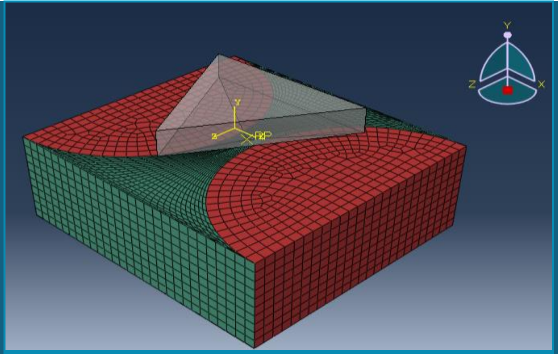
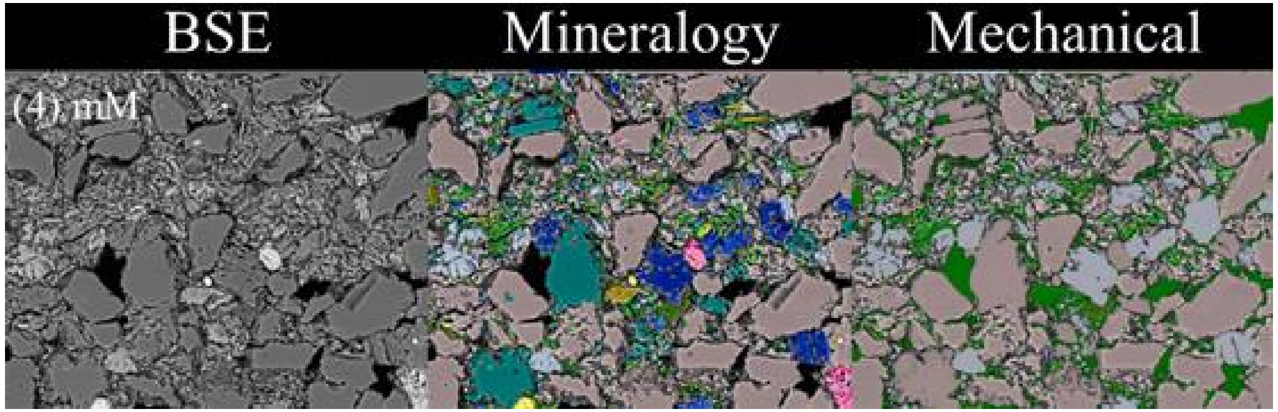
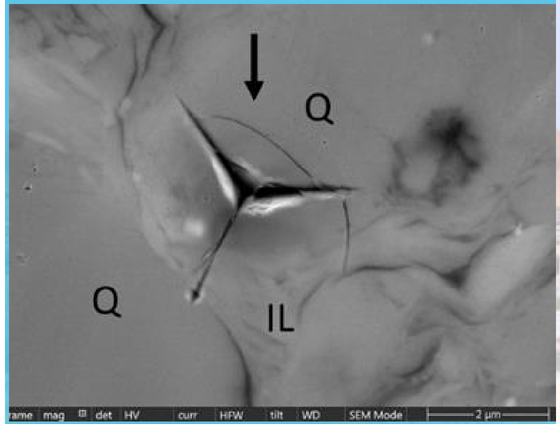
SAND2022-8286C

Multiscale mechanical properties of Mancos shale using machine learning methods







PRESENTED BY

Hongkyu Yoon & Teeratorn Kadeethum (Sandia National Laboratories)

Contributors: OhTark Kwon (KOGAS), Daniel Lizama (SNL)

William Mook (SNL), Peter Mozley (New Mexico Tech)

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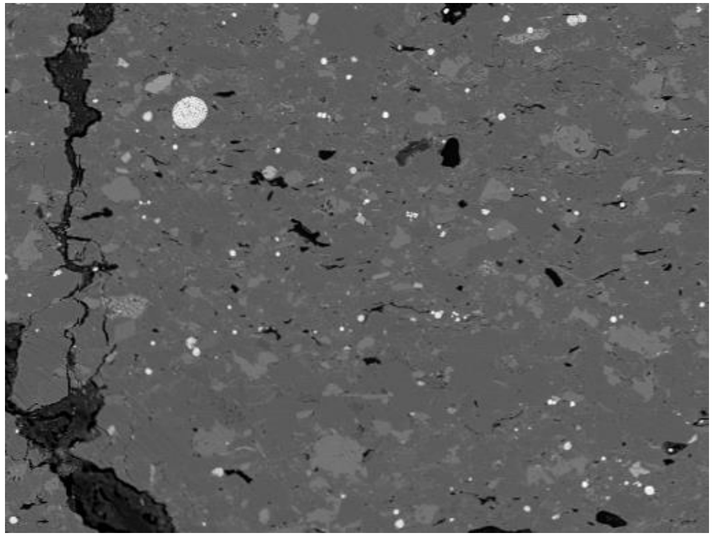
Motivations & Objectives

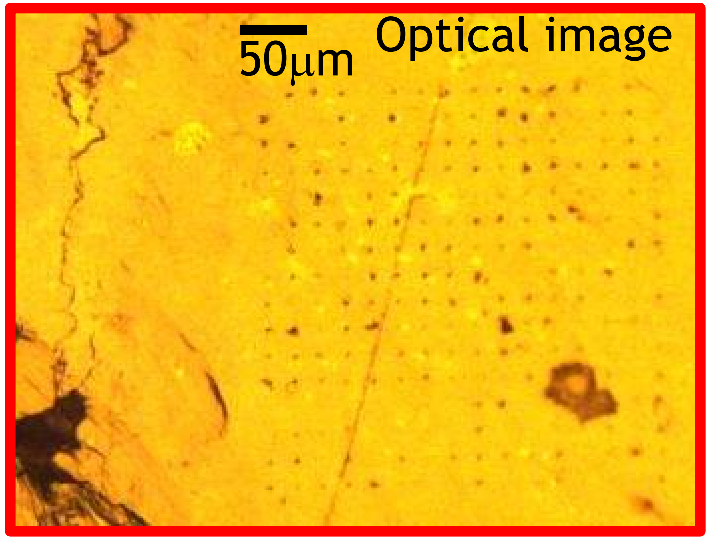
Impact of micro-lithofacial heterogeneities on mechanical properties of Mancos Shale

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

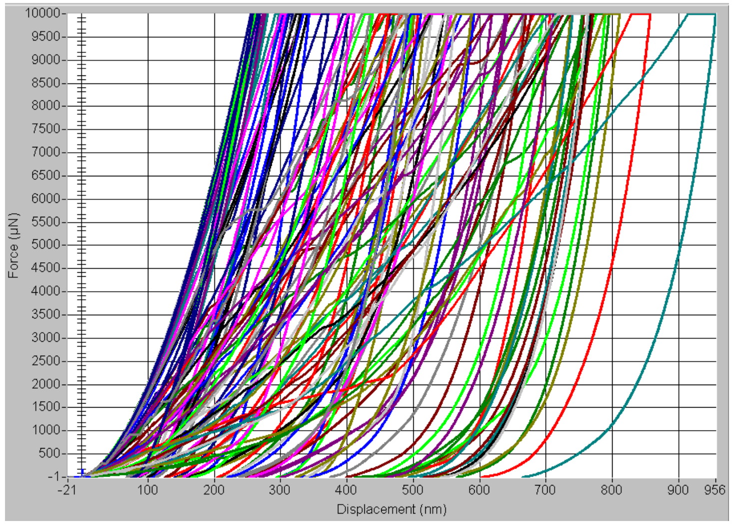
SEM image of shale



Grid nanoindentations over clay-rich area



Load-displacement curves

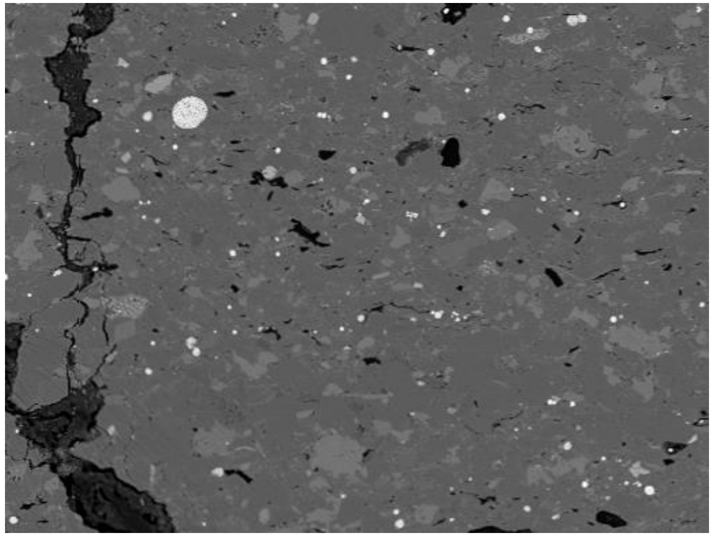


Motivations & Objectives

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)

