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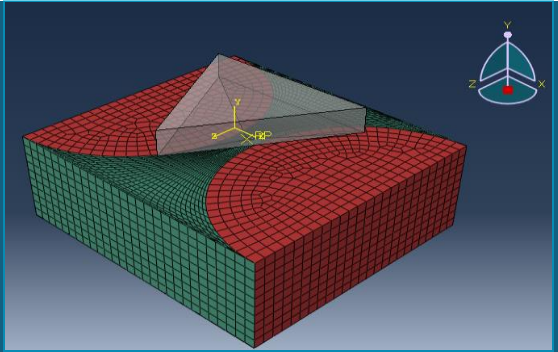
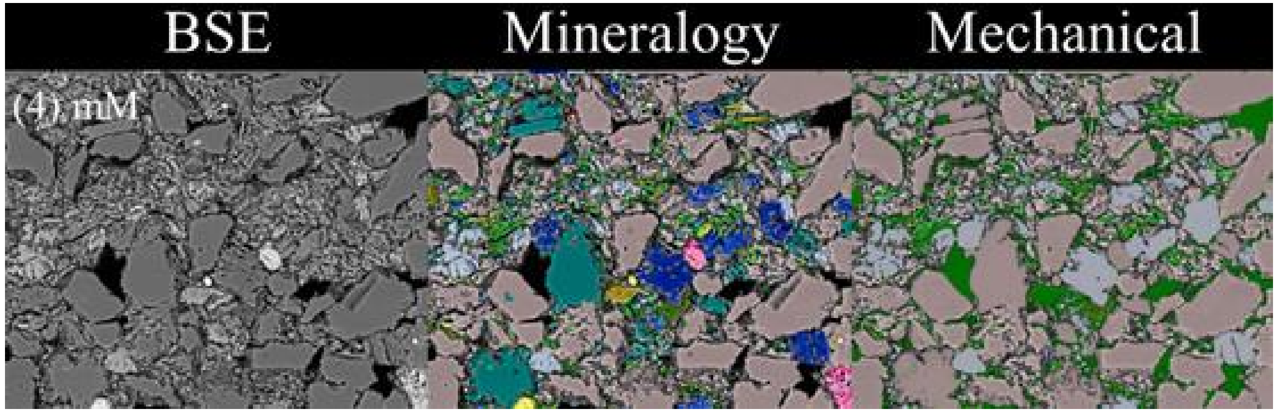
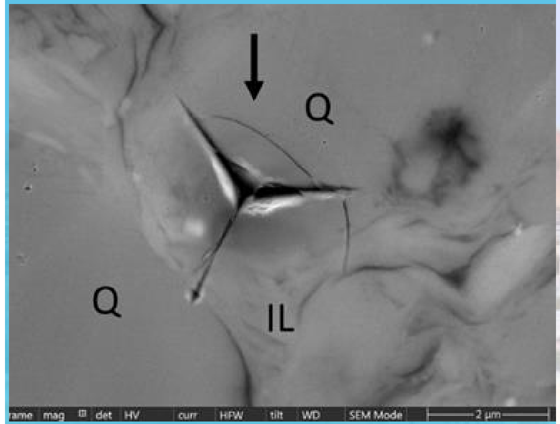
Sandia National Laboratories

Impact of Compositional and Textural Heterogeneity on Mechanical Behavior of Mancos Shale







PRESENTED BY

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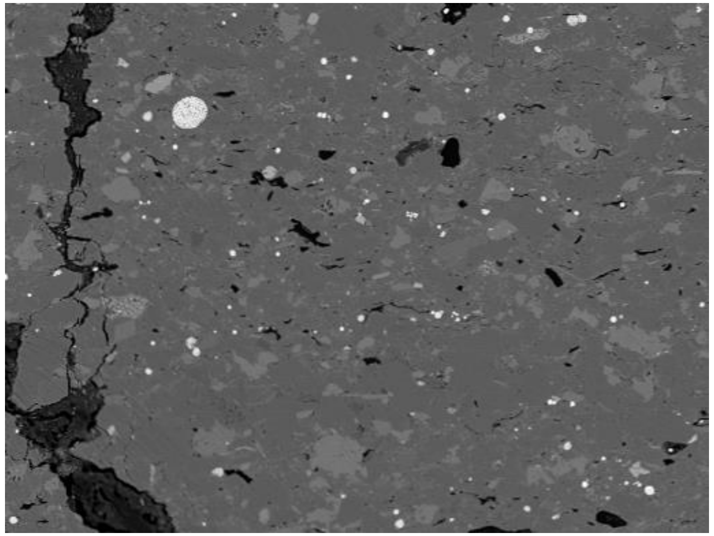
Motivations & Objectives

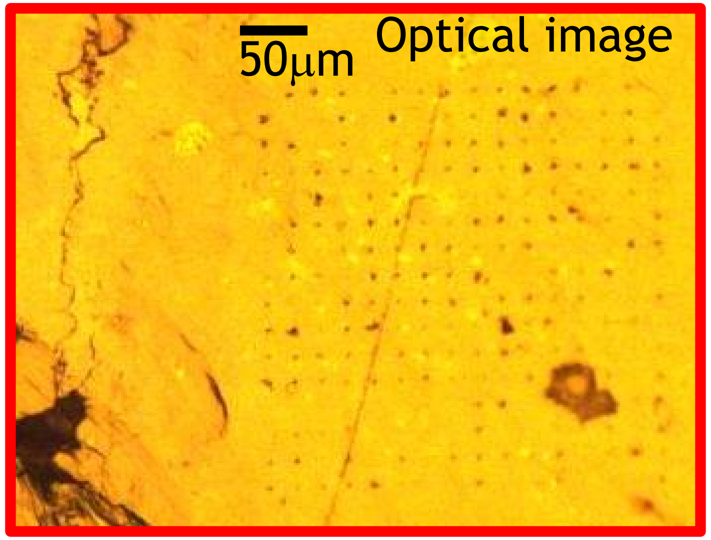
Impact of micro-lithofacial heterogeneities on mechanical properties of Mancos Shale

- Mechanical properties of fine-grained sedimentary rocks (shale and mudstone) are governed by heterogeneous mineral composition and geologic features

