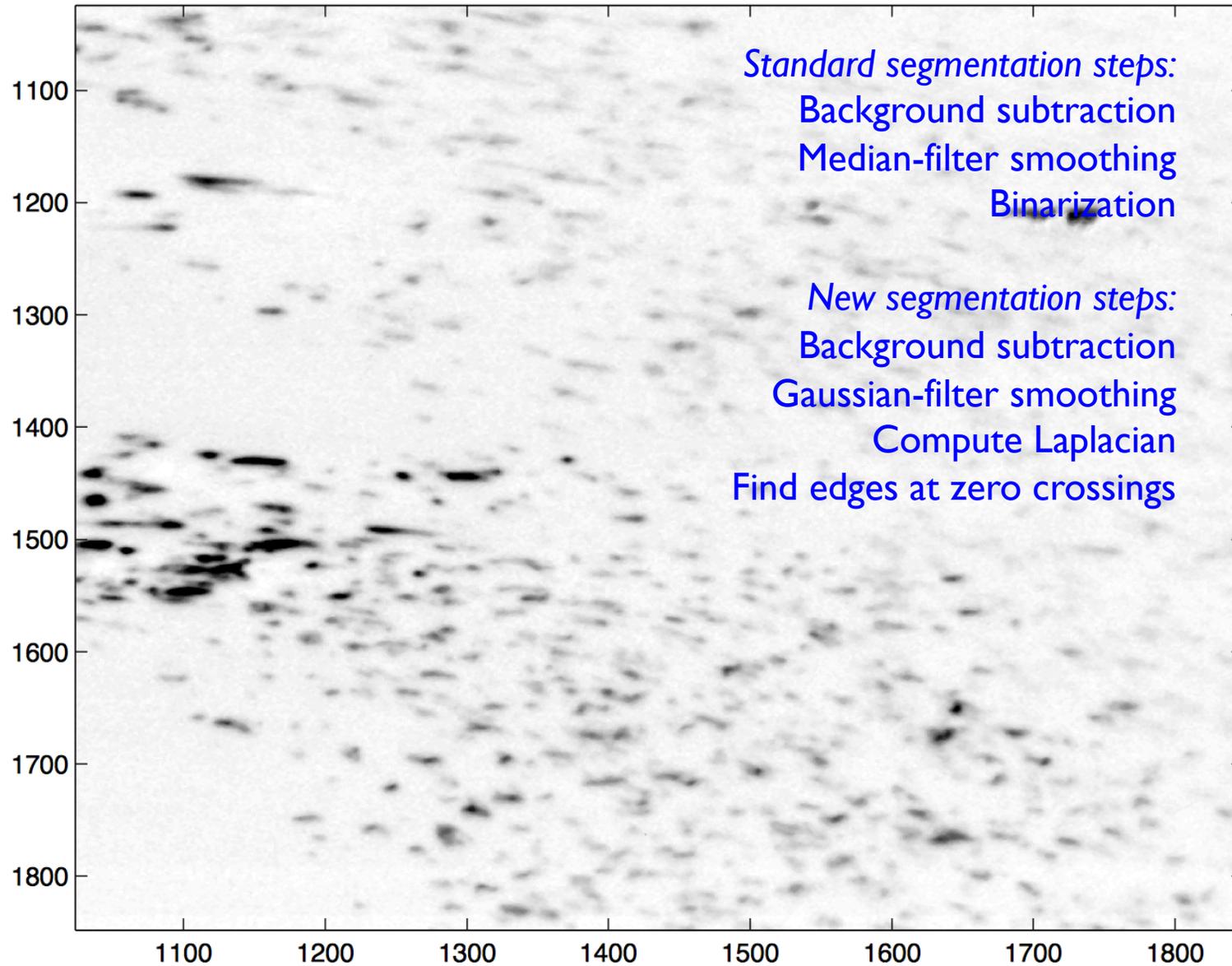
- Previous : Simple threshold (baseline + ratio)
- Risk of peak overlap, esp. strong adjacent to weak, esp. smeared peaks from plastic strain.
- Added Laplacian of Gaussian (LoG) filter
- Use $\Delta [I_m] == 0$ (crossing points) to define peak extent
- Current : Previous with low baseline + local intensity 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 $\Delta [Im] == 0$ to define peak extent



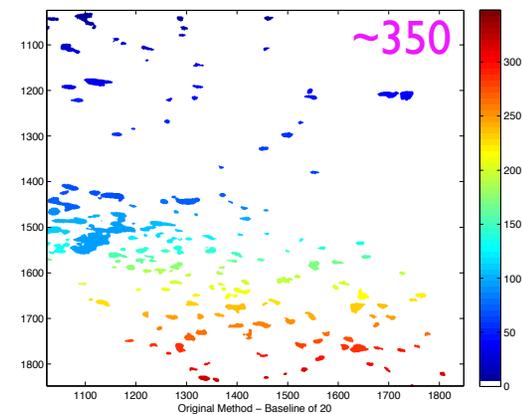
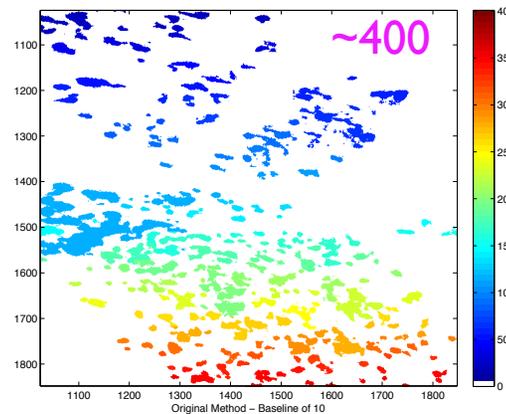
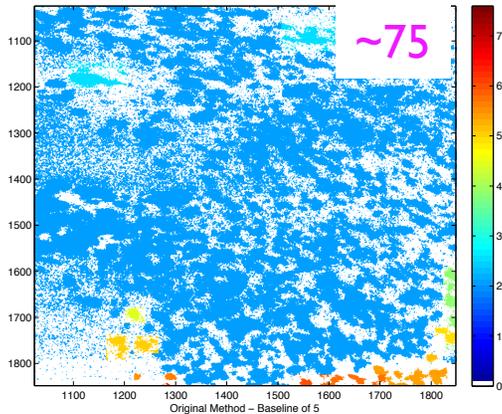
Diffractogram example