SEM image of shale



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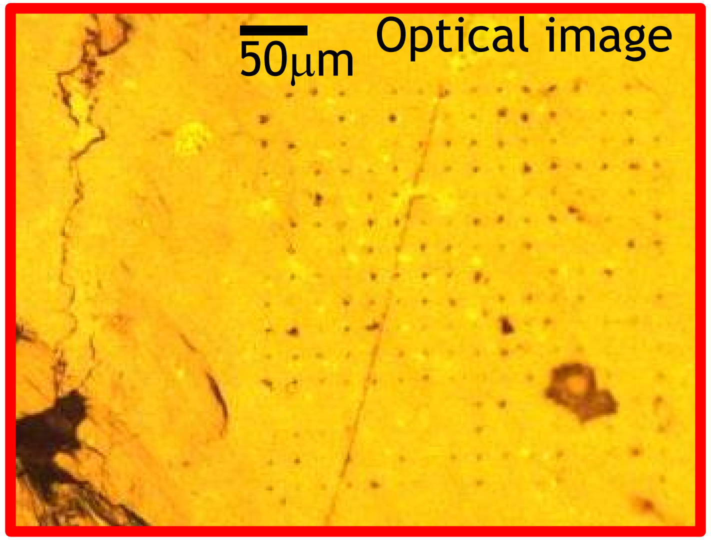

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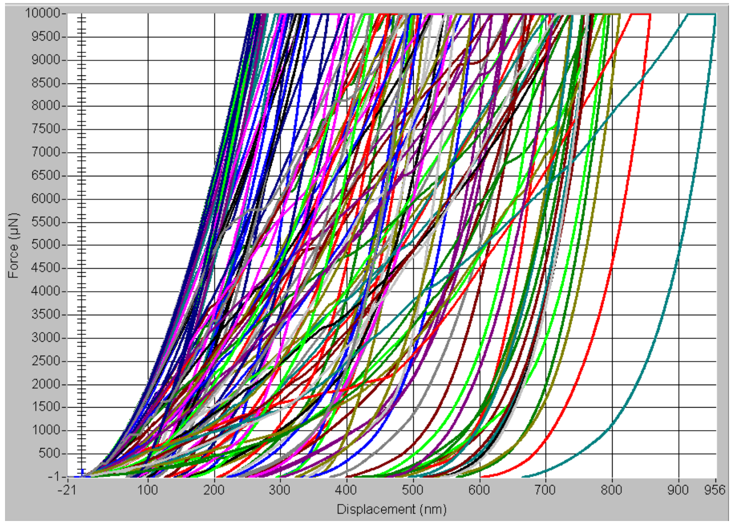


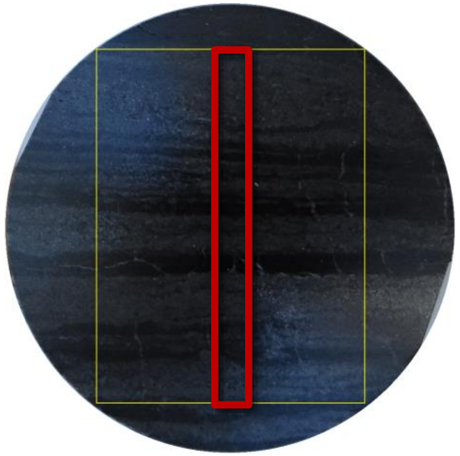
MAPS Mineralogy

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

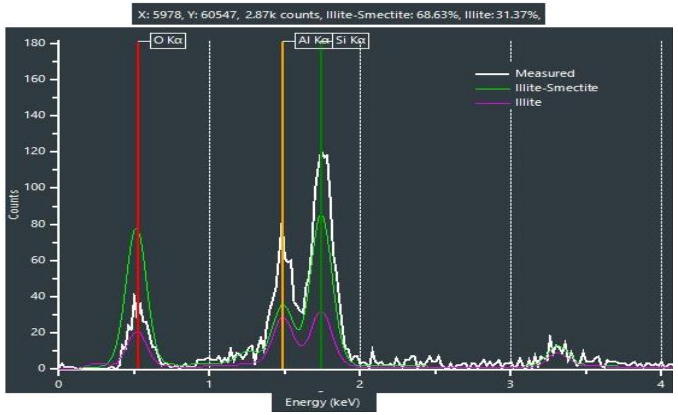
- **Mineral identification**
  - Spectral matching
  - Each pixel – single/multiple minerals

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

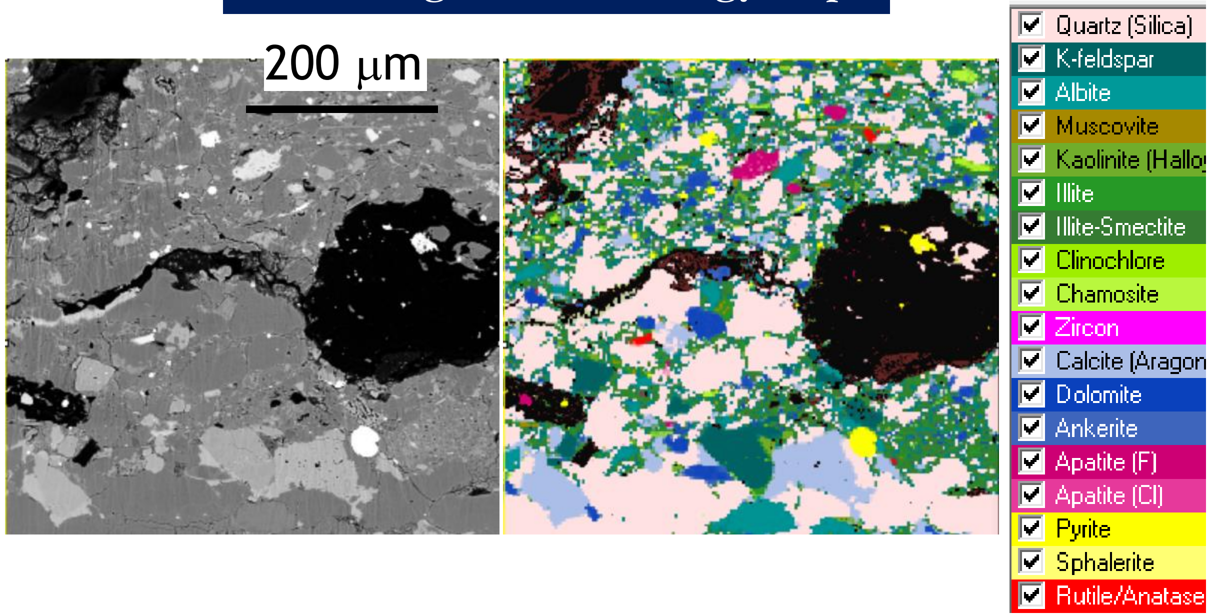
Ion-milling polished Mancos sample (2.5cm diameter)



