227-0966-00L-Quantitative Big Imaging 2015
Project presentation - Equilibrium Catalyst

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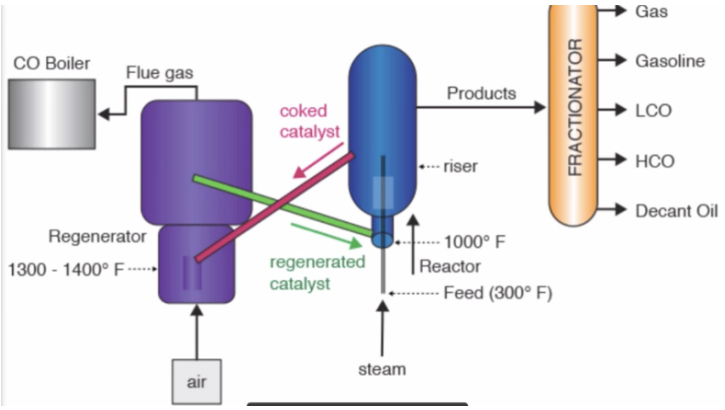
Overview

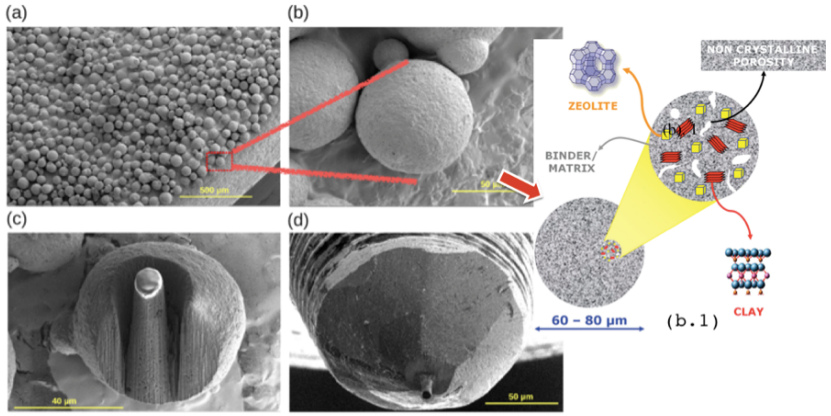
- Introduction
- Chapter 1- Noise Reduction
- Chapter 2- Basic Segmentation
- Chapter 3- Advanced Segmentation
- Chapter 4- Analysis of individual objects
- Future works

1.1 Introduction - FCC

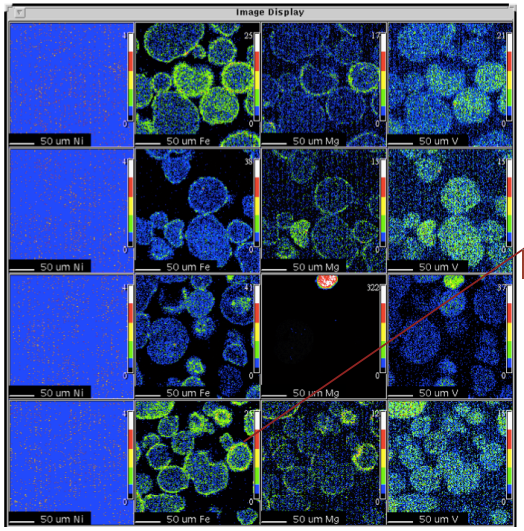
- Fluid Catalytic Cracking (FCC) catalyst (our samples)
- Catalyst used in conversion of Crude oil to Gasoline



1.2 Introduction- Samples



1.3 Introduction- Samples - EPMA analysis

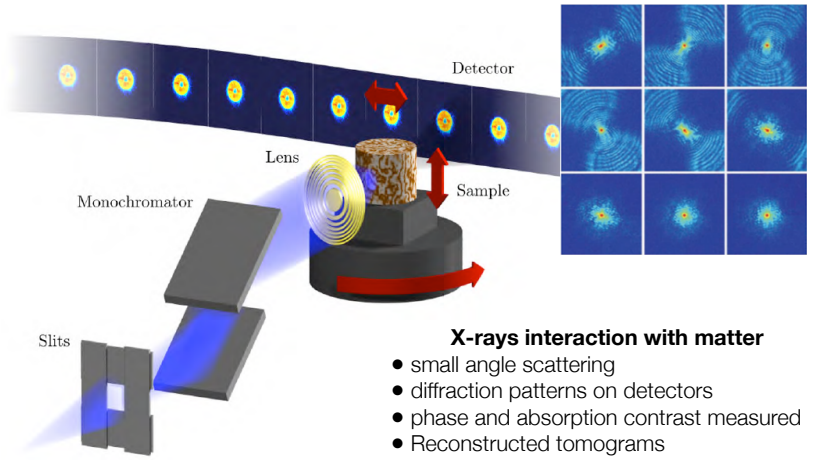


Outer Ring

Al_2O_3, %:	48.19
CaO, %:	0.23
CeO_2, %:	0.18
Fe_2O_3, %:	1.61
La_2O_3, %:	1.80
MgO, %:	1.33
Na_2O, %:	0.36
Ni, %:	0.12
RE_2O_3, %:	1.99
V, %:	0.14