Segmentation: Original vs. LoG

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

OLD

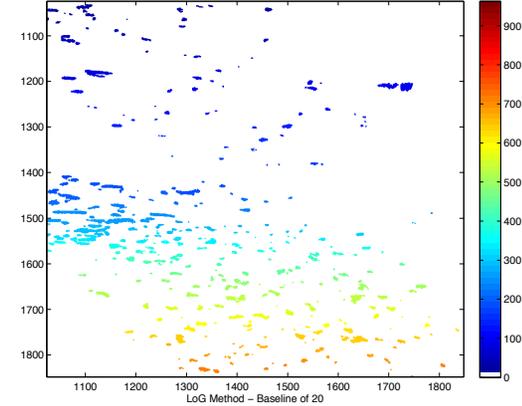
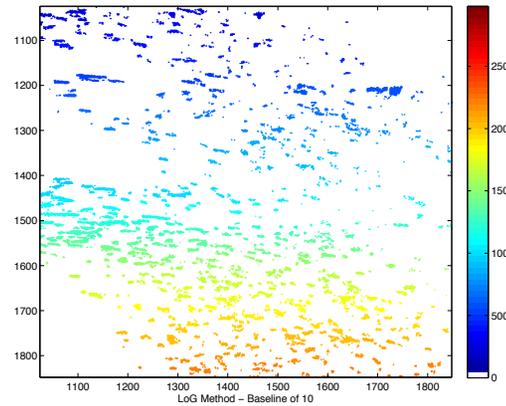
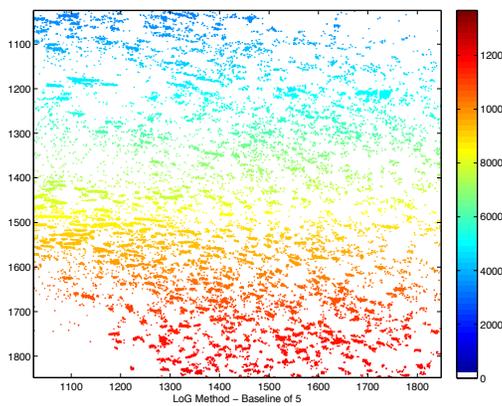


(a) ~13,000

(b) ~3000

(c) ~950

LoG

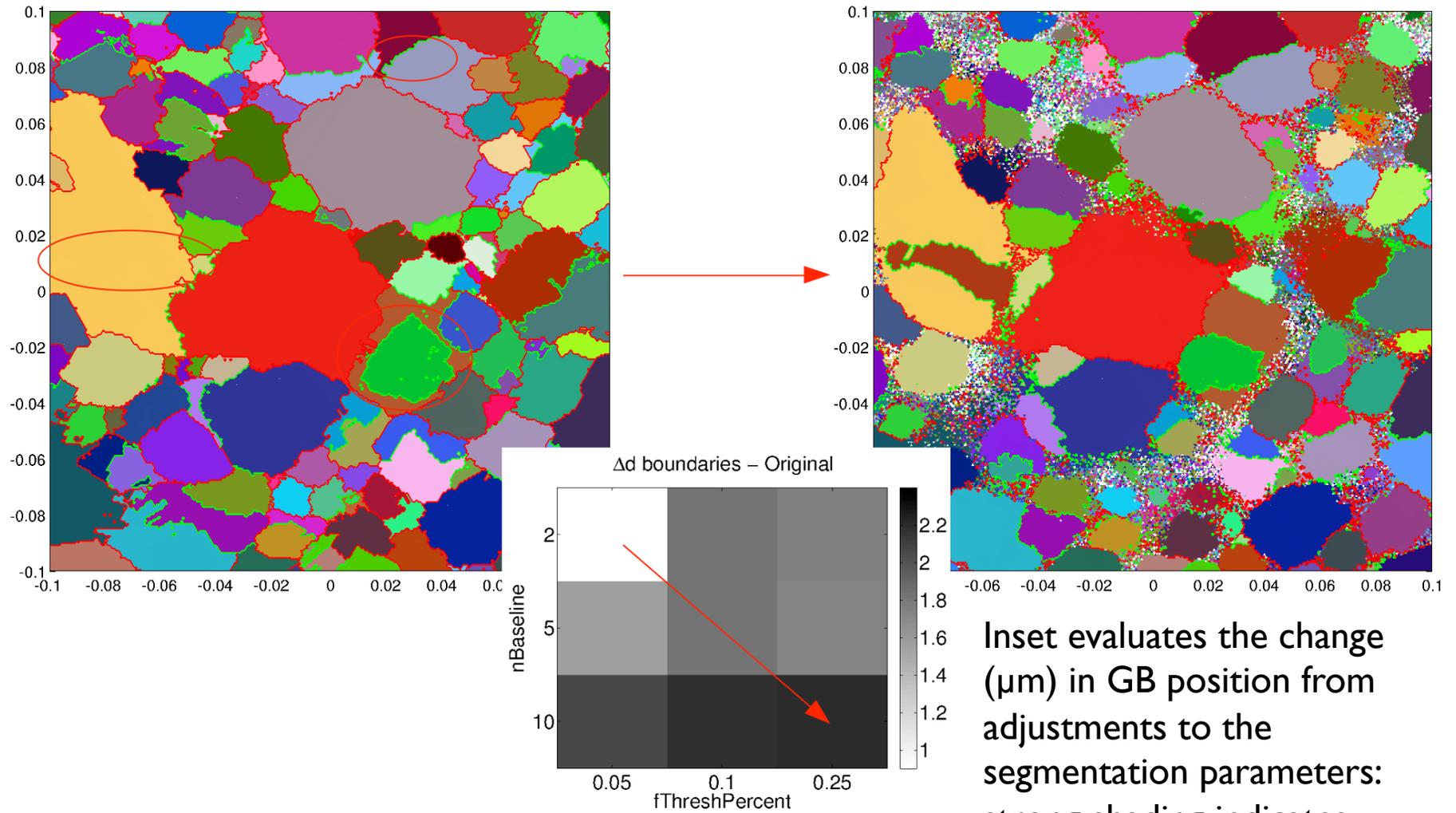


(d)

(e)