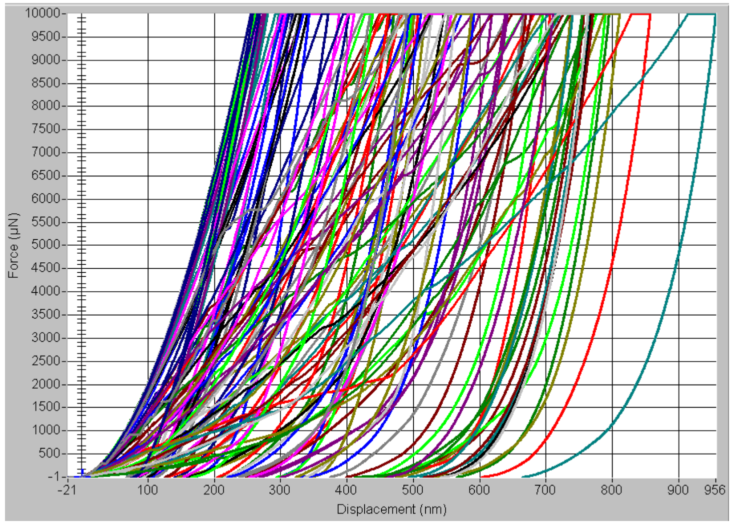
SEM image of shale



Grid nanoindentations over clay-rich area



Load-displacement curves

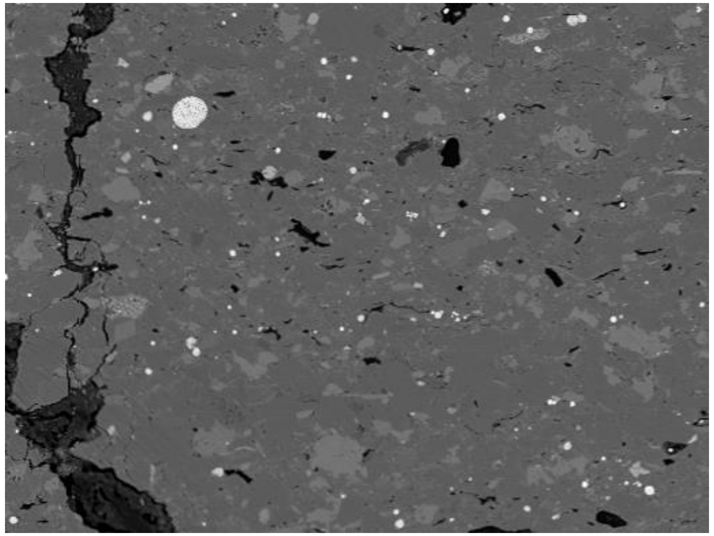


Motivations & Objectives

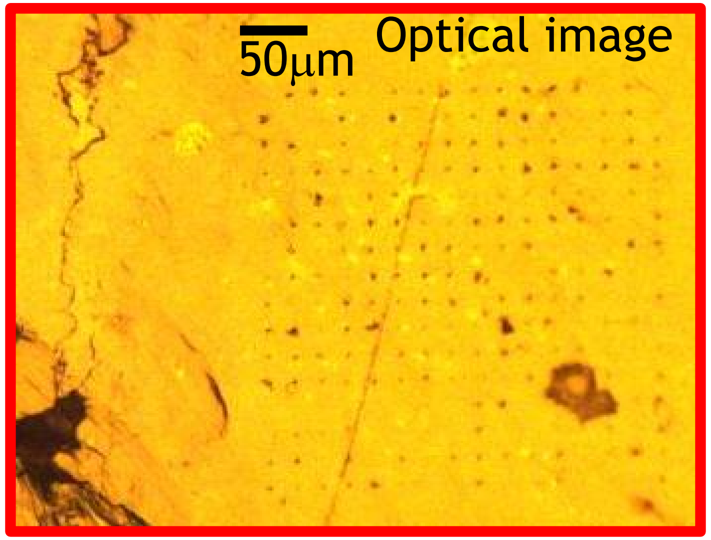
Impact of micro-lithofacial heterogeneities on mechanical properties of Mancos Shale

- ► Mechanical properties of fine-grained sedimentary rocks (shale and mudstone) are governed by heterogeneous mineral composition and geologic features
- ► Develop machine learning methods for mechanical properties by integrating high resolution mineralogy mapping, multiscale nanoindentation analysis, and (modeling)
- ► Link geological attributes to microscale mechanical properties of Mancos shale

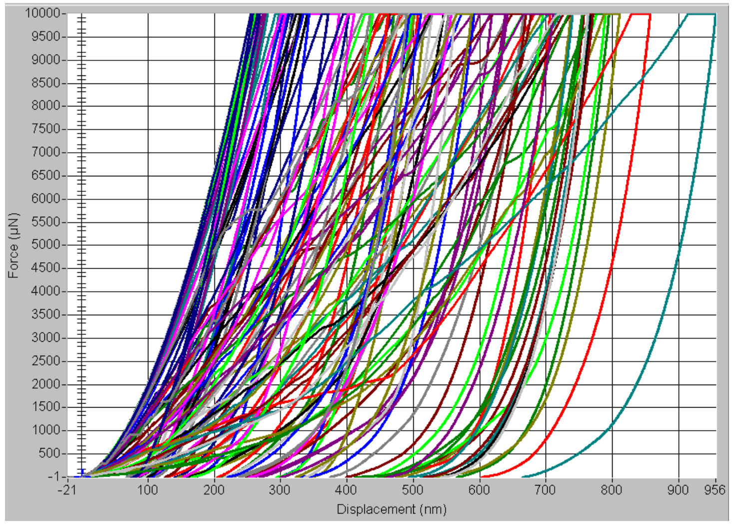
SEM image of shale



Grid nanoindentations over clay-rich area



Load-displacement curves



Integrated Approach

- **40 cm diameter core of Mancos shale**
  - Interlaminated with varying sizes of clay to sandy materials
  - 1-3 mm laminae
  - Parallel/wavy lamina, ripple forms, and bioturbation

- **Mineralogical and textural characterization***
  - **Optical petrography/microscopy**
  - **XRD/X-ray Microprobe**
  - **Back-Scattered Electron Microscopy**
  - **MAPS Mineralogy (Mineralogy mapping)**
  - Micro-CT
  - **Small Angle Neutron Scattering**
  - Focused Ion Beam-SEM

- **Mechanical Experiments**
  - **Nanoindentation**
  - Uni-/Tri-axial compression (1x2")
  - Brazilian Test (1x0.5")
- **Computational modeling**

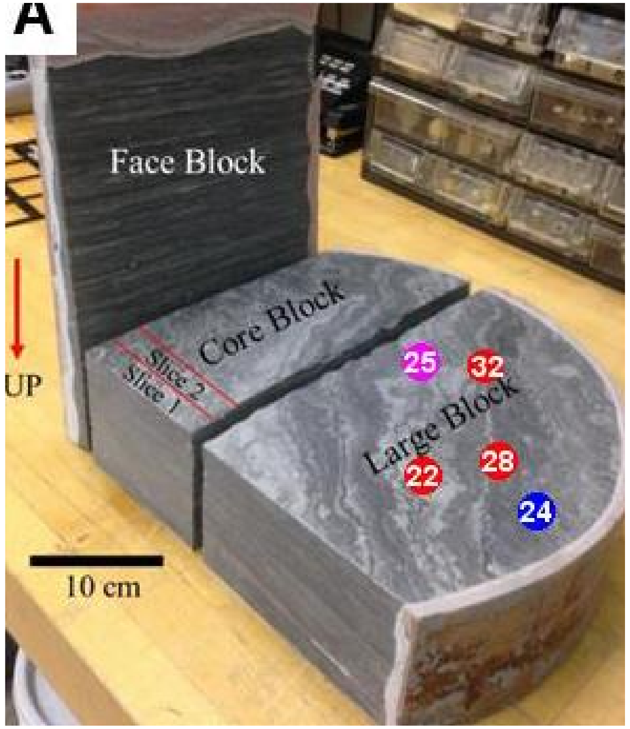


Photo of 40cm diameter block samples for small core samples for mechanical testing and characterization & thin section samples