1.4 Introduction- Measurement Technique

Ptychography at cSAXS beamline of Swiss Light Source in Paul Scherrer Institut

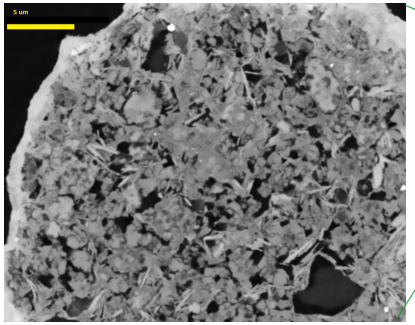


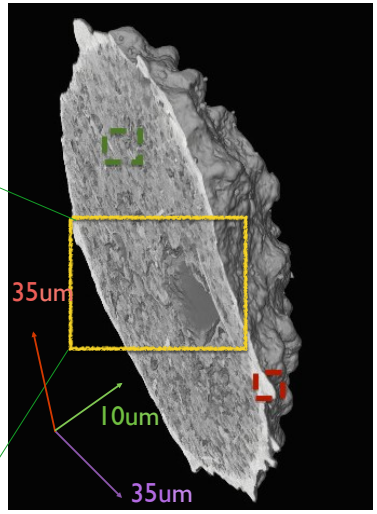
X-rays interaction with matter

- small angle scattering
- diffraction patterns on detectors
- phase and absorption contrast measured
- Reconstructed tomograms
- at High resolution - 35nm