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

Micro-lithofacies

Medium Sand

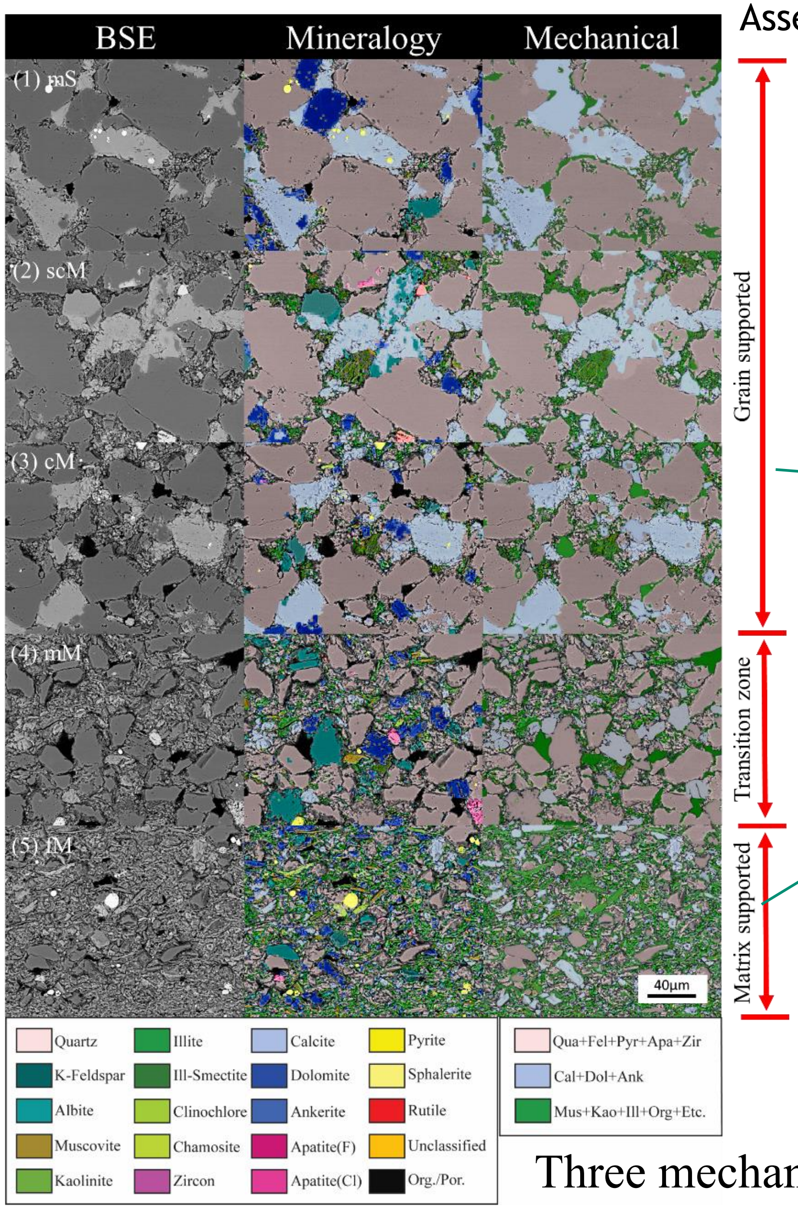
Sandy Coarse Mud

Coarse Mud

Medium Mud

Fine Mud

Mineral Assemblages

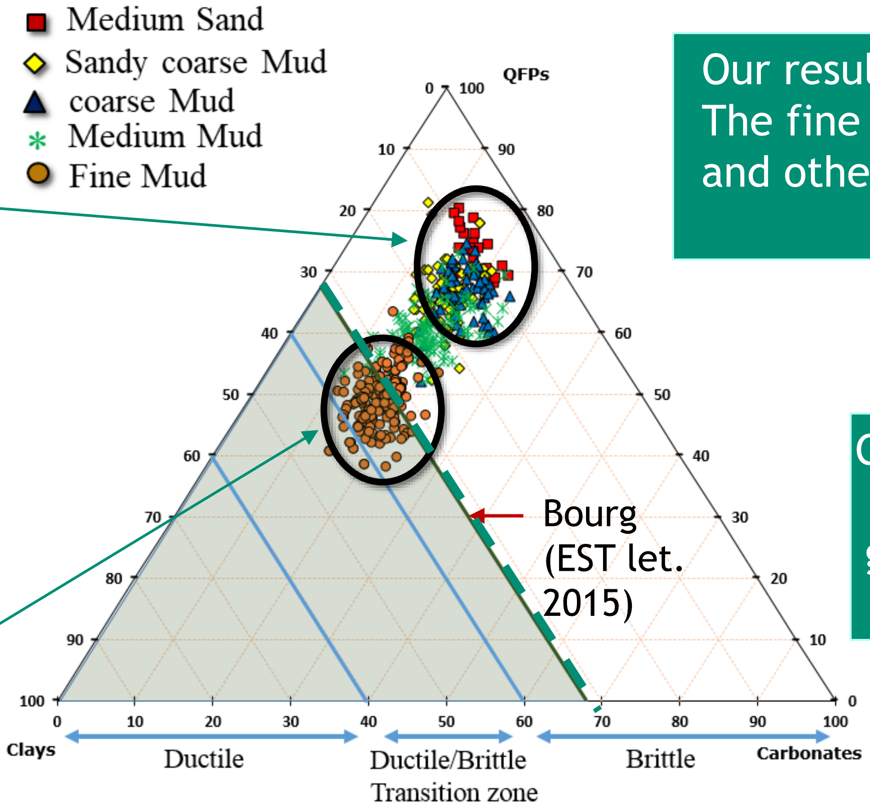


Three mechanically significant mineral assemblages

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.

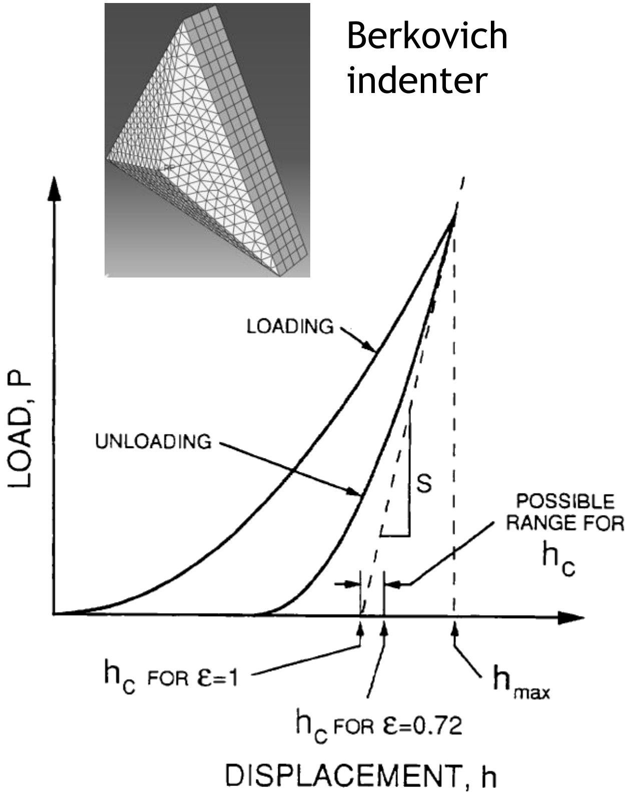
f(geological textures)? Yes

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

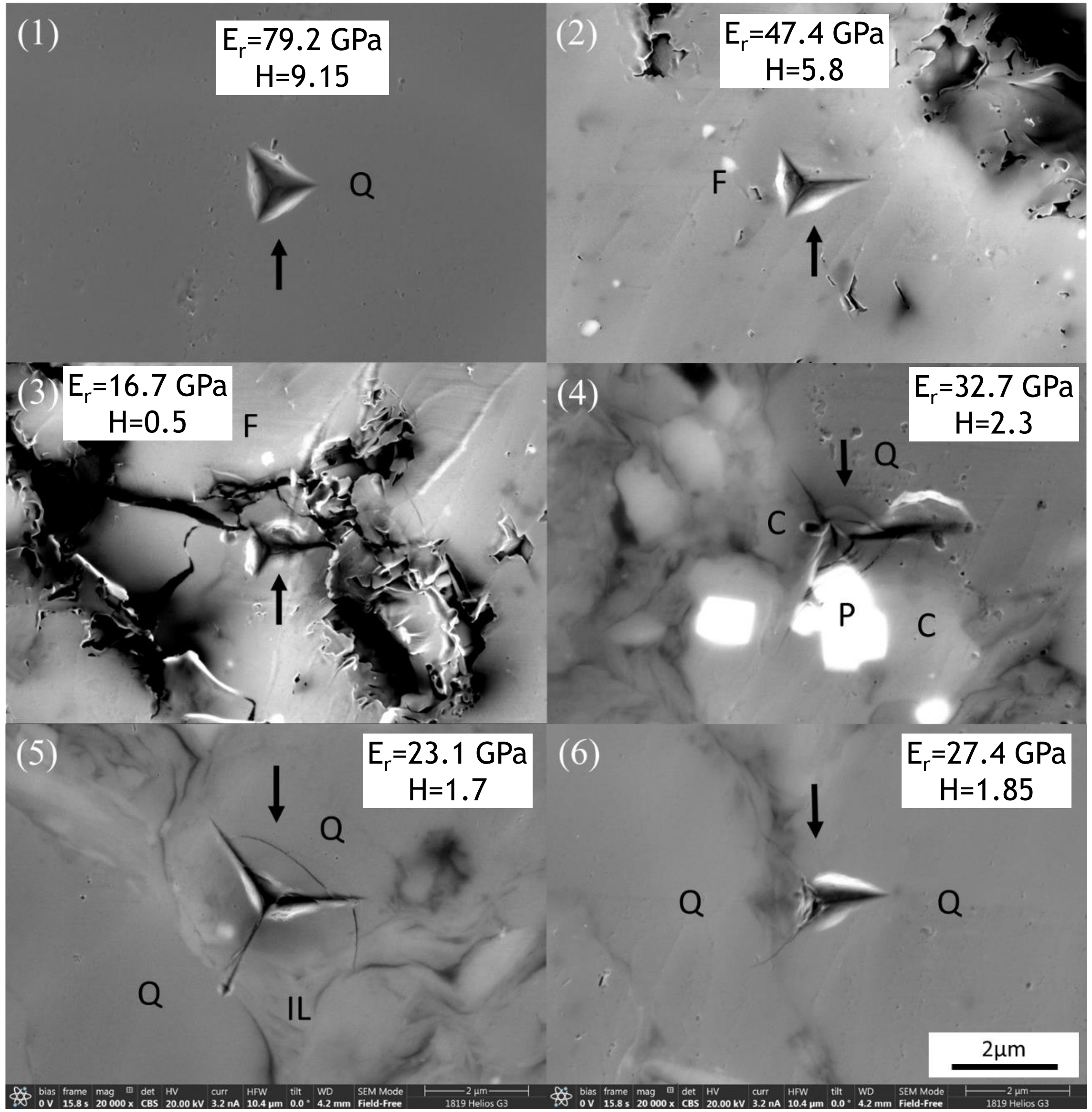
- **Analytical concept**
  - Purely elastic deformation upon initial unloading
  - Hardness = load/contact area
  - Elastic modulus determined by stiffness (S)