Yoon et al. (AAPG, Memoir 120, Chap. 8, 2020)

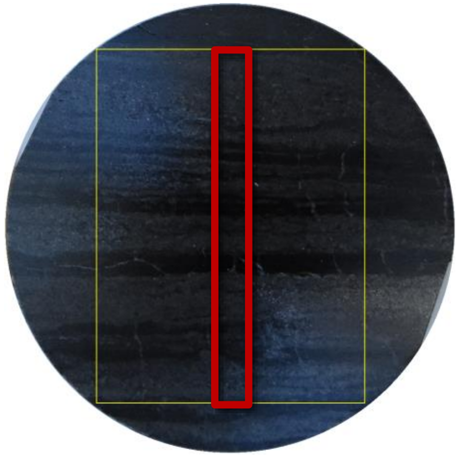
* highlighted in yellow for this presentation

MAPS Mineralogy

- **SEM-based Modular Automated Processing Systems (MAPS): mineralogical measurement, analysis, data integration**

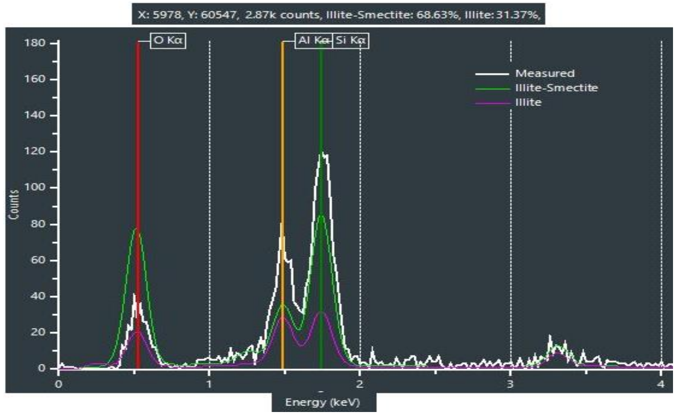
- **Mineral identification**
  - Spectral matching
  - Each pixel – single/multiple minerals

Ion-milling polished Mancos sample (2.5cm diameter)

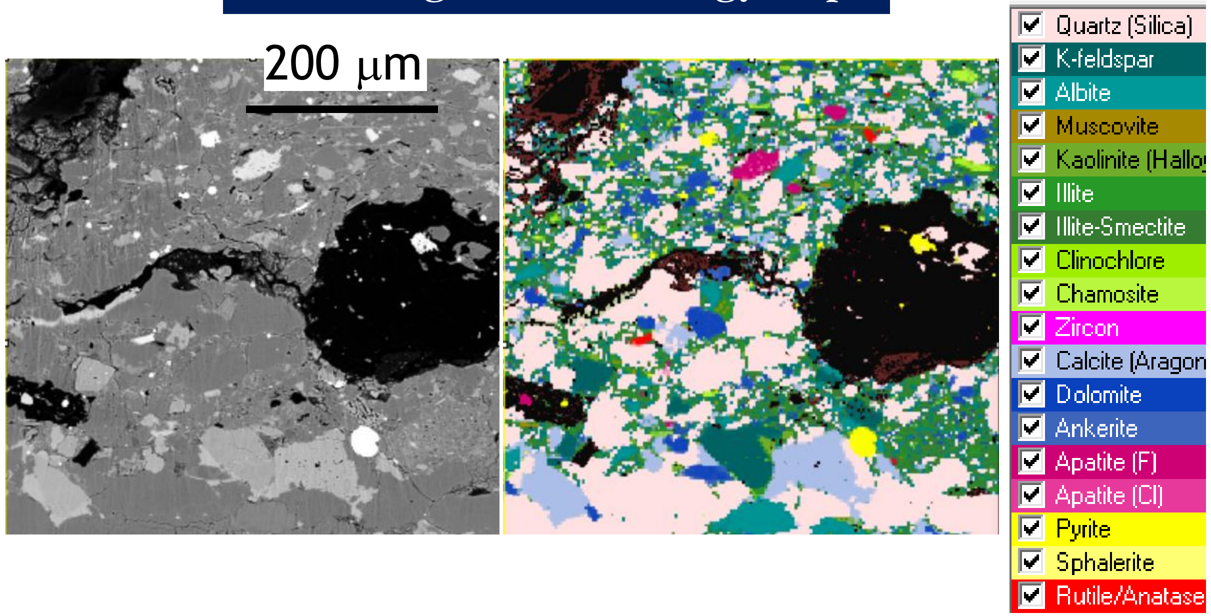


Yellow Box (1.45 x 1.98 cm):
BSE @ 1μm & MAPS @ 10μm
Red box (0.18 x 1.98 cm):
BSE @ 0.2μm & MAPS @ 2μm

