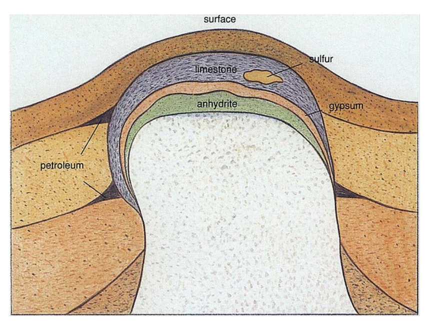
Modeling the Anisotropic Behavior of Natural Rocksalt during Creep Tests using Dislocation Density-based Crystal Plasticity

Timothy Truster, Amirsalar Moslehy, Sunday Aduloju, and Khalid Alshibli

Department of Civil and Environmental Engineering – University of Tennessee - Knoxville

Motivation



Salt domes are used as a repository for:

- Nuclear waste; Hydrocarbons; Compressed air at power plants
- Why: Low permeability and creep rate

Challenges:

- Waste are usually hot
- Storage should be impermeable
- Long-term behavior
- High earth pressure at salt dome depths

Salt domes entrap oil and gas:

- Well drilling to obtain resources

Challenges:

- Drilling through a brittle material
- Stability of the well and its casing

1. Hansen, F.D. and Leigh, C.D., 2011. *Salt disposal of heat-generating nuclear waste* (p. 110). Albuquerque, NM: Sandia National Laboratories.
2. Martinez, Joseph D. "Salt Domes." *American Scientist* 79, no. 5 (1991): 420-31. http://www.jstor.org/stable/29774476.

Objectives

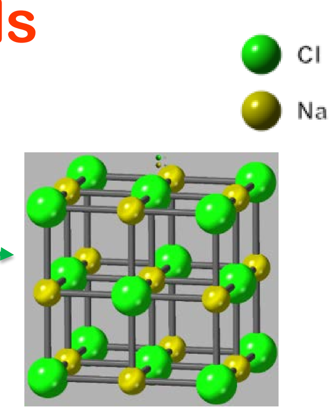
- Study the influences of anisotropy, temperature, and confinement on strength, fracture behavior, and creep rate and behavior of halite
- Develop crystal plasticity dislocation density-based model to account for plastic anisotropy along with cohesive zone model for fracture behavior on different lattice planes

Experimental Methods

Crystal Structure

Halite's crystal structure:

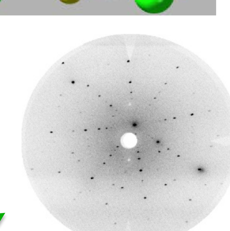
- Face centered cubical crystal structure (FCC)

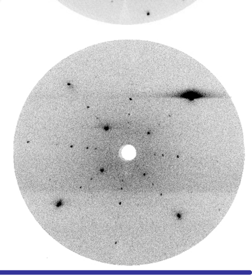


Specimens used in the study:

- Single crystal
- Natural halite usage in lieu of industrial or commercial grade
- Mineralogy and purity investigated by powder x-ray diffraction

Sodium chloride (NaCl) 99.9%



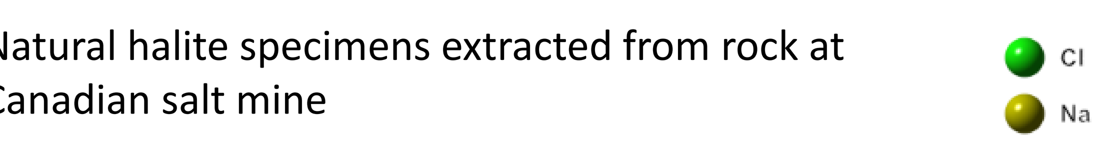


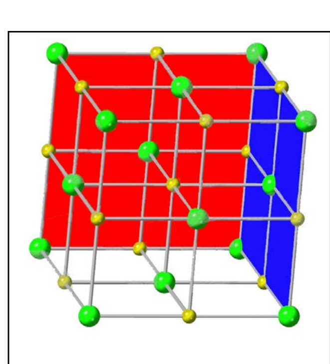
Crystal planes orientations in Laue x-ray diffraction