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



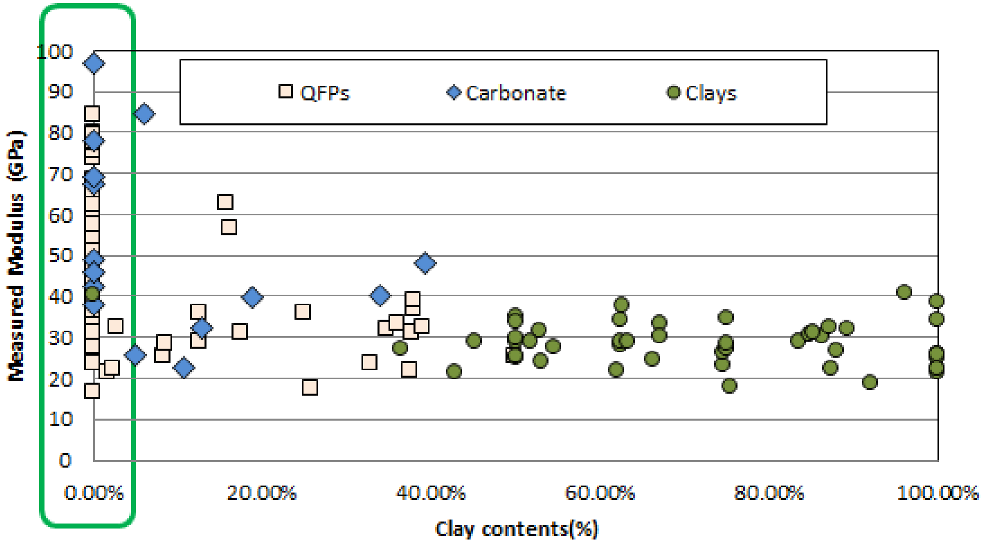
NOTE: Q=quartz, P=pyrite, C=carbonate, F=feldspar, and IL=illite)

(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.

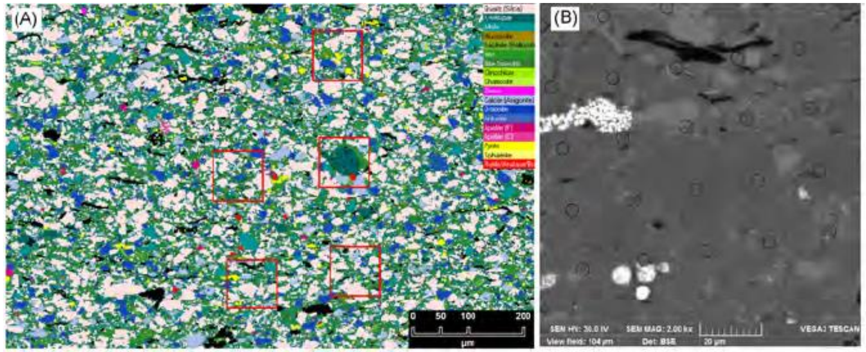


Estimation of Properties using Machine Learning

Step 1. Clustering dataset based on mineral composition

Table 1: List of mineral composition

mineral composition			
quartz	feldspar	muscovite	kaolinite
illite	smectite	Mg-chlorite	Fe-chlorite
zircon	calcite	dolomite	ankerite
apatite	monazite	pyrite	sphalerite
rutile	unclassified	porosity	organics



Step 2. Building regression models for each cluster (linear, Gaussian process, support vector machine, XG-Boost)

Hardness (H)
(input)

Cluster 1

Cluster 2

⋮

Cluster n

Reduced Young Modulus (E_r)
(output)

Kadeethum & Yoon (ARMA proceedings, 2022)

Clustering: balanced iterative reducing and clustering using hierarchies (BIRCH)

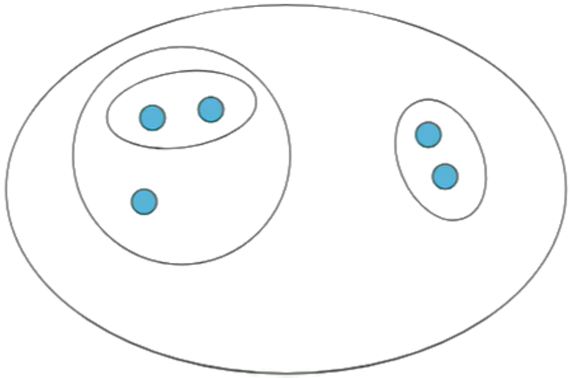
1. BIRCH has two primary hyperparameters, **threshold** and **number of clusters**. The threshold constraints a radius of the sub-cluster obtained by merging a new sample and the closest sub-cluster.

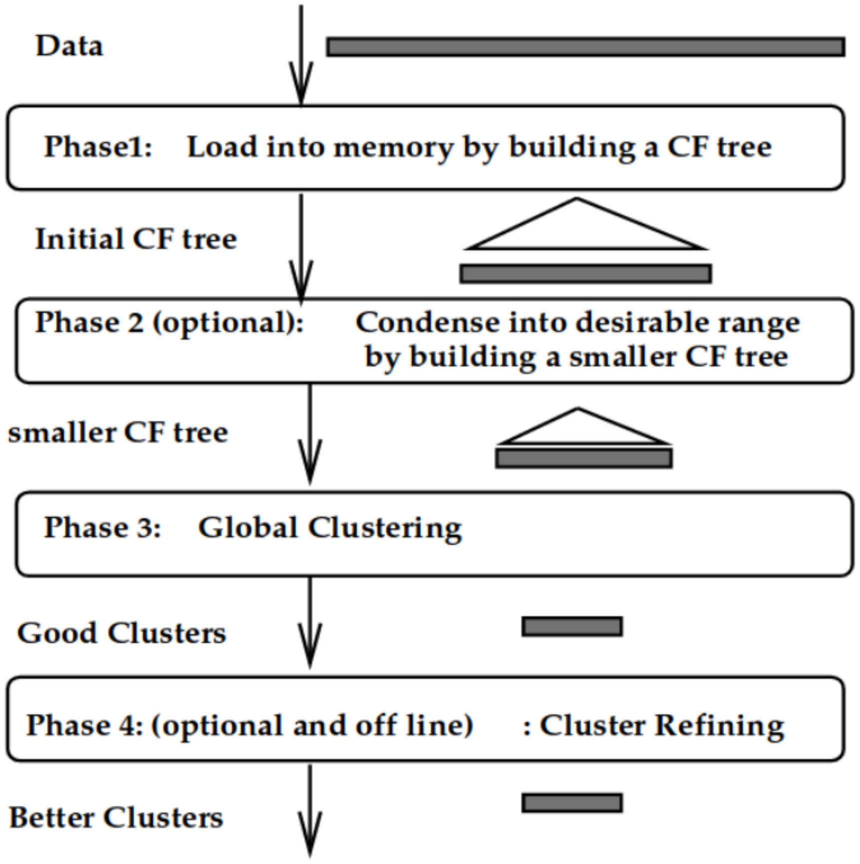
2. We set **threshold** as 0.001 throughout this study.