Spectral matching for multiple minerals @ pixel

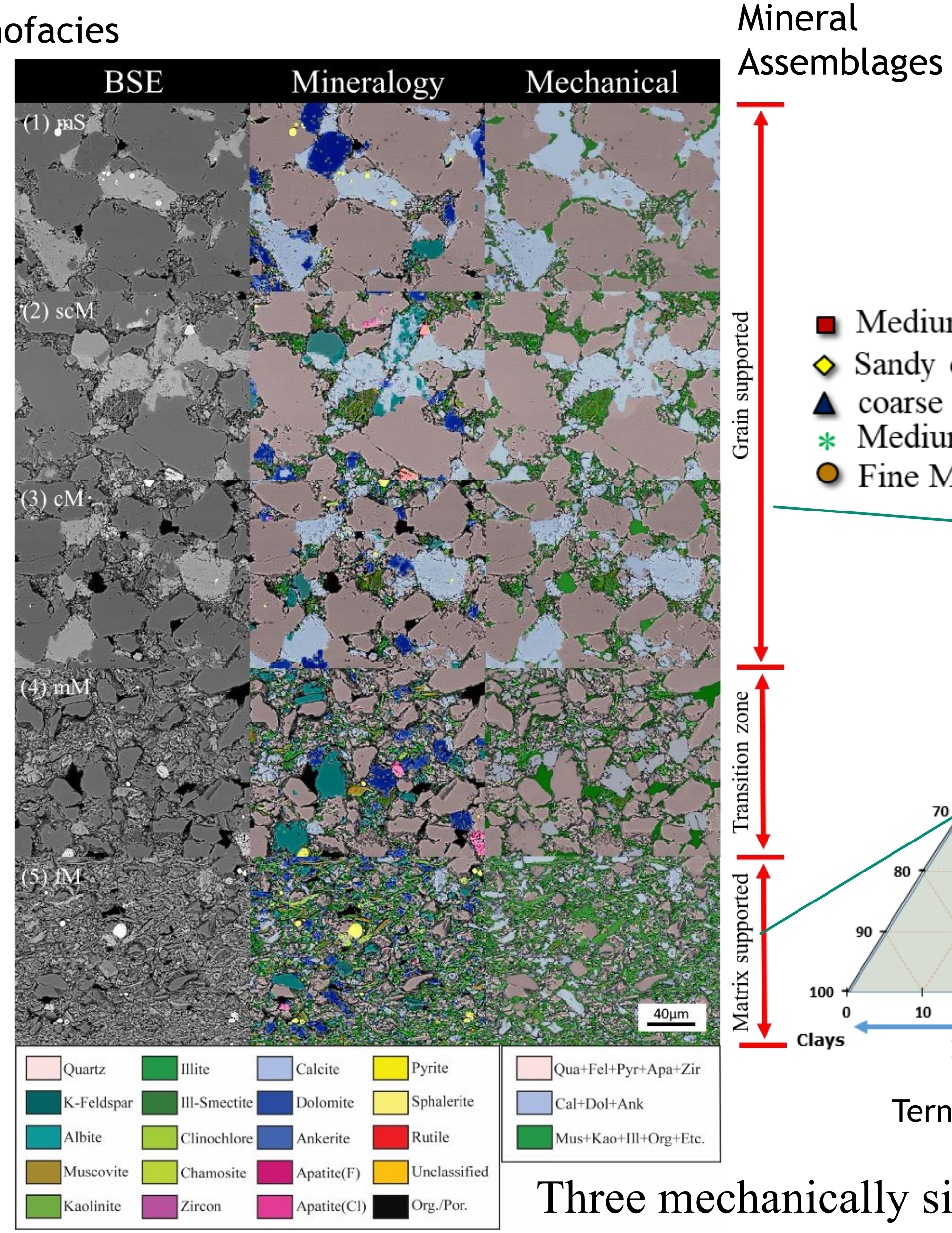


BSE image and mineralogy map



Yoon et al. (AAPG, Memoir 120, Chap. 8, 2021)

Effect of geological attributes on mechanical properties

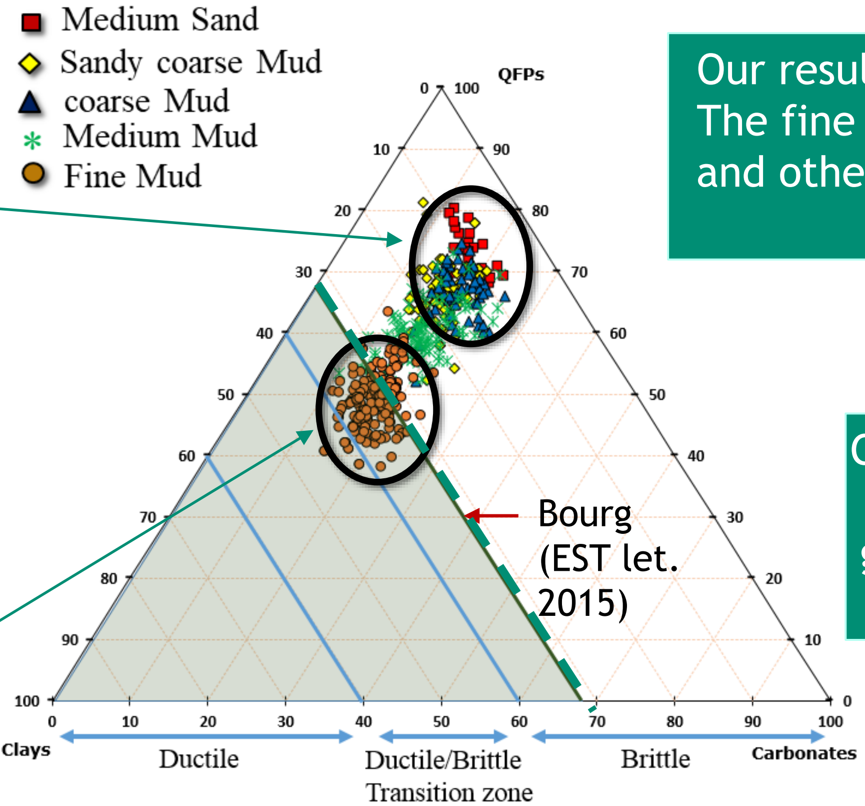


Three mechanically significant mineral assemblages

Mechanical properties = f(mineral composition)? Yes

Green line at ~33% clays rather than ~40% was suggested (Bourg, 2015) to separate the brittle shale from sealing shale.

Our results match a clay boundary of 33%. The fine mud is within the transition zone and other micro-lithofacies are within the brittle zone.



Ternary diagram after Ulmer-Scholle et al. (2014)

Comparison of BSE, mineralogy, and mechanical grouping shows geological attributes would impact mechanical properties, too.

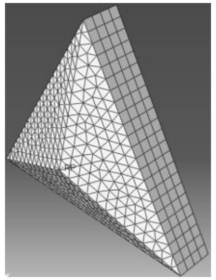
f(geological textures)? Yes

Kwon (MS, NMT, 2018)

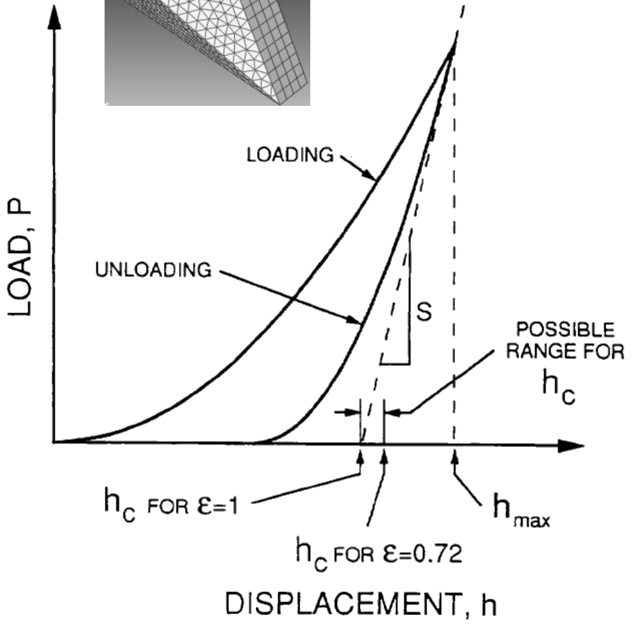
Nanoindentation

- **Depth sensing/instrumented indentation**
  - Highly accurate load-displacement record
  - Determine modulus, hardness and other mechanical properties using the load-displacement data

- **Analytical concept**
  - Purely elastic deformation upon initial unloading
  - Hardness = load/contact area
  - Elastic modulus determined by stiffness (S)