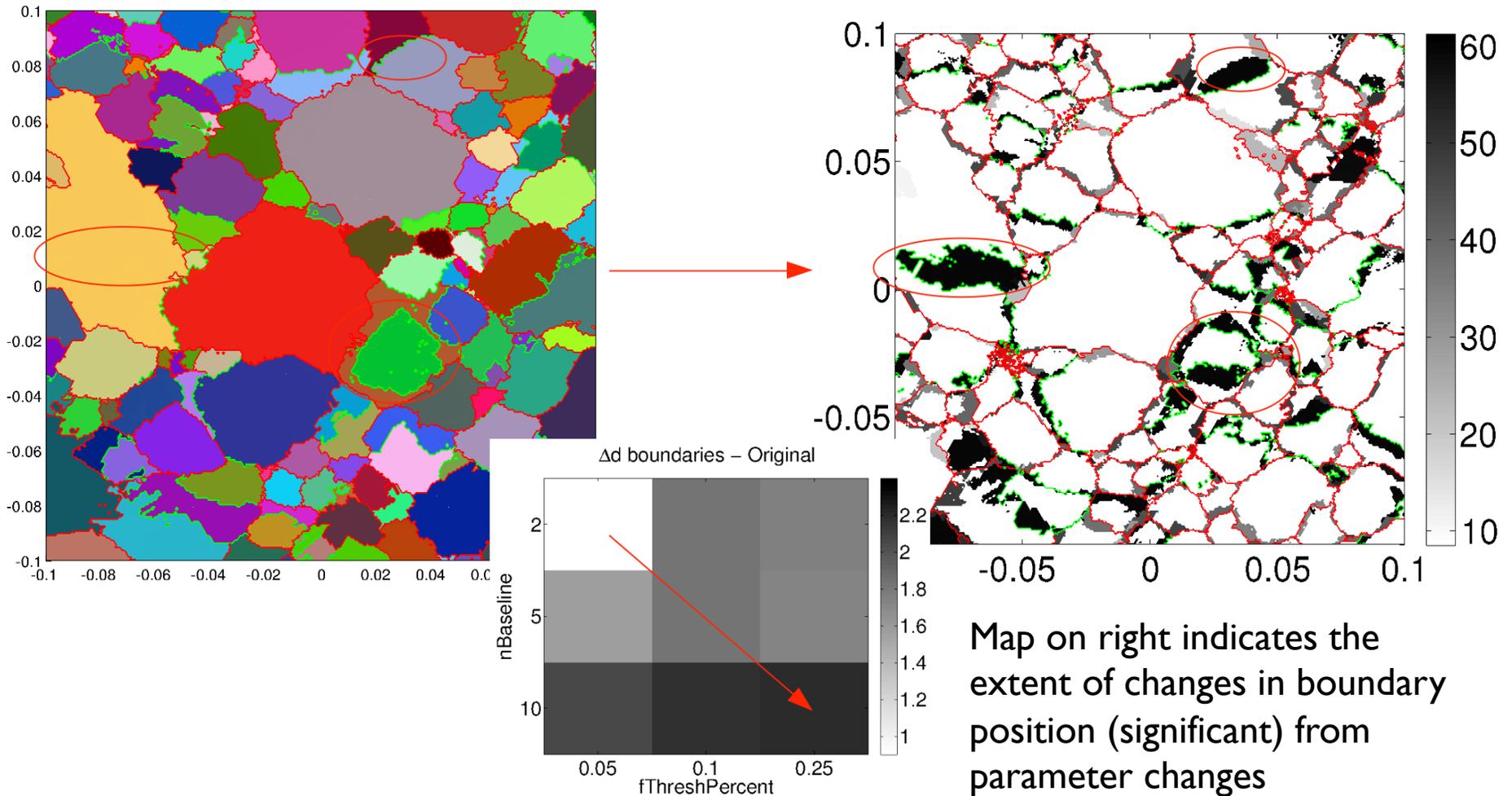
(f)

Old method (threshold)

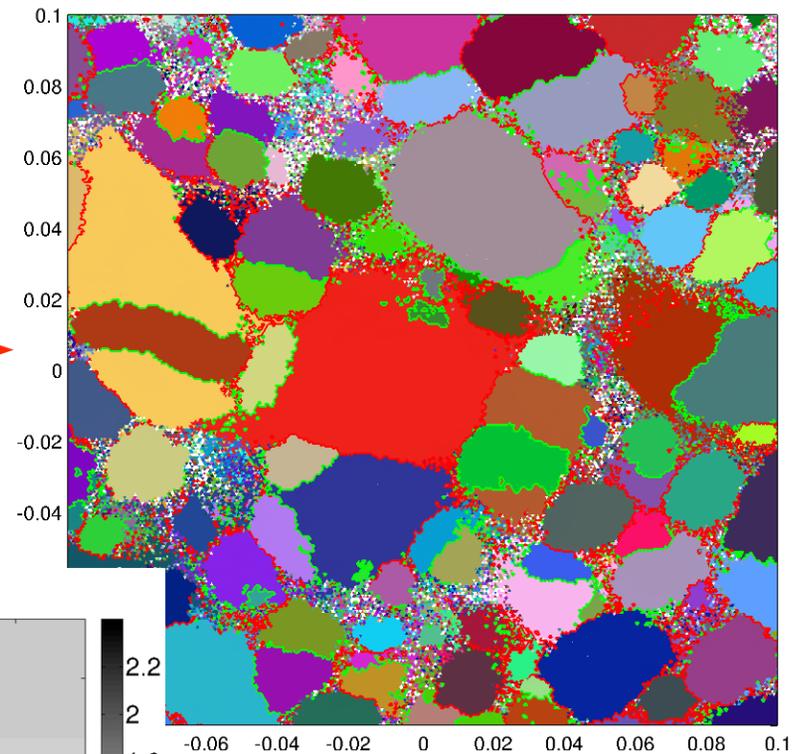
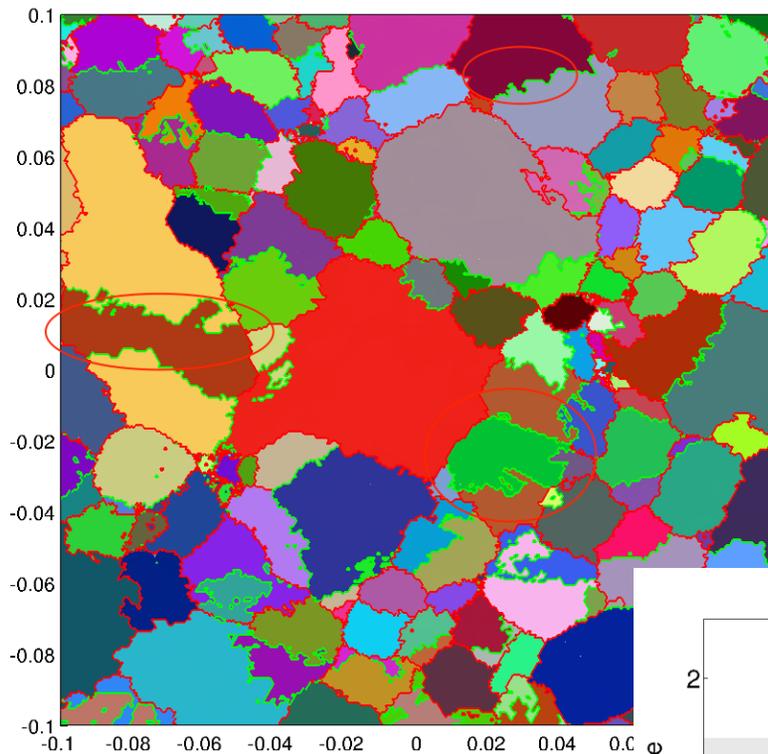