3. We have tested **number of clusters**

from 1 to 8 (but we shown our result only 1 to 5)

Hierarchical Clustering





CF: Clustering Feature

http://www.cs.uvm.edu/~xwu/kdd/BIRCH.pdf

Clustering Results

1. The training set has a total members of 237

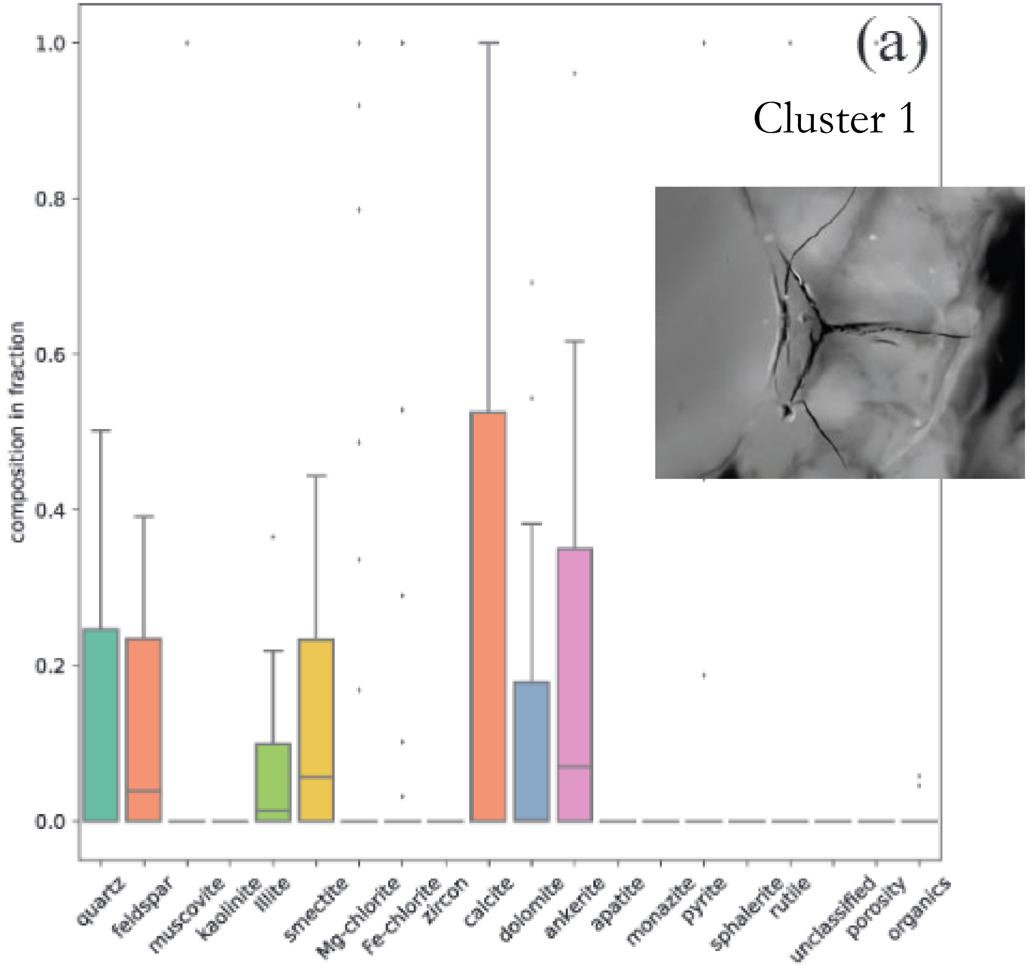
Table 4: Clustering results for the training set: we cluster the data using mineral composition.

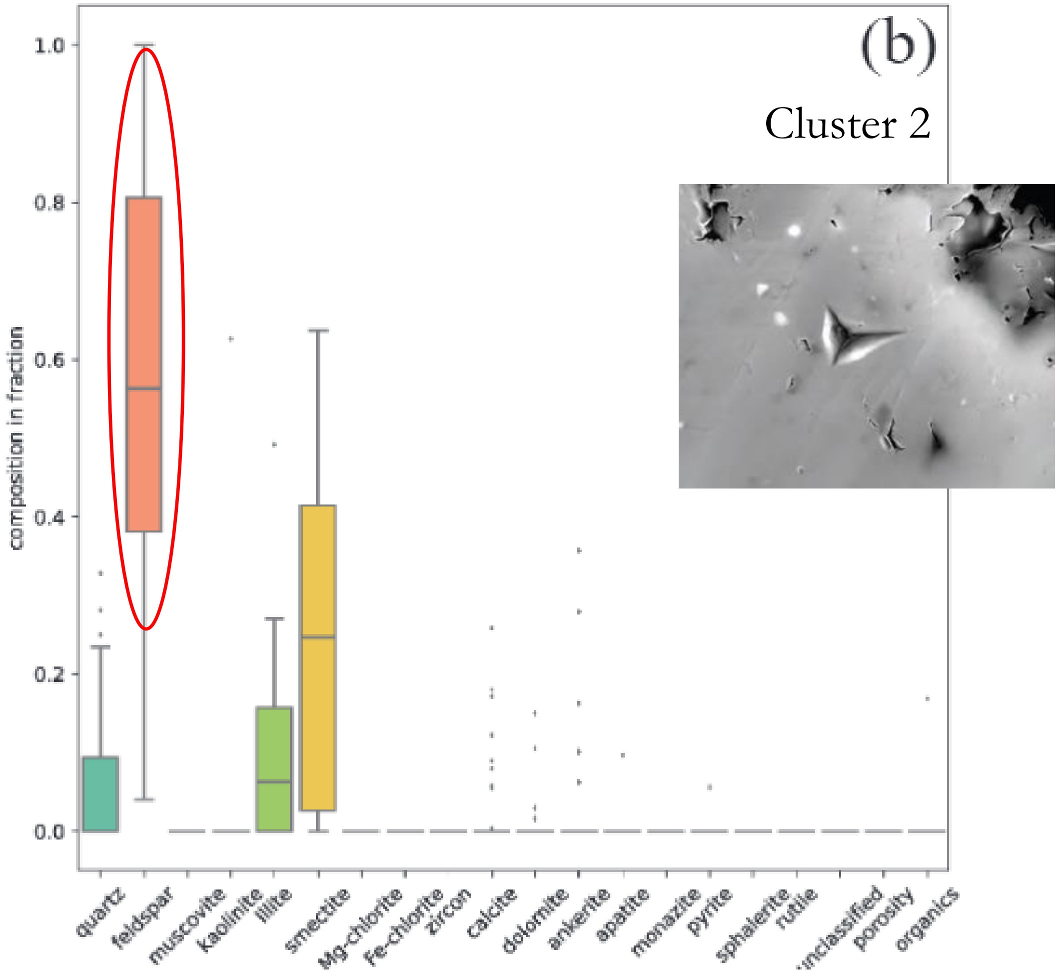
number of members for each cluster	number of clusters				
	1	2	3	4	5
1	237	x	x	x	x
2	228	9	x	x	x
3	167	61	9	x	x
4	103	64	61	9	x
5	37	66	64	61	9