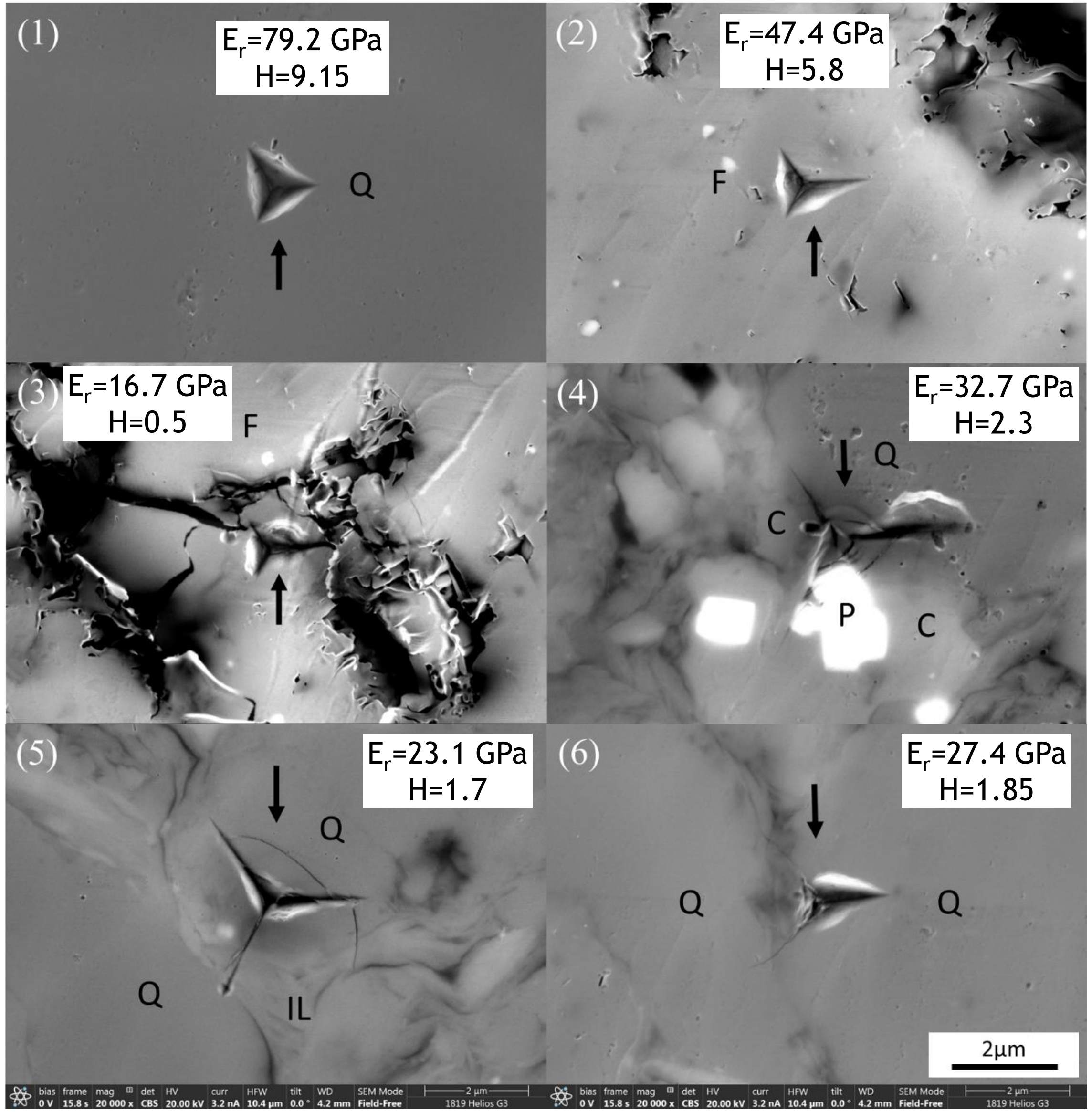
Berkovich indenter



Oliver & Pharr (1992)

[Hysitron Triboindenter 900]
Indentation strain rate = 0.1 (Oliver et al., 1997)
(current change in displacement/current total disp.)
Maximum load = 0.1,1 10 mN (multiscale indenting)
A total of >1500 indentations were performed.

Nanoindentation Impressions



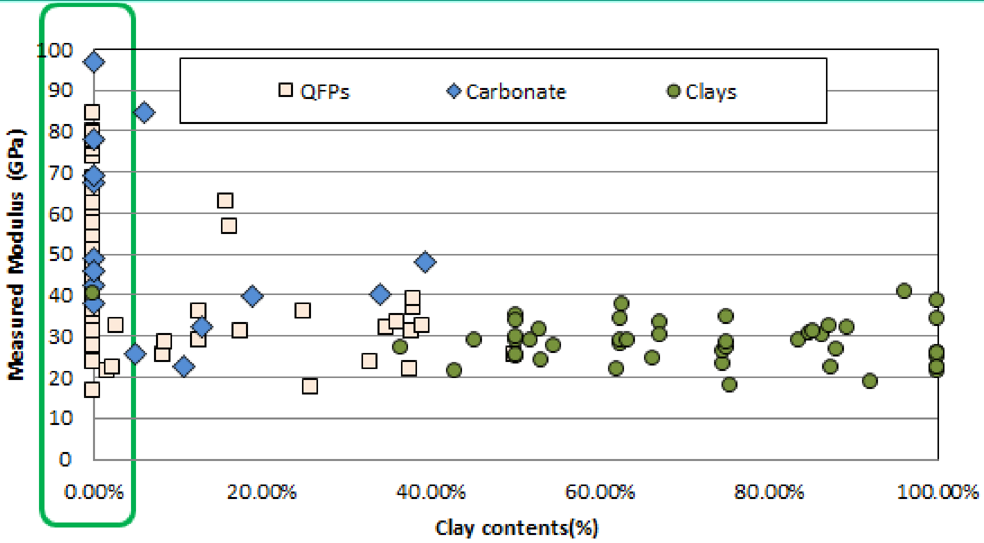
NOTE: Q=quartz, P=pyrite, C=carbonate, F=feldspar, and IL=illite)

(1-2) Low-clay contents: surface of pure quartz and feldspar having higher values of mechanical properties such as elastic modulus and hardness

(3) Dissolution surface of feldspar (mechanical properties are weaker)

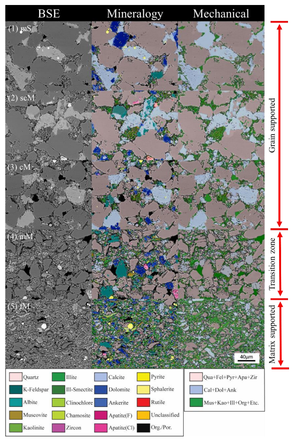
(4-6) Grain-to-grain boundary and edge-of-grain, which have lower mechanical properties values