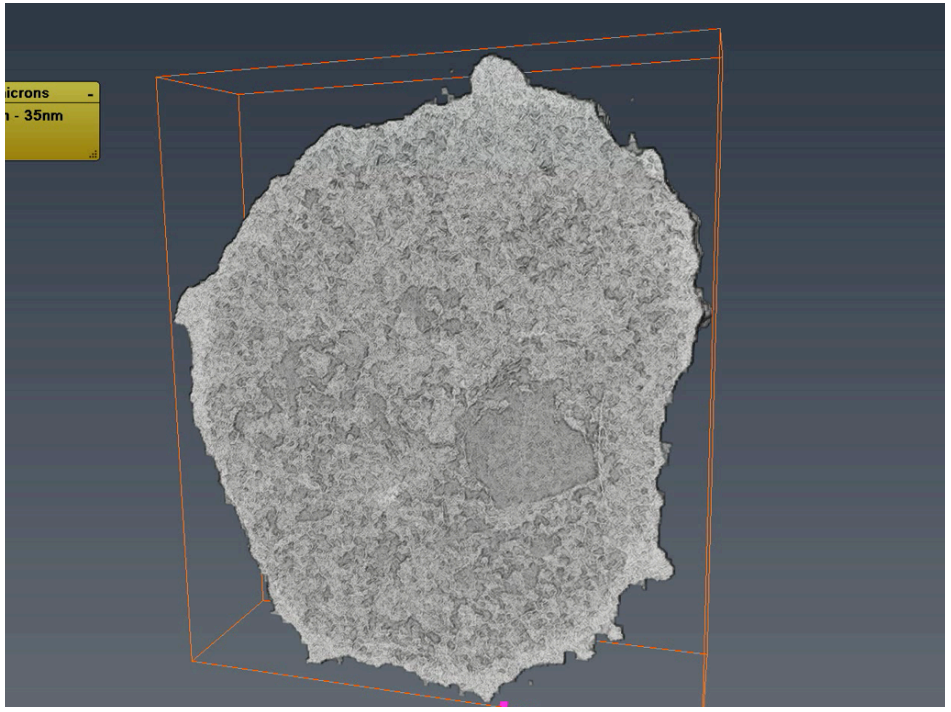
1.4 Introduction- Nanotomograms

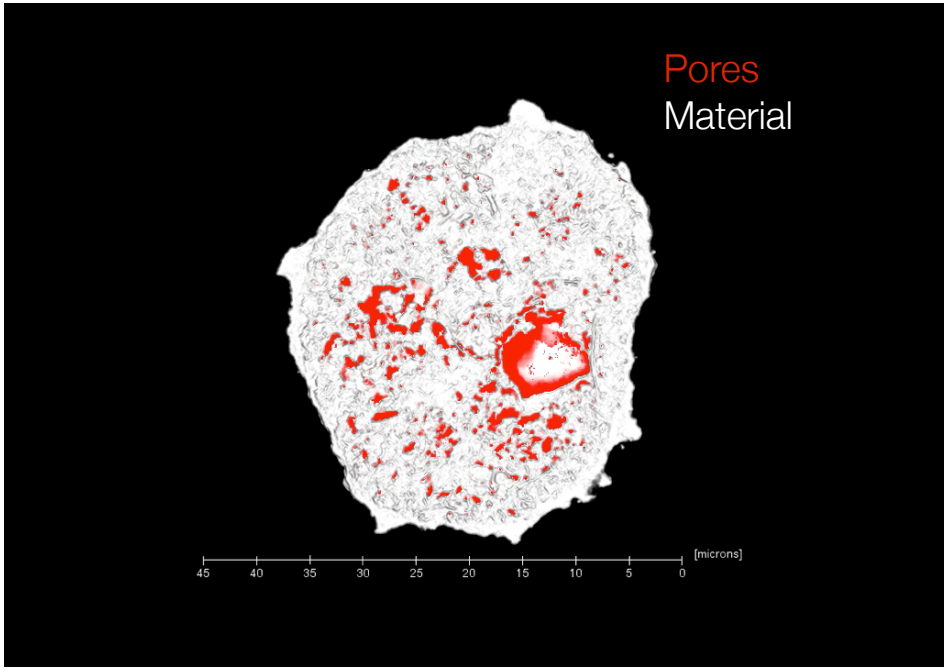
- 1/3rd of an individual particle measured
- Sample Volume
  - 35 x 35 x 10μm^3
- Voxel Dimension
  - 21.35 nm
- 3D resolution
  - 35 nm





2034 x 2034 x 520 x 16bit voxels = 53 hours measurement





1.5 Target

ETH zürich — PAUL SCHERRER INSTITUT PSI

Questions attempted to solve from the measured nanotomography of deactive catalyst

Material identification | Porosity/Particle Analysis | Distance Maps

Deposits	• What material ? • What structure ? • Where ?
Outer ring	• Is outer ring Fe ? How does is affect poisoning catalyst • What oxidation state of Fe? • Is outer ring single new phase or mixture ?
Zeolites	• position of La can be used to localize Zeolites
Fe/V/Ni	• Metal poisoning/intrusion effect on deactivating catalyst

1.5 Target

ETH zürich — PAUL SCHERRER INSTITUT PSI

Questions attempted to solve from the measured nanotomography of deactive catalyst.

Material identification | Porosity/Particle Analysis | Distance Maps

Pore Characterization	• Pore Size and Connectivity Distribution ? • Inner vs Outer core comparison? • Pore Shape Distribution ? bottlenecks? constrictions ? • Change in porosity due to metal intrusions ? • What size of molecules can diffuse through the particle? What size gets blocked ?
Particle Characterization	• Particle Size Distribution ?

1.5 Target

ETH zürich — PAUL SCHERRER INSTITUT PSI

Questions attempted to solve from the measured nanotomography of deactive catalyst.

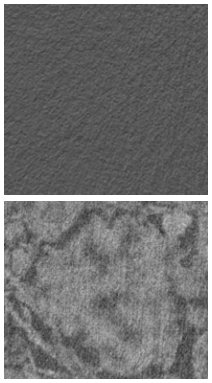
Material identification | Porosity/Particle Analysis | Distance Maps

Radial Distributions	• Void Volume Fraction • Pore Location Distribution • Relative Particle concentration v/s dist. from surface
Inter-particle Distribution	• Inter particle porosity