Clustering Results

1. Cluster 1 represents the most **heterogeneous materials** where **many minerals co-exist**

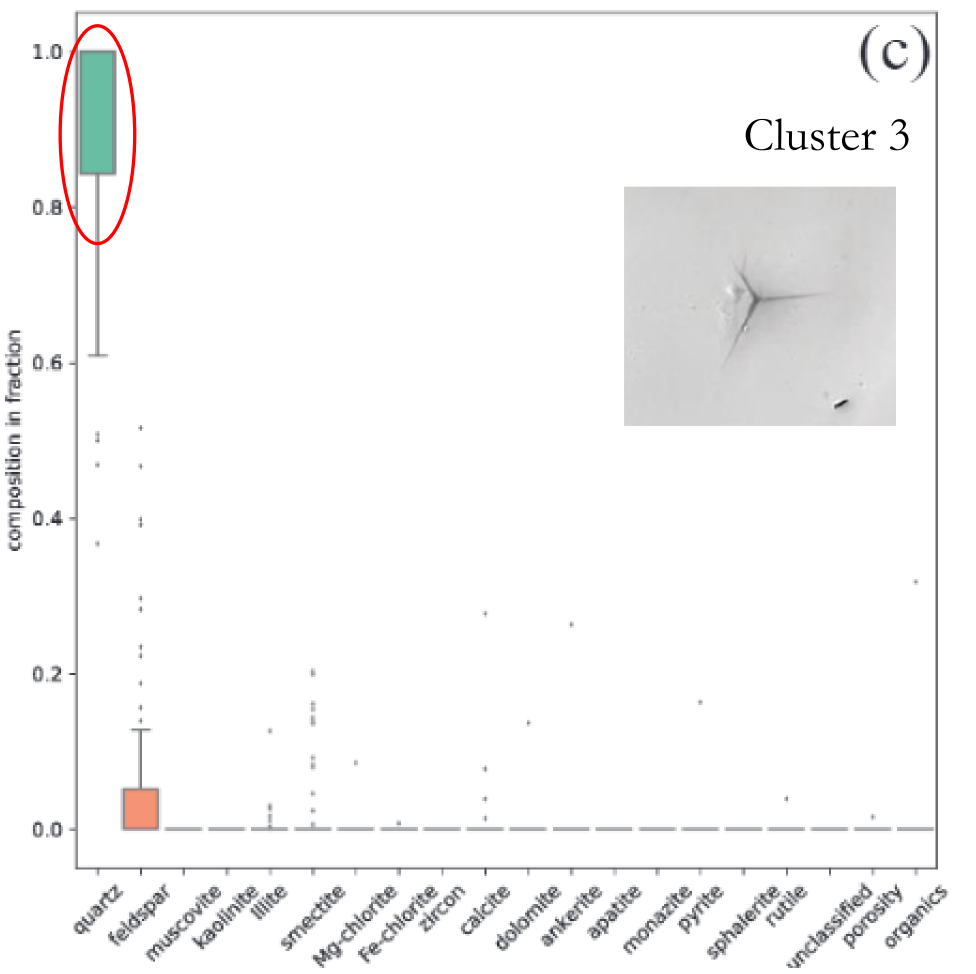
2. Cluster 2 is dominated by **feldspar & clays**

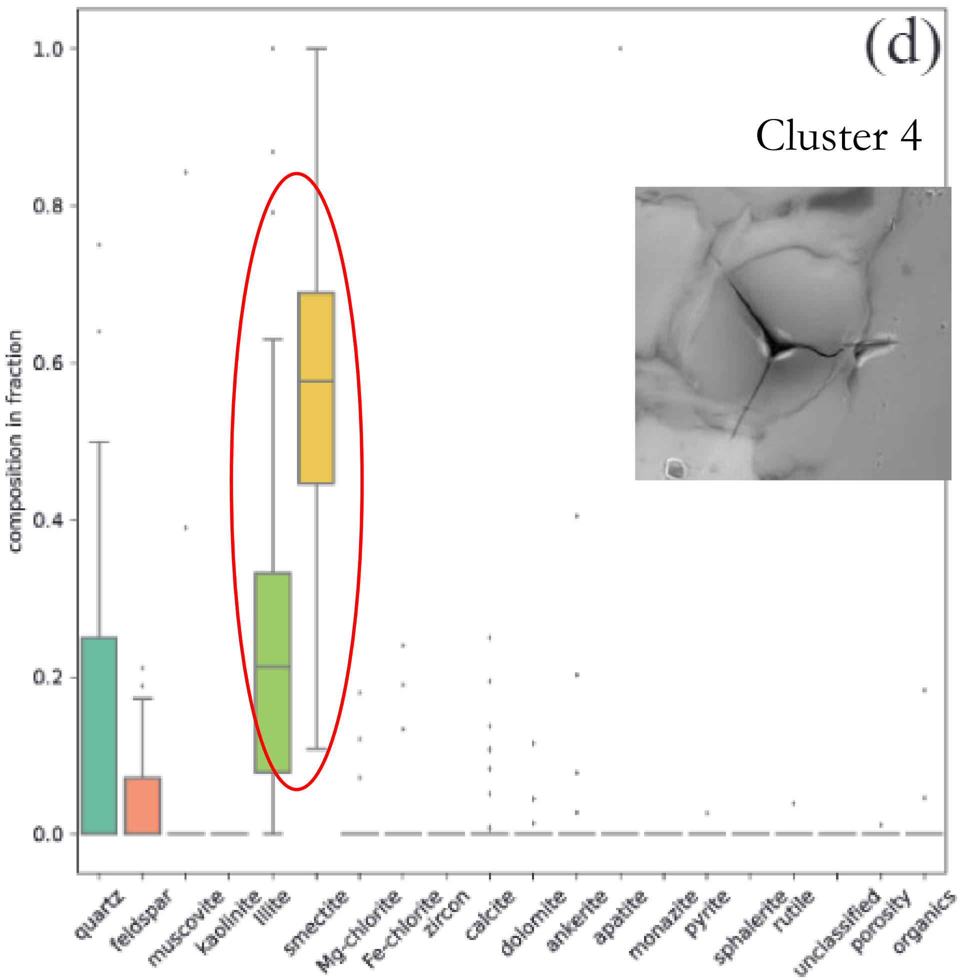




Clustering Results

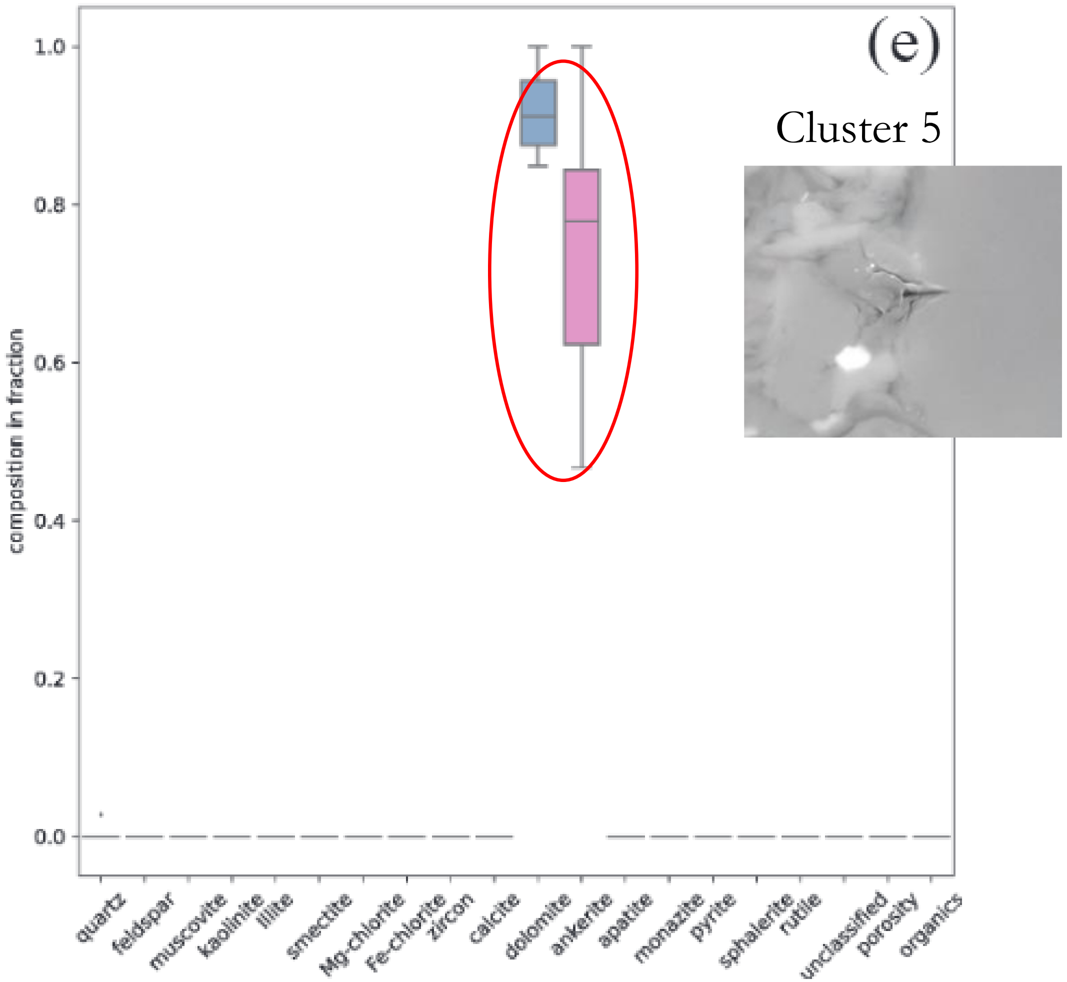
1. Cluster 3 is predominantly **quartz**
2. Cluster 4 contains a high fraction of **smectite/illite**