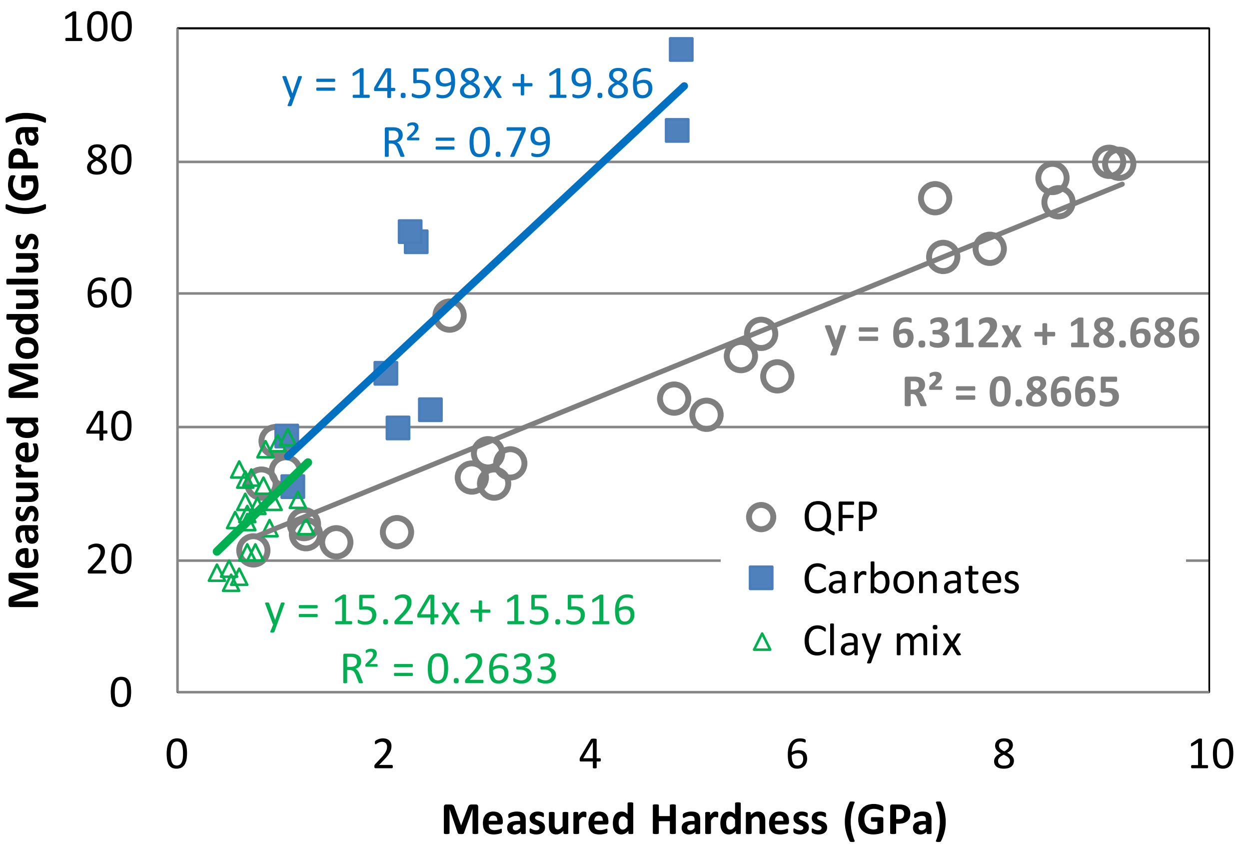
Variations of measured modulus at low clay contents came from geological textures such as boundary of grains, dissolution of grain etc. that are likely to form during diagenesis. These results indicate the important role of geological attributes in mechanical properties of mudstone.



Clustering results

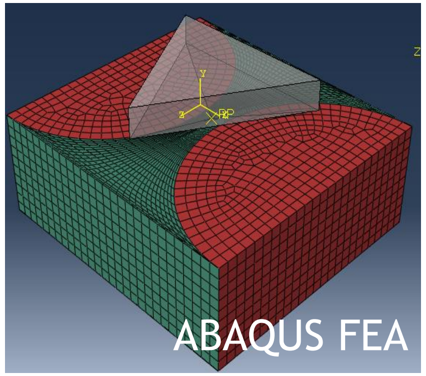
1. Overall, clustering based regression match experimental data much better
2. For low hardness data where clay mix is dominant, regression needs to be improved