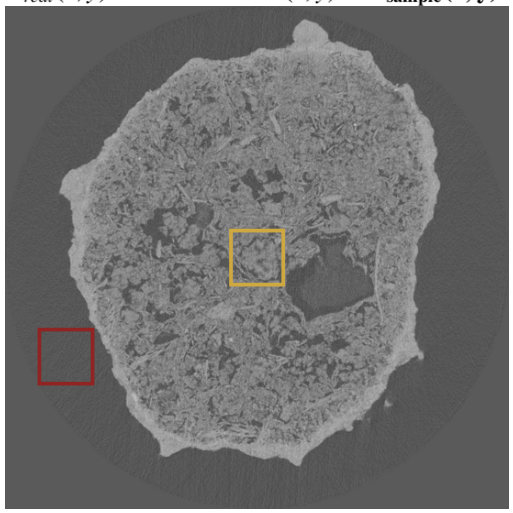
Chapter 1- Noise Reduction

- $Filter * I_{measured}(x, y) = Filter * I_{real}(x, y) + Filter * \text{Noise}(x, y) \rightarrow \mathbf{I_{sample}(x, y)}$

$$SNR_{db} = 20 \log \frac{\mu_{\text{Foreground}}}{\sigma_{\text{Background}}}$$

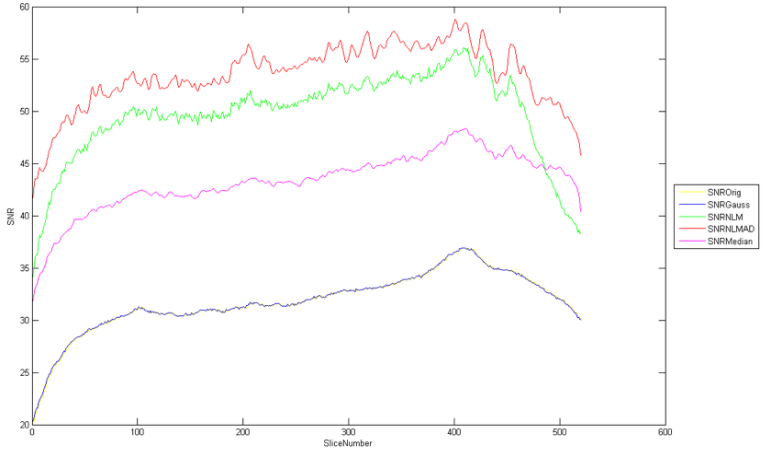


Structured / Correlated Noise



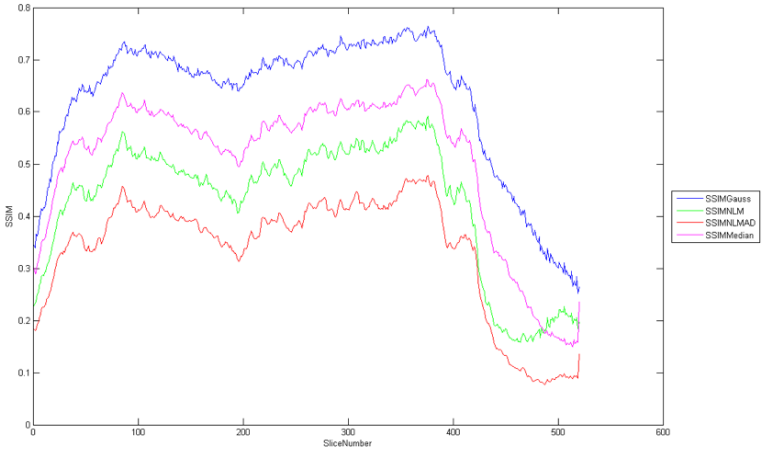
Chapter 1- Noise Reduction

$$SNR_{db} = 20 \log \frac{\mu_{\text{Foreground}}}{\sigma_{\text{Background}}}$$



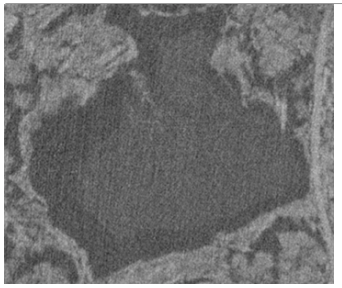
Chapter 1- Noise Reduction

- SSIM

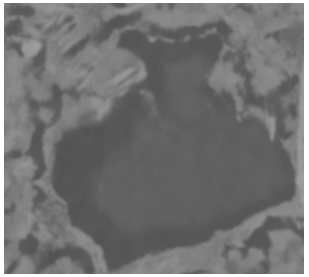


Chapter 1- Noise Reduction

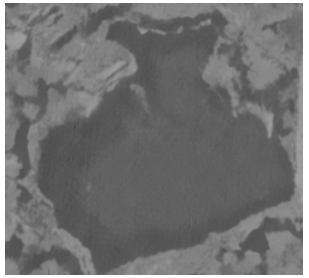
- Results comparison - NLM v/s NLM AD - Over Smoothing