Inset evaluates the change (μm) in GB position from adjustments to the segmentation parameters: strong shading indicates sensitivity

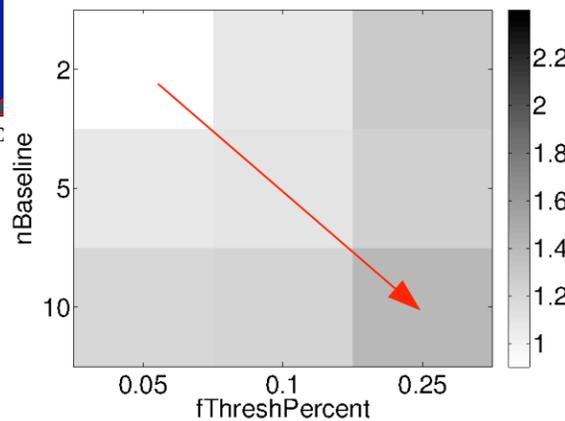
Old method (threshold)



New Method (LoG)

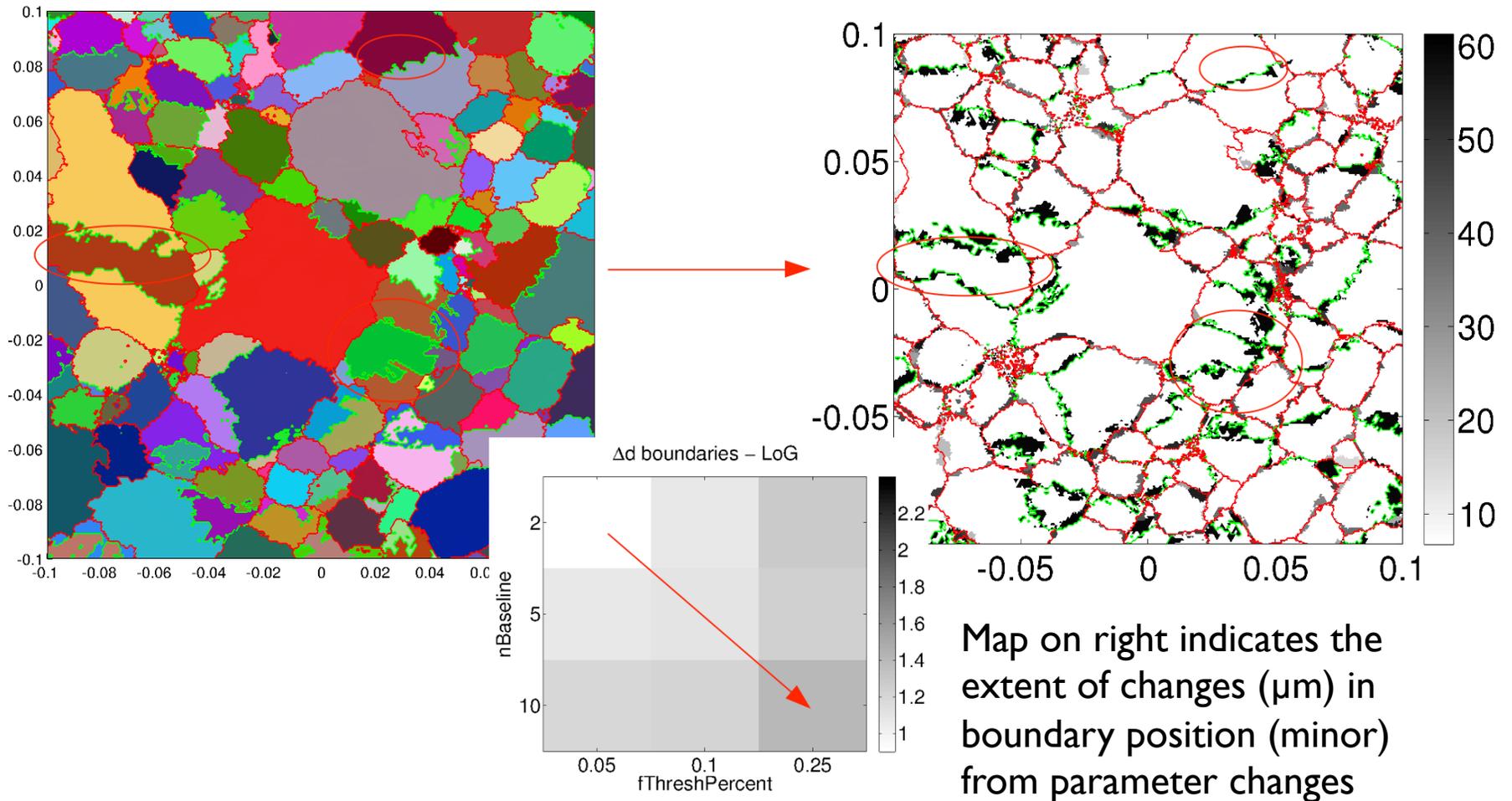


Δd boundaries - LoG

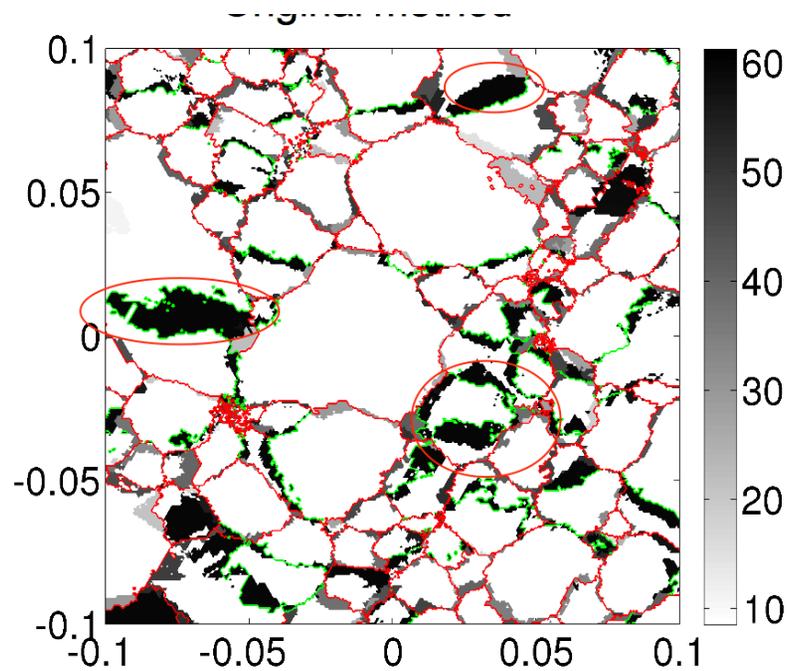


Inset evaluates the change (μm) in the result from adjustments to the segmentation parameters: light shading indicates lesser sensitivity