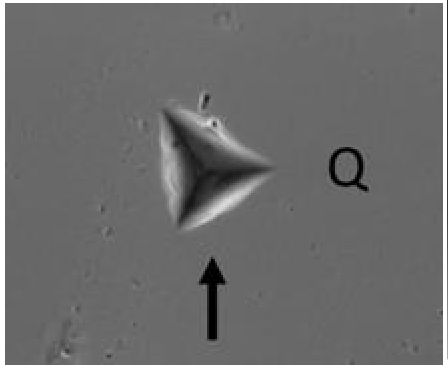


Simulation of Nanoindentation

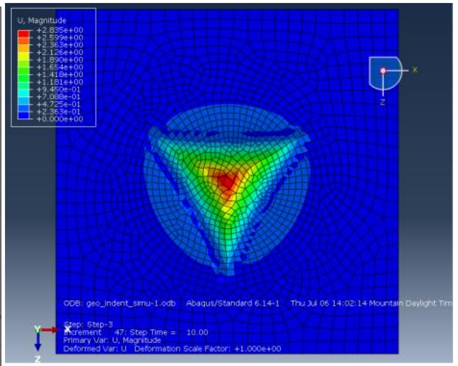
Model setup

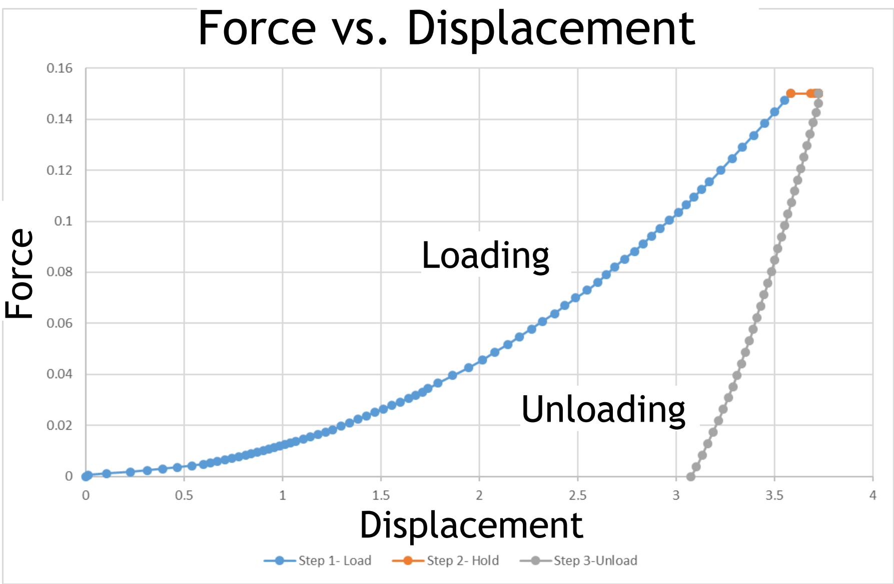


Indentation impression

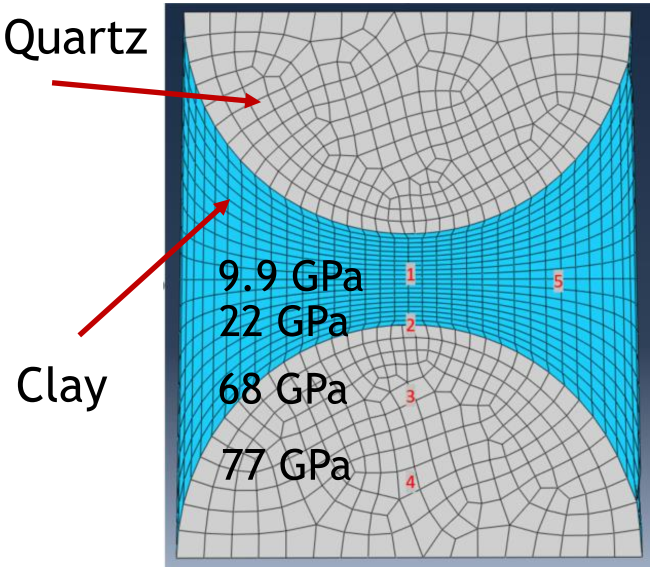


Simulated Indentation mark





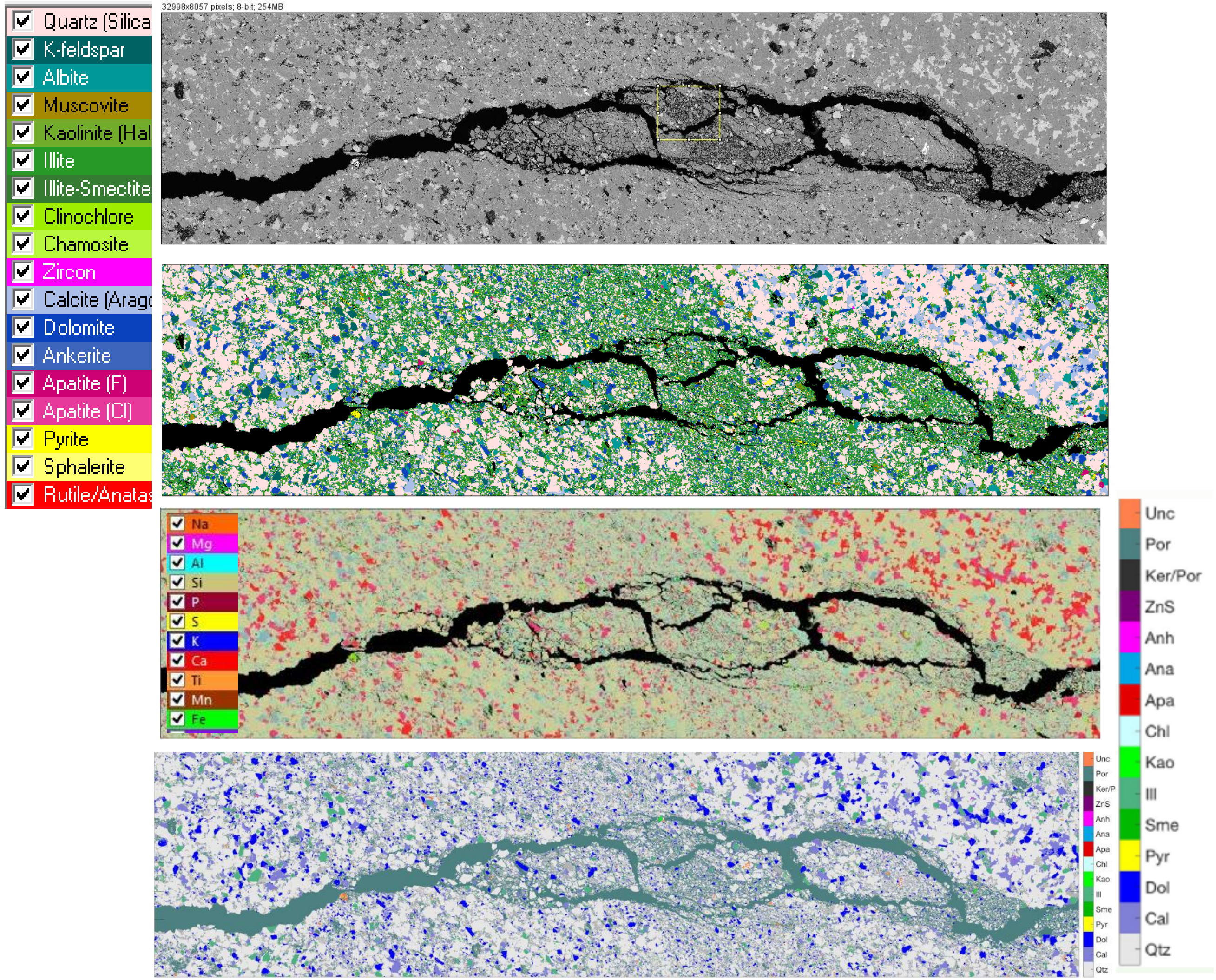
Elastic Modulus



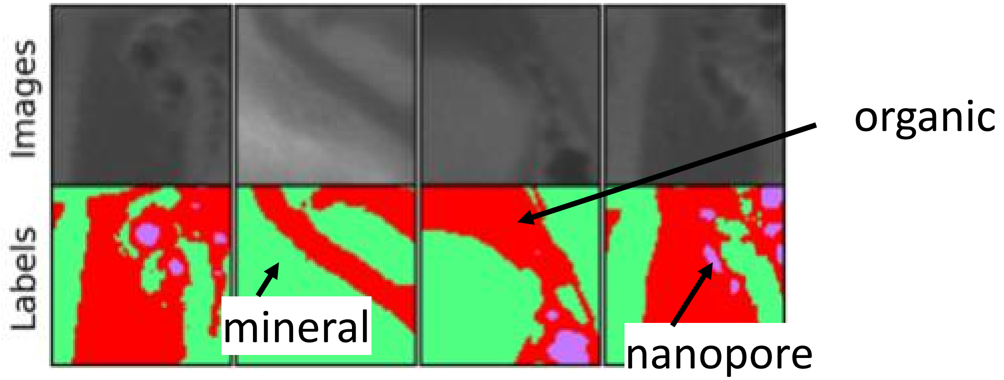
- Simulated indentation mark mimics an ideal indentation mark on quartz well
- Simulation results clearly show that calculated elastic modulus at different locations from the center of quartz to clay decrease
- This clearly demonstrates that the precise location of indentation (in other words, compositional heterogeneity) impacts estimated mechanical properties significantly

Deep Learning-based Analysis

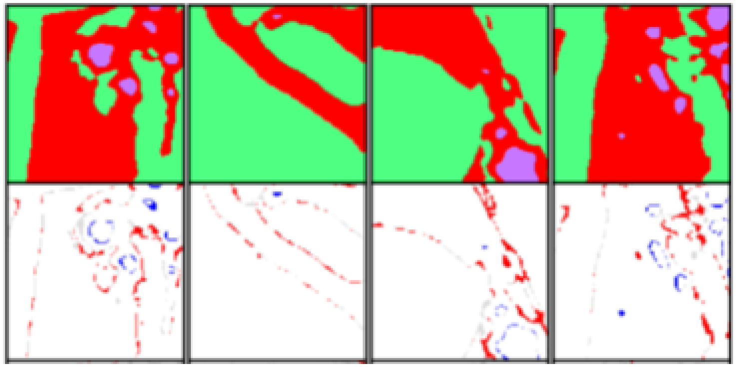
Multi-label classification (Convolutional neural network)
Input: BSE image, 15 elemental maps, elemental ratio
Output: multiple (15) minerals per pixel