Original



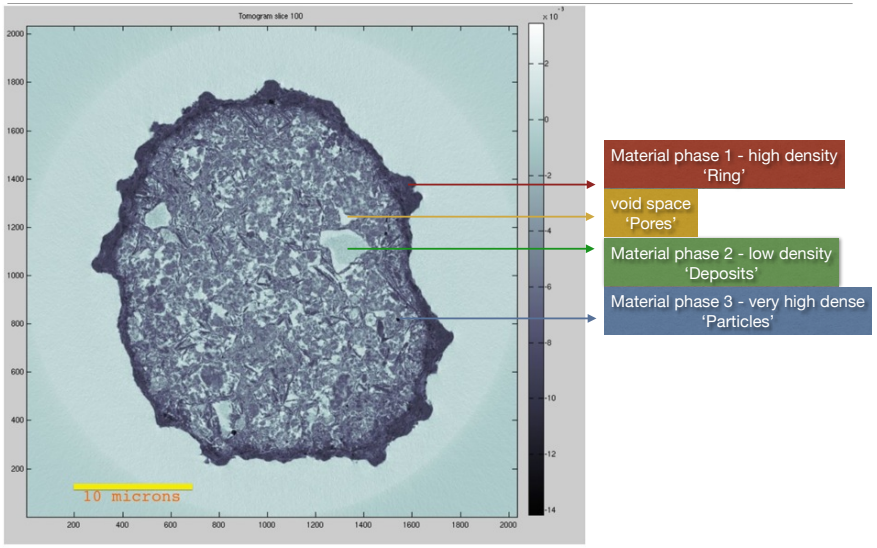
OverSmoothed NLM



Edges Enhanced NLM+AD

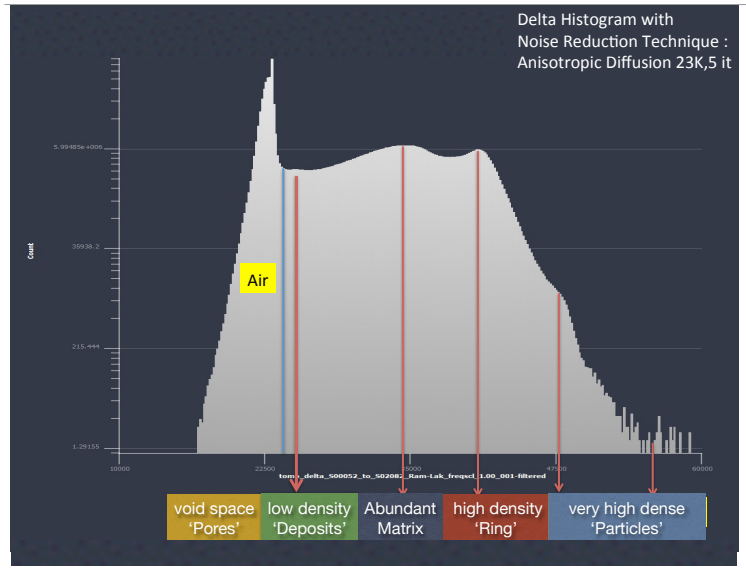
Chapter 2- Basic Segmentation

- Visual identification



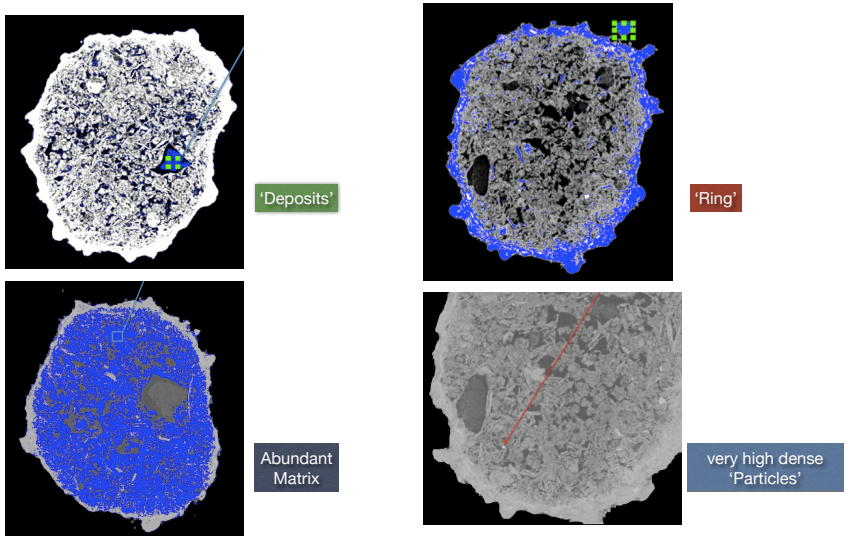
Chapter 2- Basic Segmentation

- Histogram



Chapter 2- Basic Segmentation

- Result based Segmentation- small regions chosen for investigation



Chapter 2- Basic Segmentation

- Result based Segmentation- small regions chosen for investigation

- Phase shift

$$\phi(x,y) = -\frac{2\pi}{\lambda}\int \delta(\mathbf{r})dz,$$