Clustering Results

1. Cluster 5 is dominated by carbonates (**dolomite/ankerite)**



Building a regression model for each cluster

- Four types of regressors: 1. linear regression (LR), 2. support vector regression (SVR), 3. Gaussian process regression (GP), and 4. extreme gradient boosting regression (XGBoost)

- For SVR, we utilize a quadratic polynomial kernel with an independent term of one, a **regularization parameter of 100**, and a kernel coefficient of one over number explanatory variables

- For GP, we use **normal prior bias** and **white noise kernel**

- For XGBoost, we **use 100 weaker estimators** with **maximum tree depth of five**, and two regularization parameters (1.0 & 0.0)

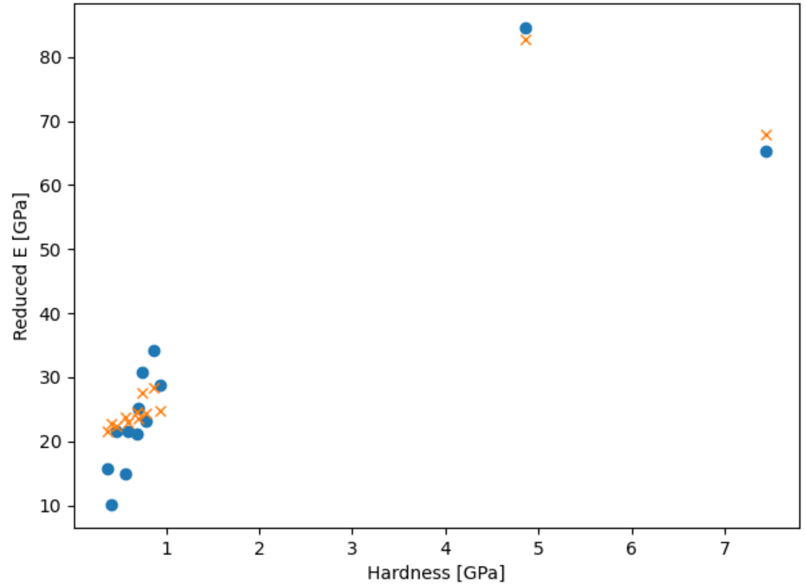
Regression model results

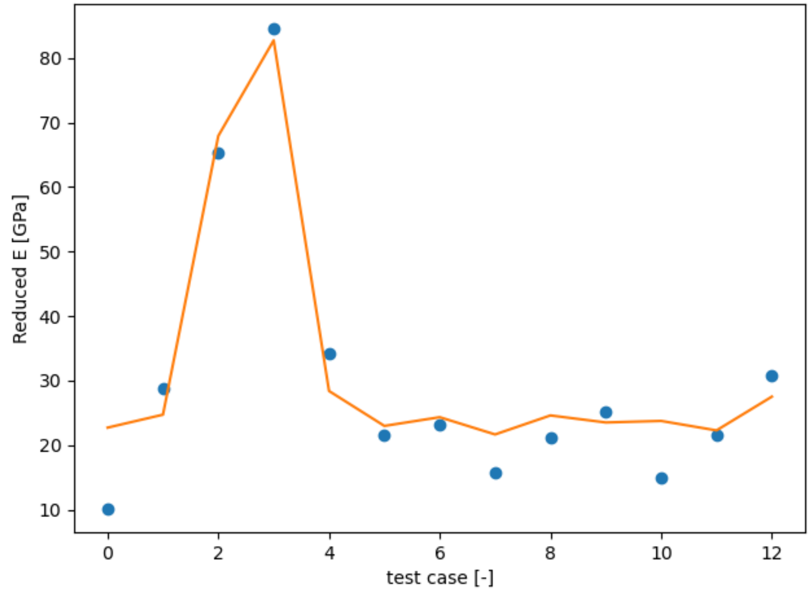
- Overall, Case with 5 clusters yields the best results
- Tentative results: linear regression (LR) performs well
- CF with explicit coordinates in an Euclidean space may work well with LR
- Due to a small testing data this comparison needs to be performed more comprehensively

Table 3: R^2 results of different models using hardness (H) as input and reduced Young's modulus (E_r) as output. We cluster the data using mineral composition.

number of clusters	R^2			
	LR	SVR	GP	XGBoost
1	0.717	0.722	0.717	0.649
2	0.921	0.906	0.921	0.923
3	0.921	0.906	0.921	0.916
4	0.923	0.915	0.924	0.905
5	0.933	0.925	0.933	0.906

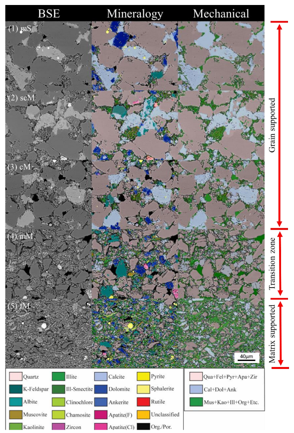
Testing results (Linear Regression)