Multi-label segmentation



MultiResUnet **97.13% accuracy**

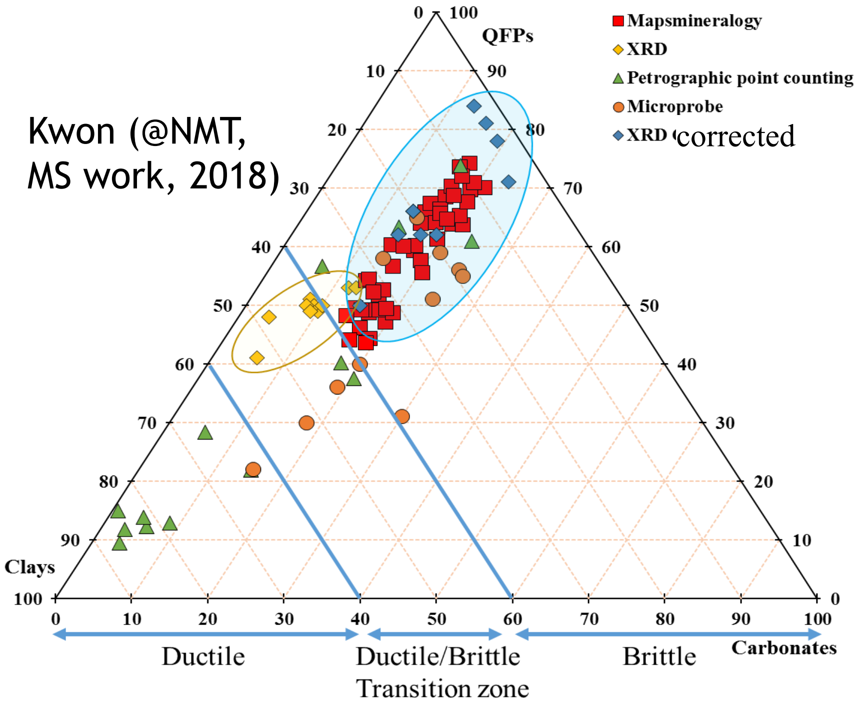


Summary & Conclusions

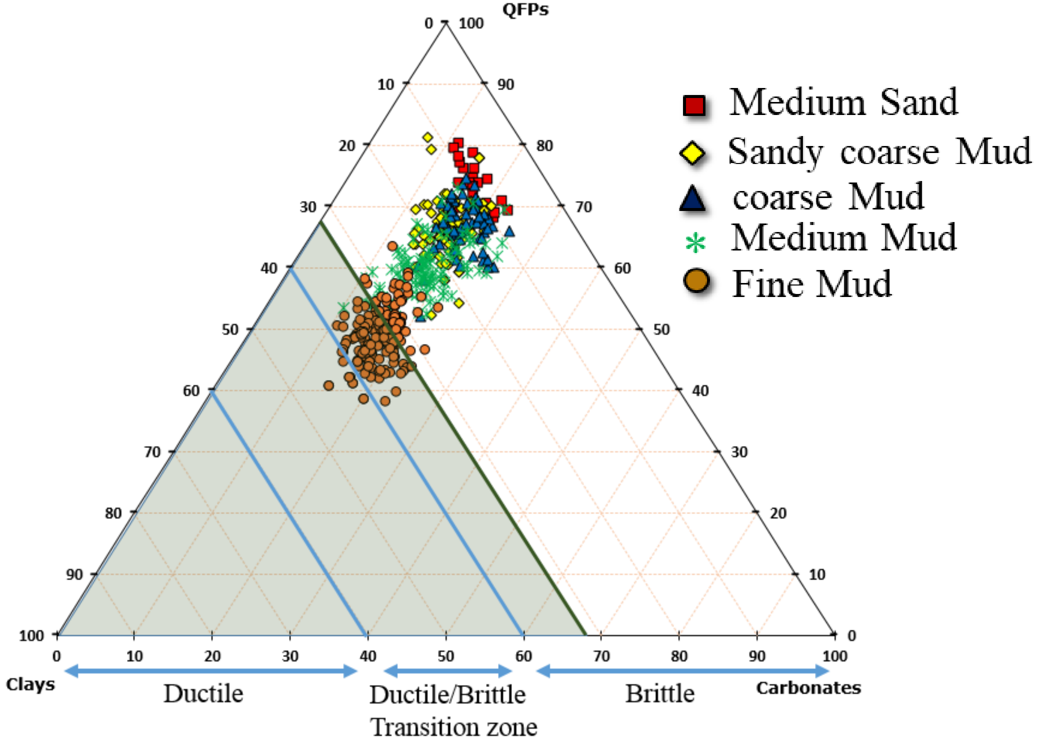
- Integrated multiscale imaging and mechanical testing with numerical simulation provides a robust approach to advancing our understanding of mechanical properties of Mancos shale
- Texture/mineralogical characterization
  - Recent advances in mineralogical mapping with high resolution imaging over the large area
  - Multiscale mineralogical and geologic features lead to considerable heterogeneity of mechanical properties.
- Nanoindentation
  - Both mineralogy and its distribution govern distinctively different mechanical properties
  - Mechanical map and nanoindentation test suggest the important role of geological attribute to mechanical properties of mudstone
  - Microscopic heterogeneity of mechanical properties can control the spatial distribution of fractures
  - This heterogeneity should be taken into account for realistic mechanical modeling and can scale up by rigorous numerical modeling & machine learning appraoches

Key reference: Yoon et al., 2020, Impact of depositional and diagenetic heterogeneity on multiscale mechanical behavior of mancos shale, New Mexico and Utah, USA, in W. Camp, K. Milliken, K. Taylor, N. Fishman, P. Hackley, and J. Macquaker, eds., Mudstone diagenesis: Research perspectives for shale hydrocarbon reservoirs, seals, and source rocks: AAPG Memoir 120. Chapter 8 p. 121–148. [if there is any question including the preprint version of the chapter, please contact hyoon@sandia.gov]

Mineralogy Mapping: Scale/methods dependent



Ternary map after Ulmer-Scholle et al. (2014)



MAPS data over 50 x 50 μm^2 with 2 μm resolution)

- Ternary diagram with QFPs (quartz, feldspars, pyrite), clays, and carbonates for mechanical properties (brittle to ductile)
- Petrographic point count can't distinguish fine particles/crystalline from clays
- Original XRD/microprobe analysis tend to overcount clay fraction (due to inaccurate mineral assumption and low resolution)

- MAPS data shows five micro-lithofacies that fall within a siliceous mudstone and brittle zone on the ternary diagram
- A fraction of quartz (QFPs) decreases with decreasing the grain size (clays in an opposite trend)
- Feldspars and carbonates are relatively evenly distributed