- Electron Density

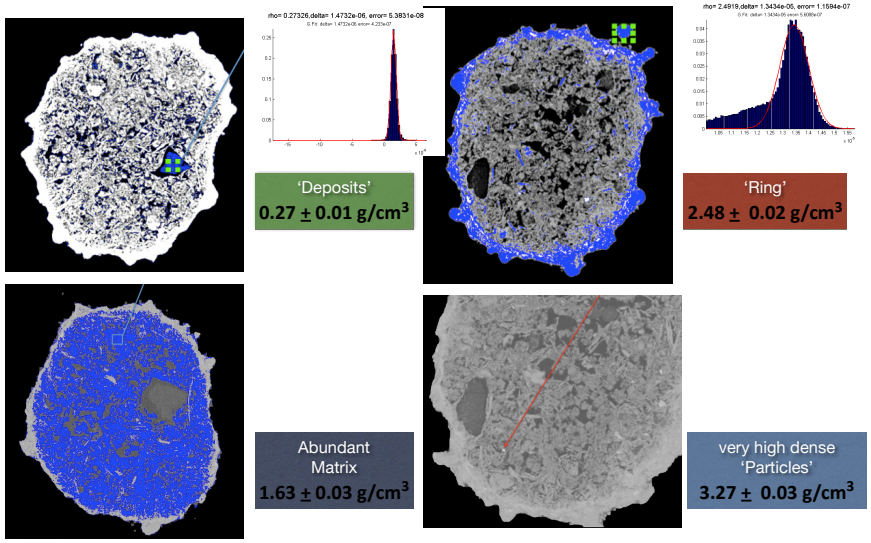
$$n_e(\mathbf{r}) = \frac{2\pi\delta(\mathbf{r})}{\lambda^2 r_0},$$

- Mass Density

$$\rho = \frac{n_e A}{N_A Z},$$

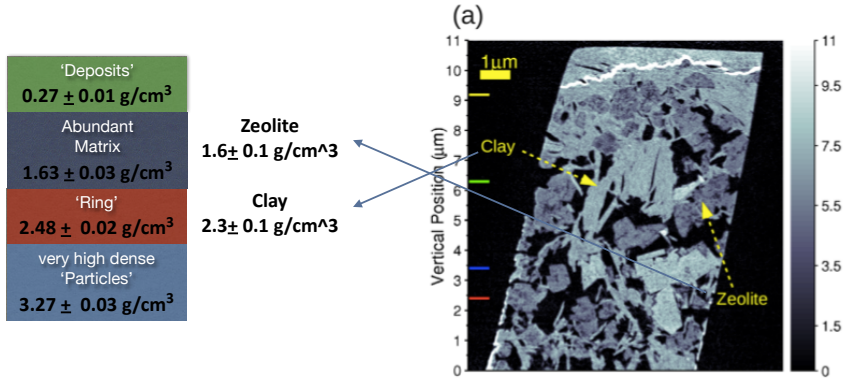
Chapter 2- Basic Segmentation

- Result based Segmentation- Gaussian Fit of Mass Density (g/cm^3)



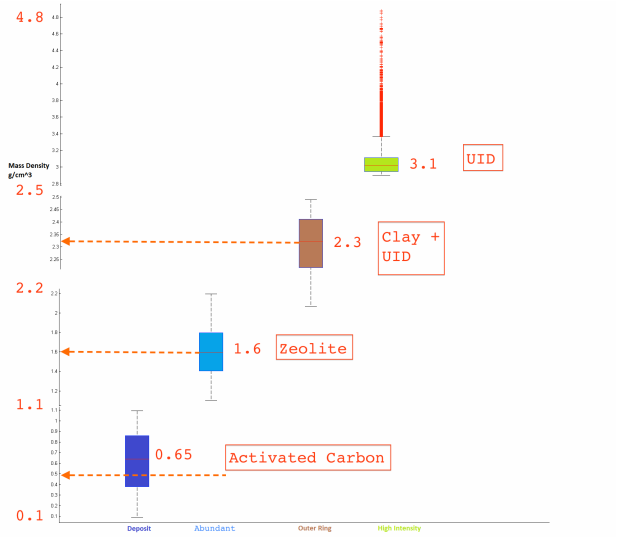
Chapter 2- Basic Segmentation

- Result based Segmentation- Mass Density (g/cm^3) - Verification
  - Using apriori information
  - Previously measured sample