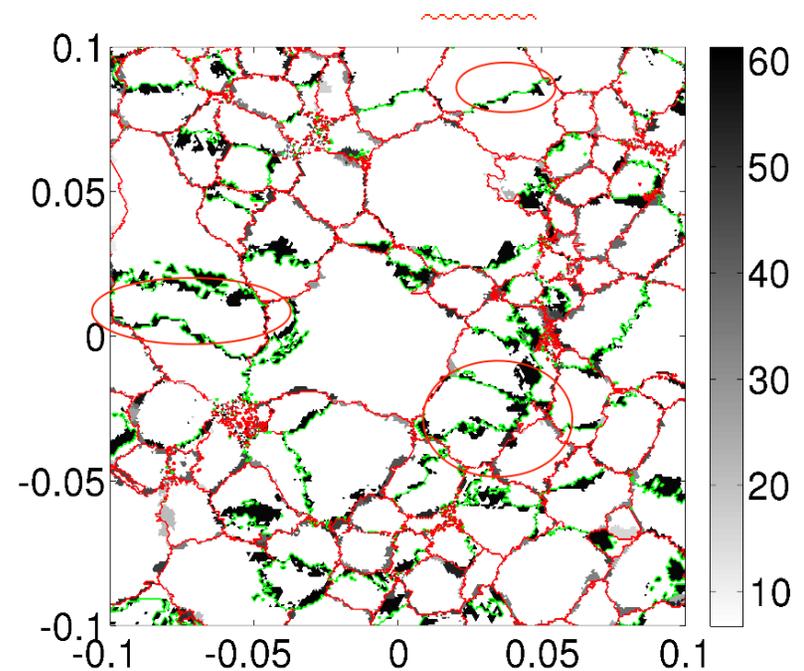
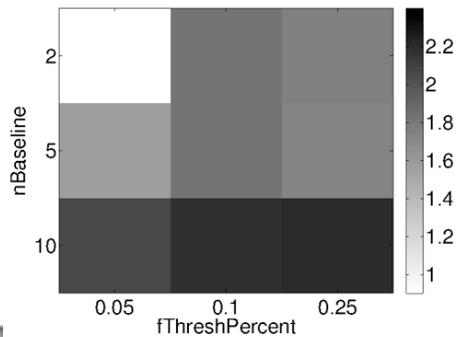
LoG – Quality map