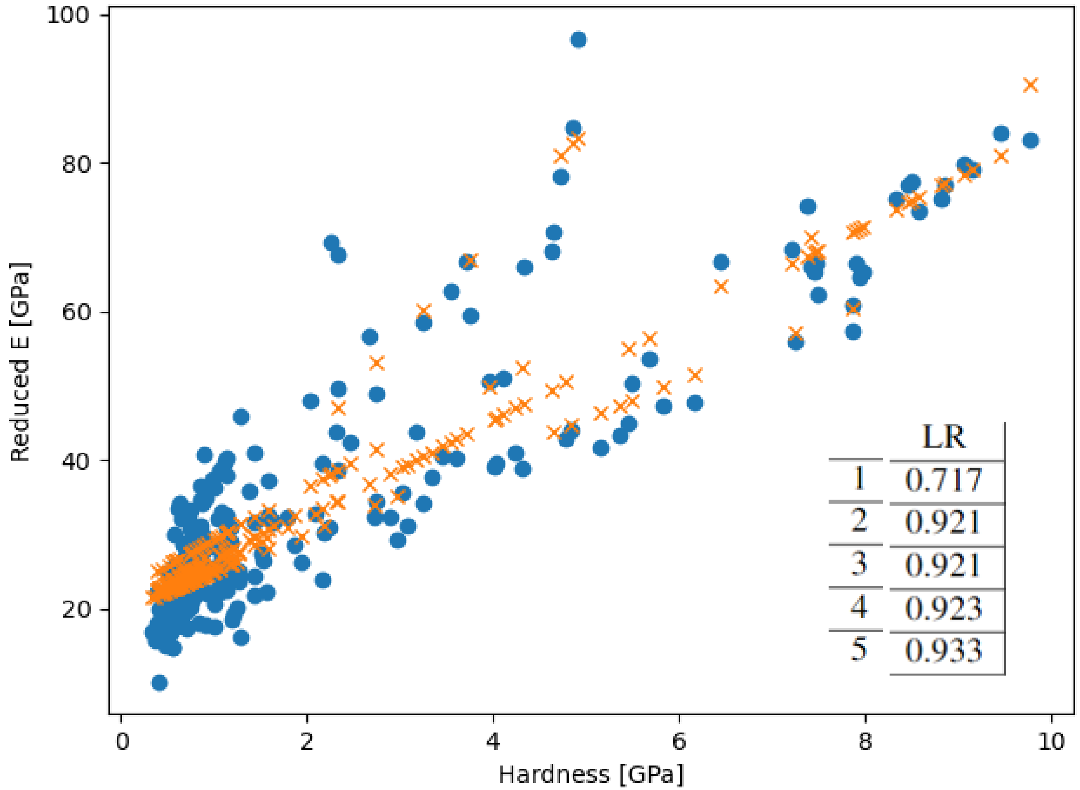


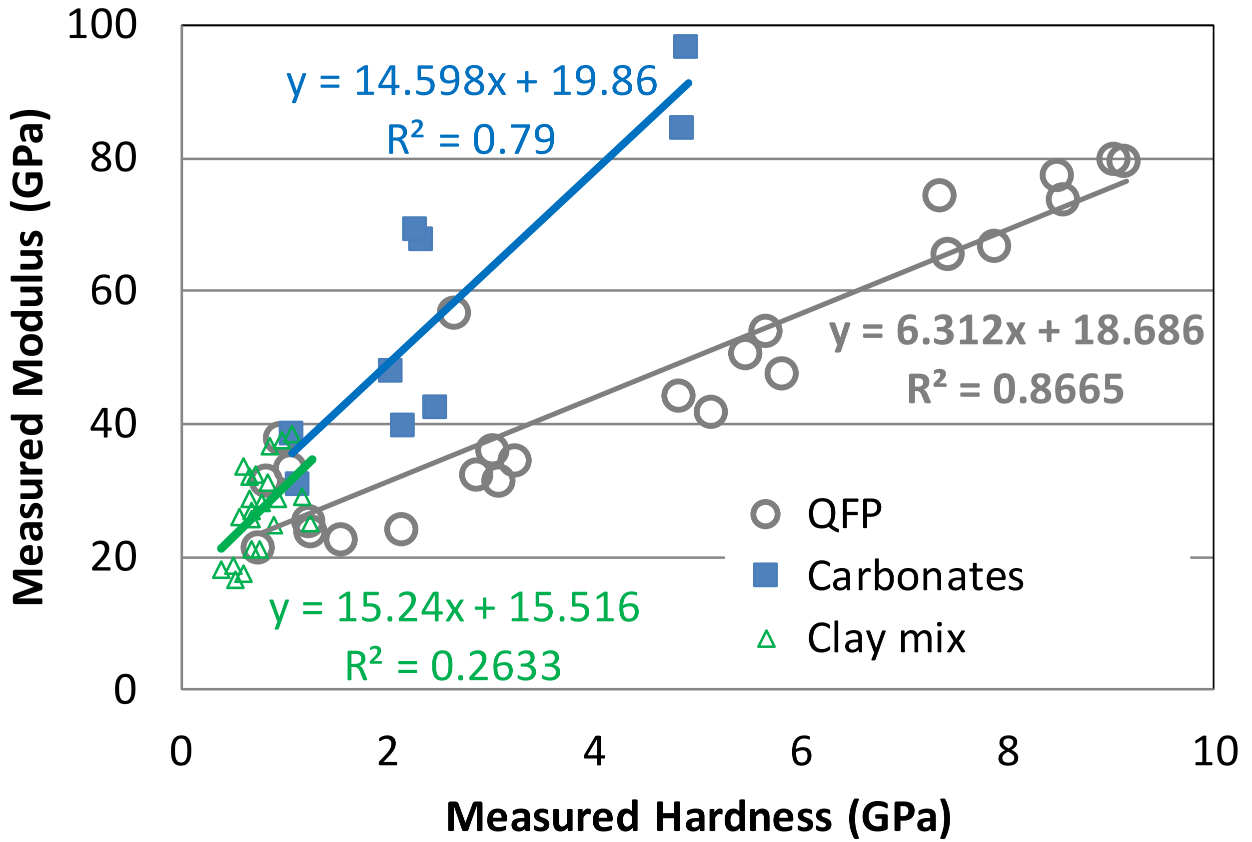
Regression model results

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



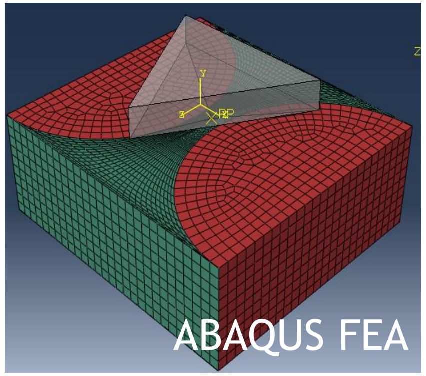
Training & testing results (Linear Regression)



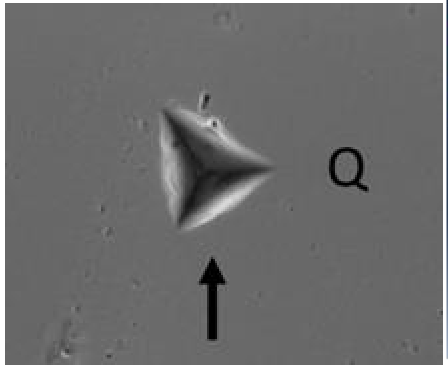


Simulation of Nanoindentation

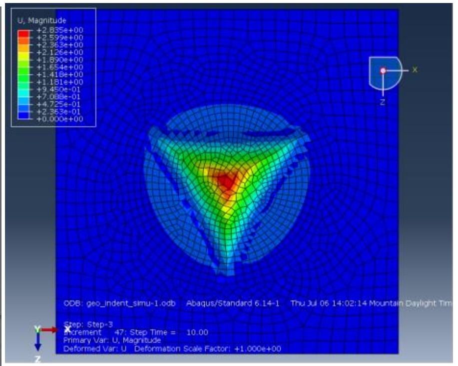
Model setup

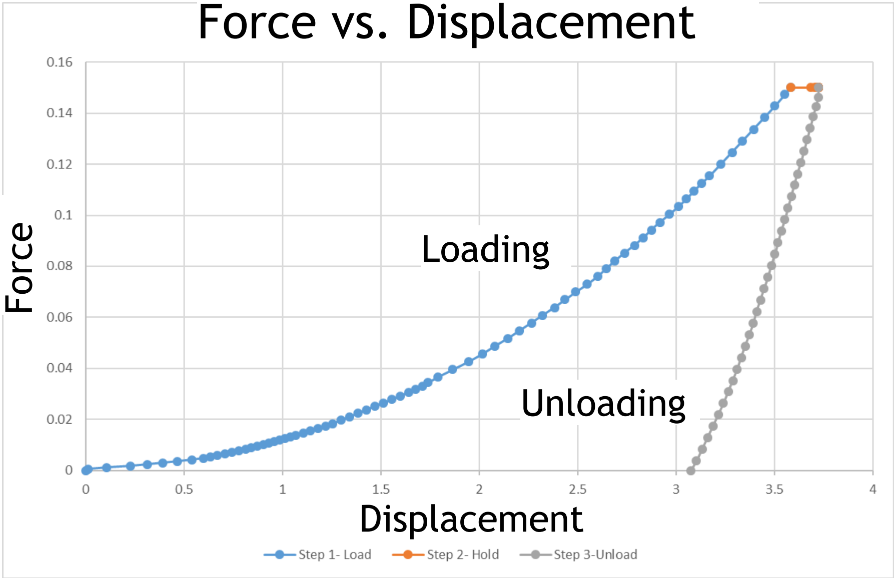


Indentation impression

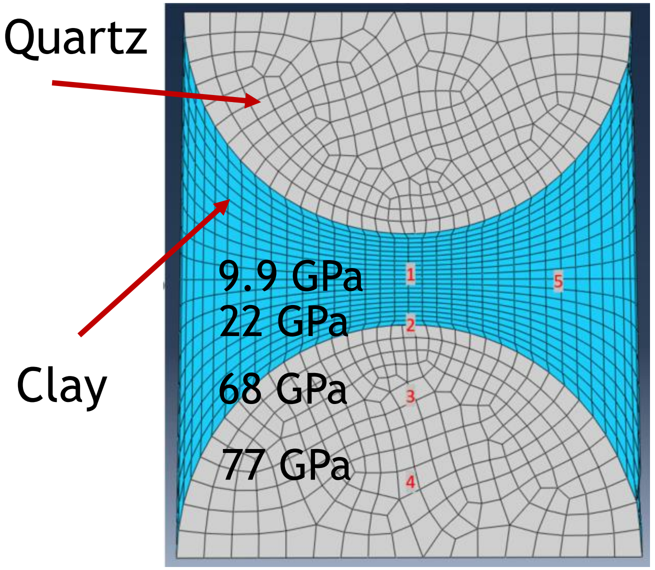


Simulated Indentation mark





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

Summary

- The balanced iterative reducing and clustering using hierarchies (BIRCH) with multiple regressors (LR, GPR, SVR) perform well to predict the reduced Young's modulus of highly heterogeneous materials from nanoindentation experiments.
- Clustering was performed with mineralogy compositions
- Five clusters tend to work well and could be represented by mineralogy distribution
- In the future, we plan to perform conditional variational autoencoder (cVAE) to develop a more robust model to account spatial distribution of mineralogy and geologic attributes

Summary

- The balanced iterative reducing and clustering using hierarchies (BIRCH) in conjunction with linear regression or Gaussian process regression can be very accurate to predict the reduced Young's modulus of highly heterogeneous materials from nanoindentation experiments.

- 2. We cluster the dataset from mineralogy classification through scanning electron microscope (SEM) images.

- 3. We observe that the number of clusters of five delivers the most accurate results.

- 4. We also illustrate these five clusters could be represented by the physical mineralogy.