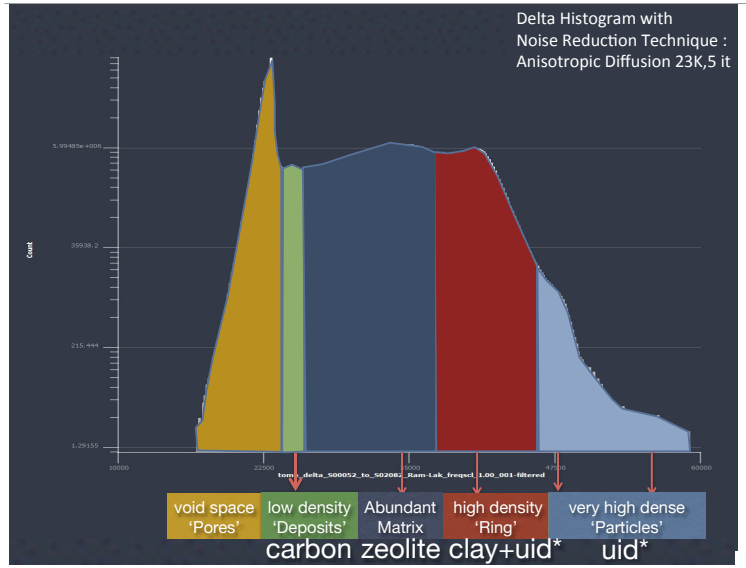
Chapter 2- Basic Segmentation

- Result based Segmentation- Mass Density plot of Full tomogram



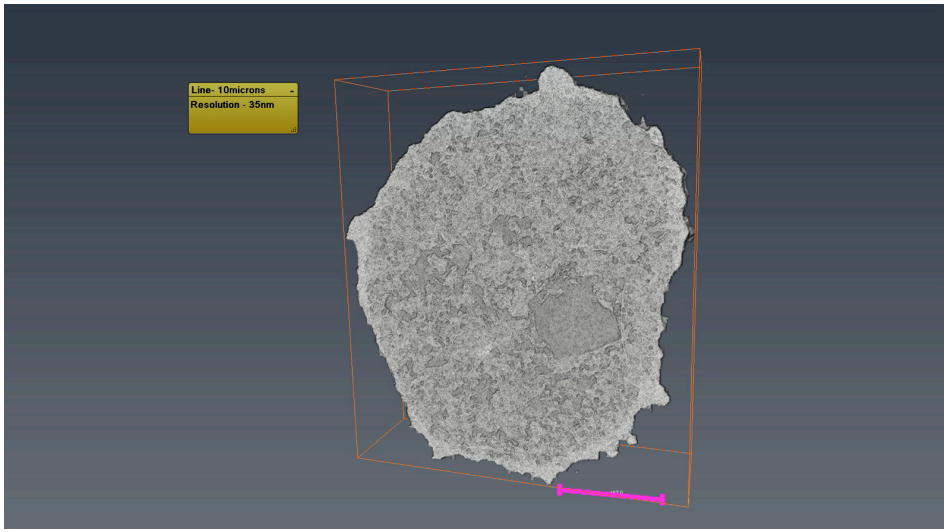
Chapter 2- Basic Segmentation

- Histogram based segmentation



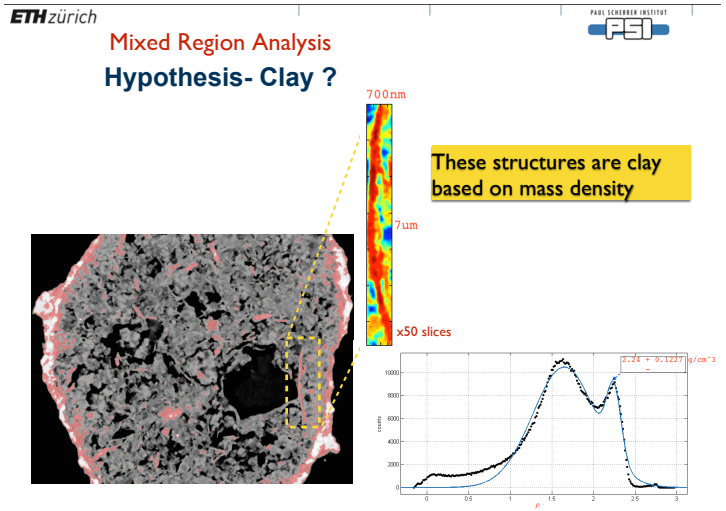
Chapter 2- Basic Segmentation

- Histogram based segmentation- Material Phases



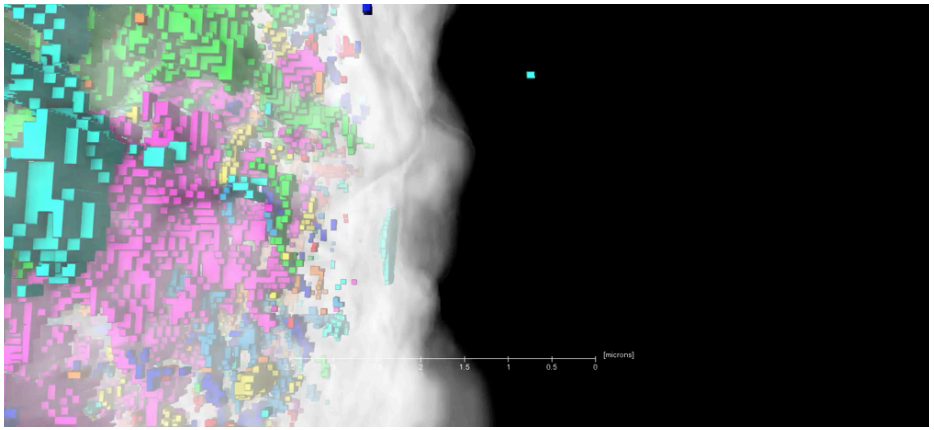
Chapter 3- Advanced Segmentation

- Region Growing



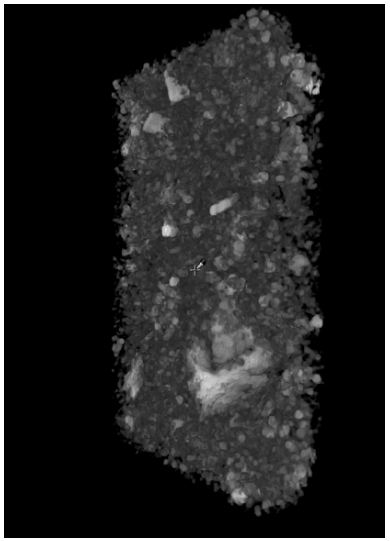