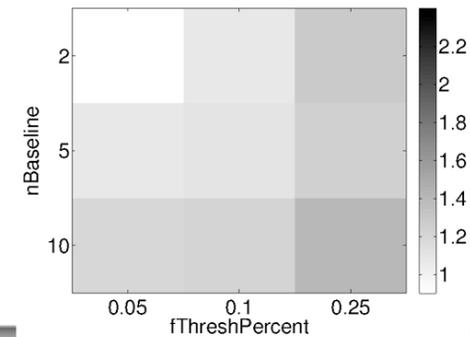
Compare Old vs LoG methods



Δd boundaries – Original

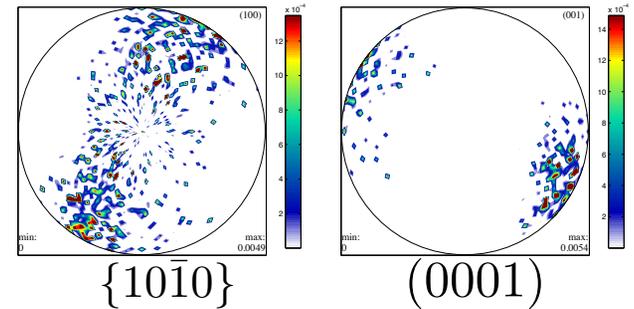


Δd boundaries – LoG



HEDM of Tensile Test on Zr

- Initial goal was to correlate void formation with microstructural features

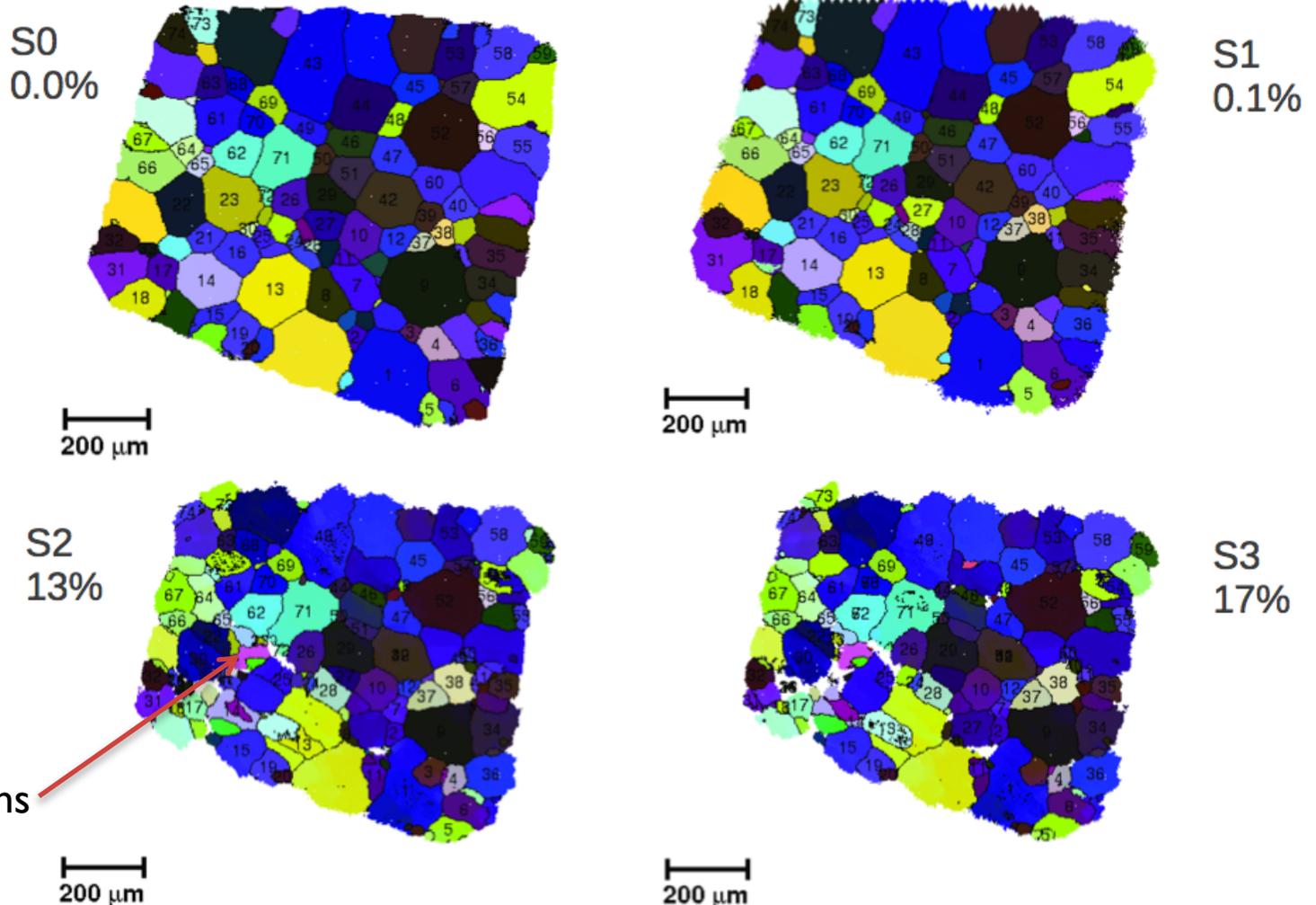


- Dogbone design but with rectangular cross-section

- HEDM snapshots at: 0%, 0.1%, 13% and 17%

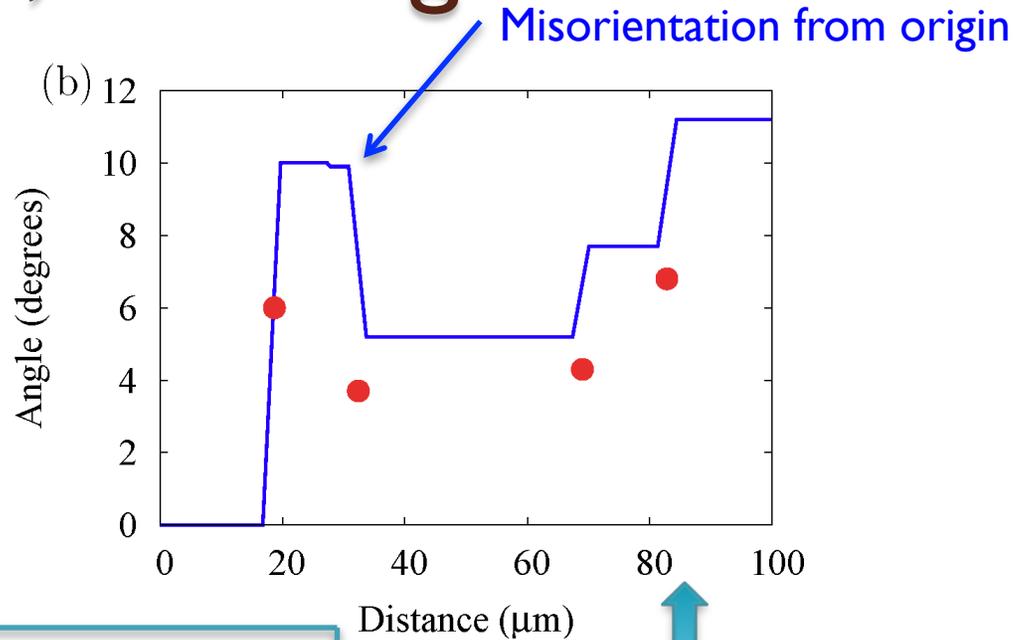
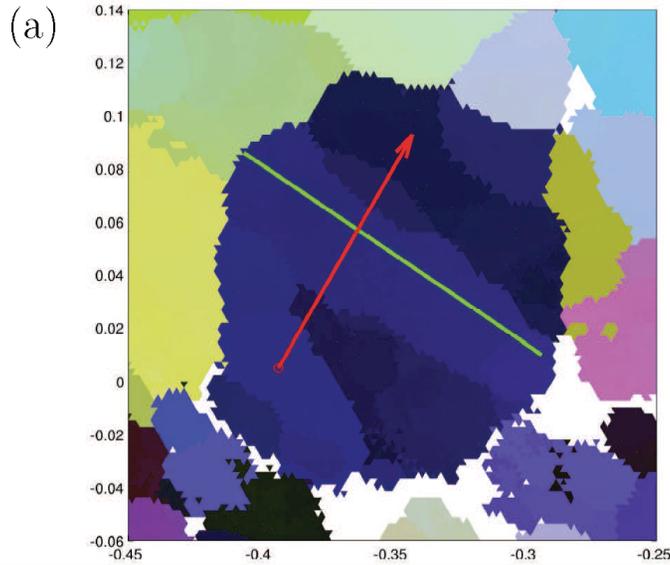
- Note near-plane strain

Mechanical Twins

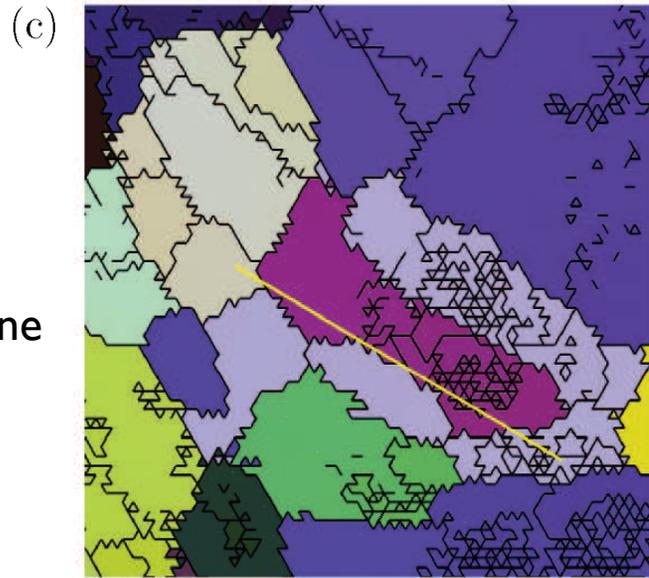


“Tensile twin nucleation events coupled to neighboring slip observed in 3D”, Lind et al., *Acta mater.*, 74 213-220 (2014)