Chapter 4- Analyze individual objects

- Pores - Component Labeling **Kevin Mader (uFOAM software)*



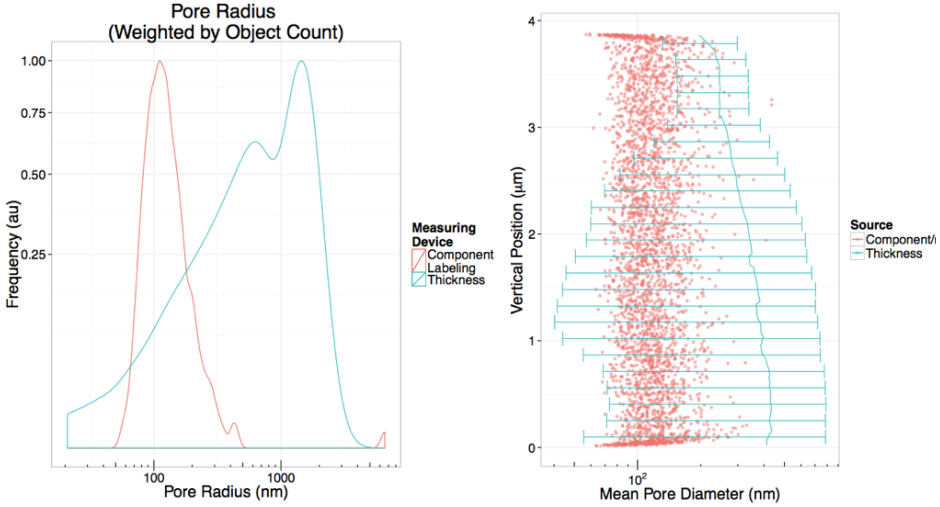
Chapter 4- Analyze individual objects

- Pores - Thickness Analysis **Kevin Mader (uFOAM software)*



Chapter 4- Analyze individual objects

- Pores Size distribution **Kevin Mader (uFOAM software)*



Future Works

- Advanced Segmentation for Mixed region analysis
- Inter particle porosity
- Pore connectivity
- Percolation
- Diffusivity
- Tortuosity