Zr: Rotation axes, twinning

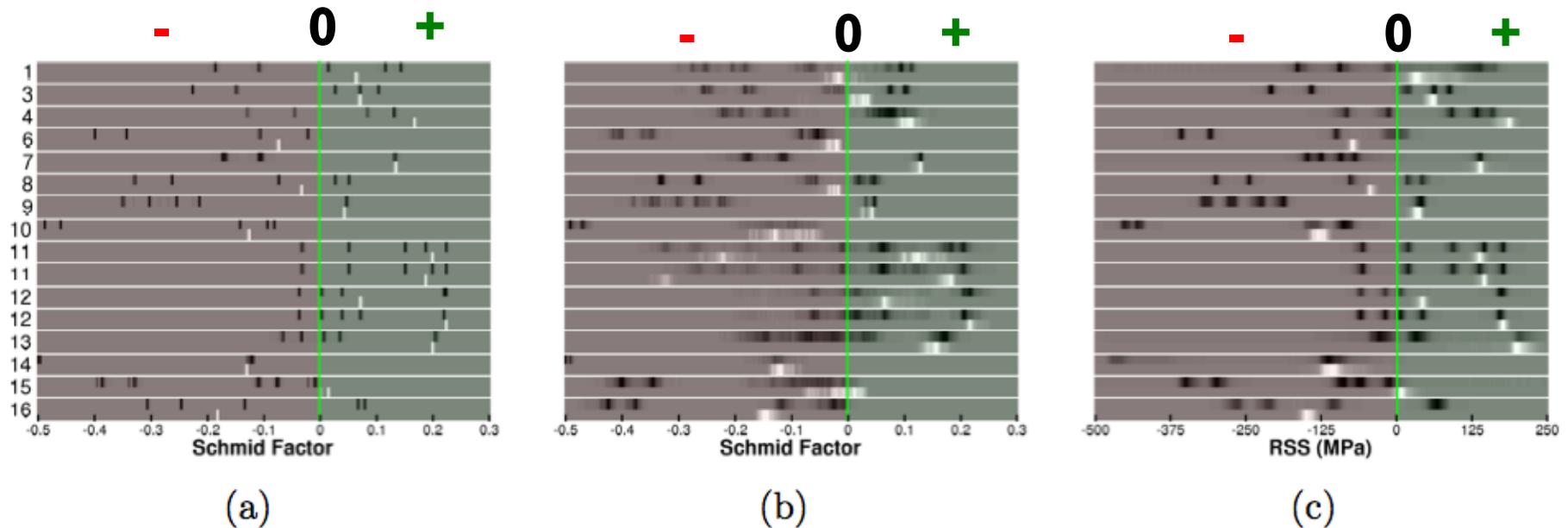


Magenta: twin
Yellow line:
{1012} twin plane



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

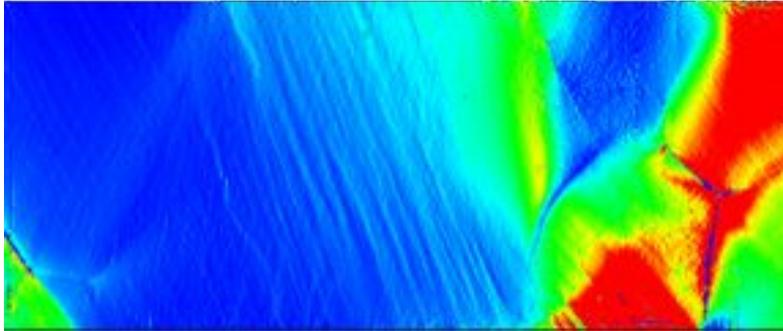
Schmid factors, Resolved Shear Stress



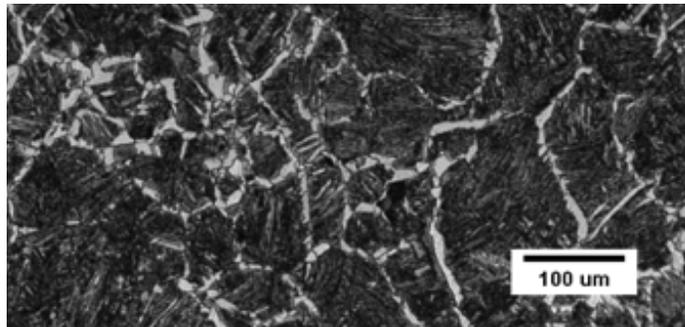
Schmid factors at 0 % - Schmid factors at 13 % – Resolved Shear Stress

- 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* \Rightarrow Plasticity influences twinning
- (Anisotropic) elastic stress-strain fields computed with FFT method

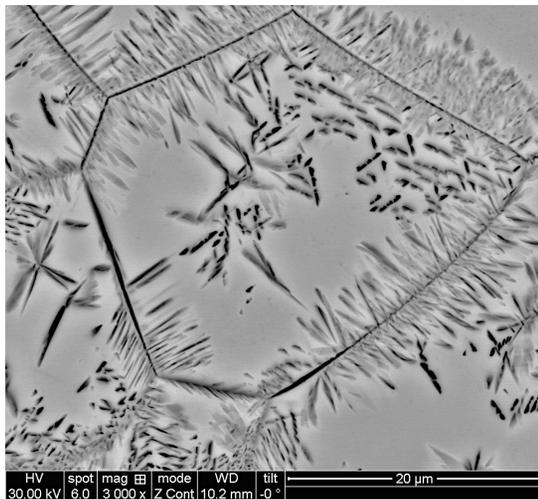
Other Image Challenges



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



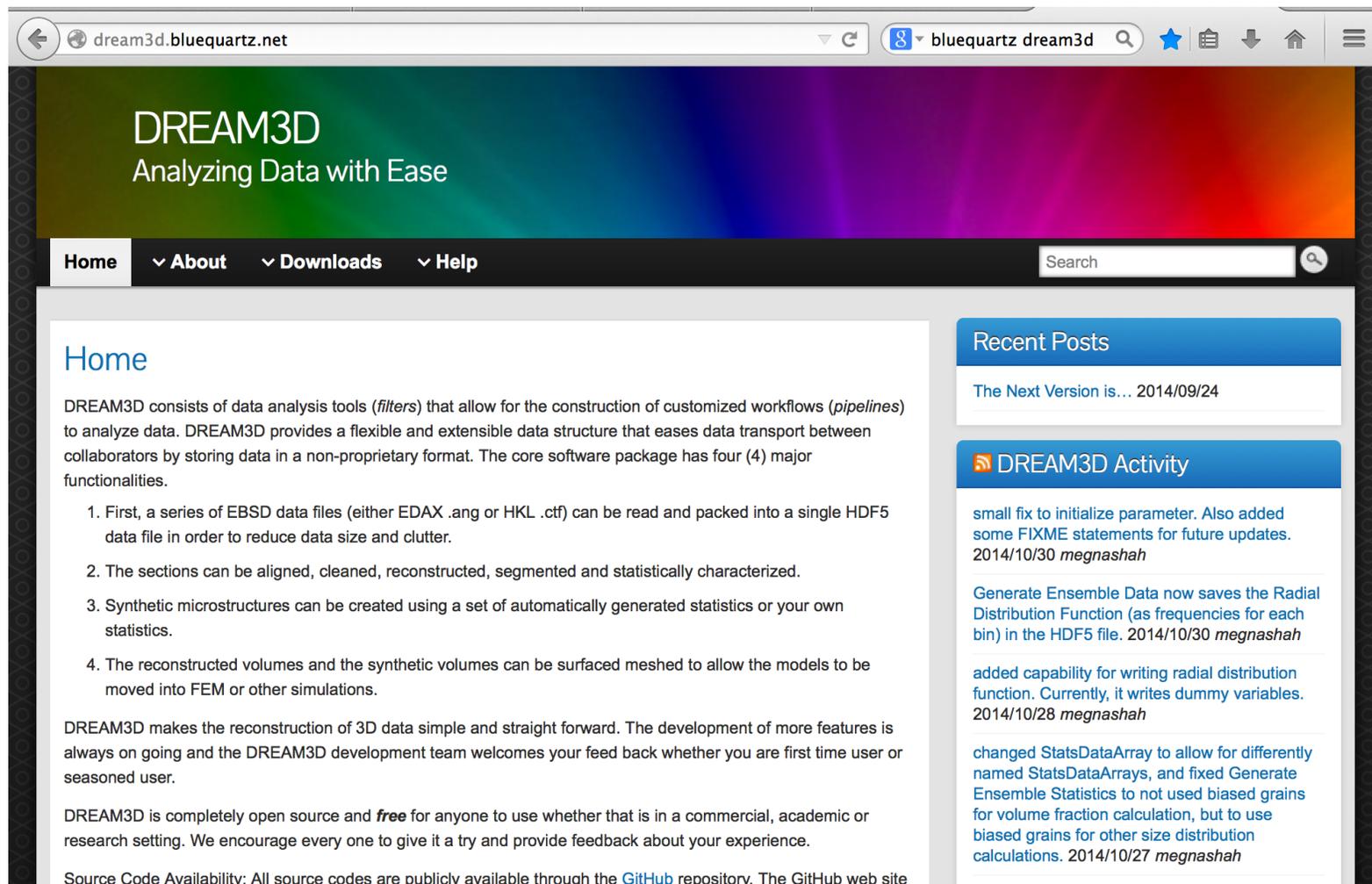
Deformed metal reveals a grain structure but the **boundaries** (white lines) are incomplete: how to complete the network?



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.



The screenshot shows the homepage of the DREAM3D website. The browser address bar displays 'dream3d.bluequartz.net'. The main header features the text 'DREAM3D Analyzing Data with Ease' against a colorful gradient background. Below the header is a navigation menu with 'Home', 'About', 'Downloads', and 'Help' options, along with a search bar. The main content area is divided into two columns. The left column contains the 'Home' section, which describes the software's purpose and lists four major functionalities: 1. Reading and packing EBSD data files into a single HDF5 file. 2. Aligning, cleaning, reconstructing, segmenting, and characterizing sections. 3. Creating synthetic microstructures from statistics. 4. Surfacing and meshing reconstructed volumes for simulation. The right column contains 'Recent Posts' and 'DREAM3D Activity' sections, listing updates such as 'The Next Version is...' and 'small fix to initialize parameter'.

Home

DREAM3D consists of data analysis tools (*filters*) that allow for the construction of customized workflows (*pipelines*) to analyze data. DREAM3D provides a flexible and extensible data structure that eases data transport between collaborators by storing data in a non-proprietary format. The core software package has four (4) major functionalities.

1. First, a series of EBSD data files (either EDAX .ang or HKL .ctf) can be read and packed into a single HDF5 data file in order to reduce data size and clutter.
2. The sections can be aligned, cleaned, reconstructed, segmented and statistically characterized.
3. Synthetic microstructures can be created using a set of automatically generated statistics or your own statistics.
4. The reconstructed volumes and the synthetic volumes can be surfaced meshed to allow the models to be moved into FEM or other simulations.

DREAM3D makes the reconstruction of 3D data simple and straight forward. The development of more features is always on going and the DREAM3D development team welcomes your feed back whether you are first time user or seasoned user.

DREAM3D is completely open source and **free** for anyone to use whether that is in a commercial, academic or research setting. We encourage every one to give it a try and provide feedback about your experience.

Source Code Availability: All source codes are publicly available through the [GitHub](#) repository. The GitHub web site

Recent Posts

The Next Version is... 2014/09/24

DREAM3D Activity

small fix to initialize parameter. Also added some FIXME statements for future updates. 2014/10/30 *megnashah*

Generate Ensemble Data now saves the Radial Distribution Function (as frequencies for each bin) in the HDF5 file. 2014/10/30 *megnashah*

added capability for writing radial distribution function. Currently, it writes dummy variables. 2014/10/28 *megnashah*

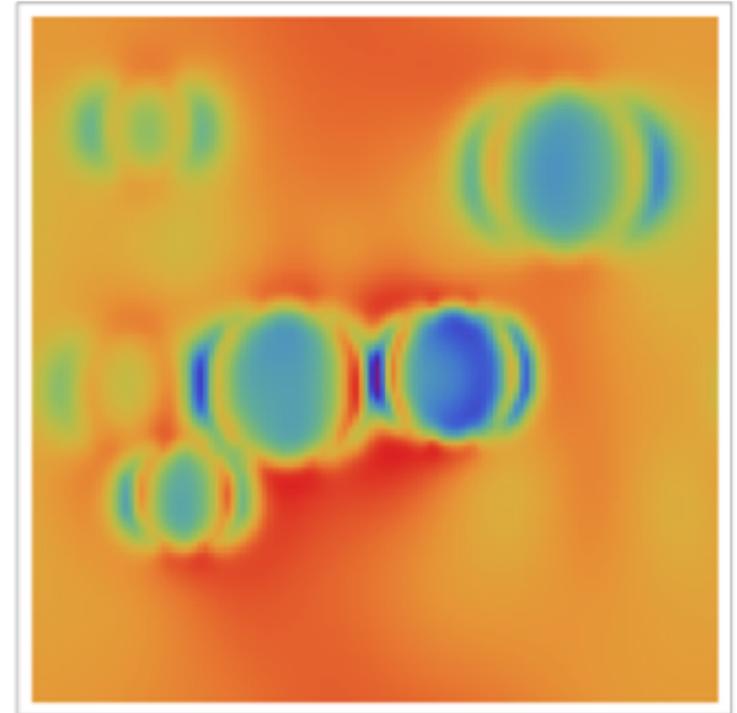
changed StatsDataArray to allow for differently named StatsDataArrays, and fixed Generate Ensemble Statistics to not use biased grains for volume fraction calculation, but to use biased grains for other size distribution calculations. 2014/10/27 *megnashah*

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.