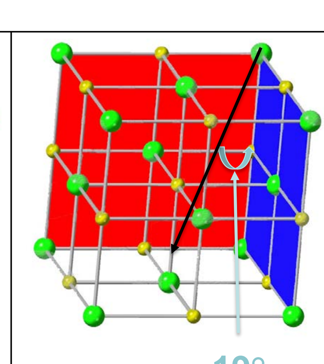
- Cut in cuboidal shapes on certain crystal planes
- Laue x-ray diffraction => confirm the orientations of the crystal planes with respect to specimens' surfaces

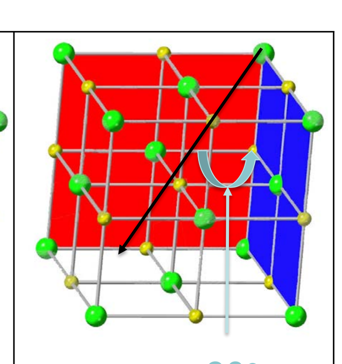
Specimens for Creep and Unconfined Compression Tests

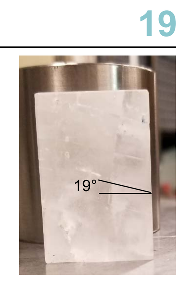
Natural halite specimens extracted from rock at Canadian salt mine







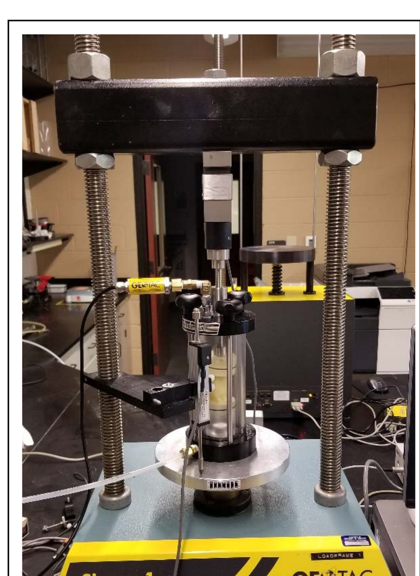




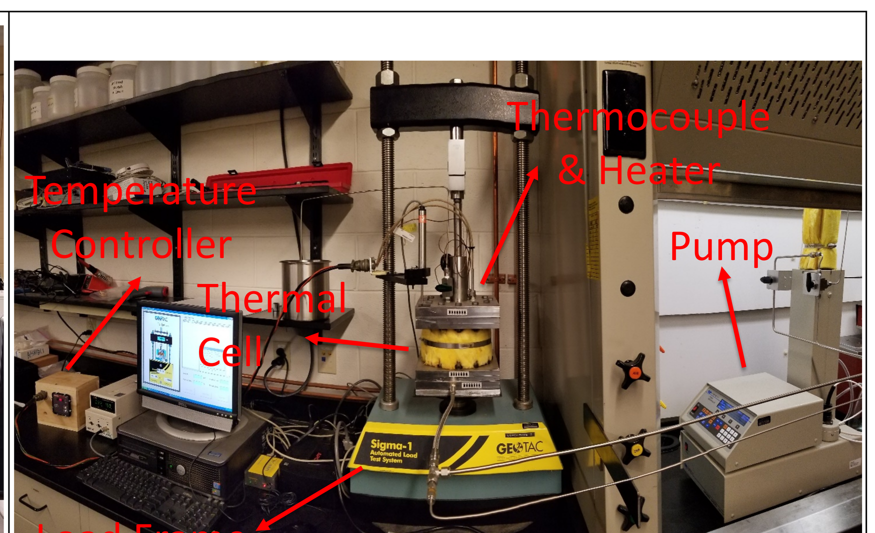
Parallel [1 0 0]	19° to (1 0 0) in (0 1 0)	30° to (1 0 0) in (0 1 0)

- 2" by 1"x1" rectangular specimens
- Orientations chosen to target plastic deformation to isolated or multiple crystal slip systems

Test Setups and Procedures



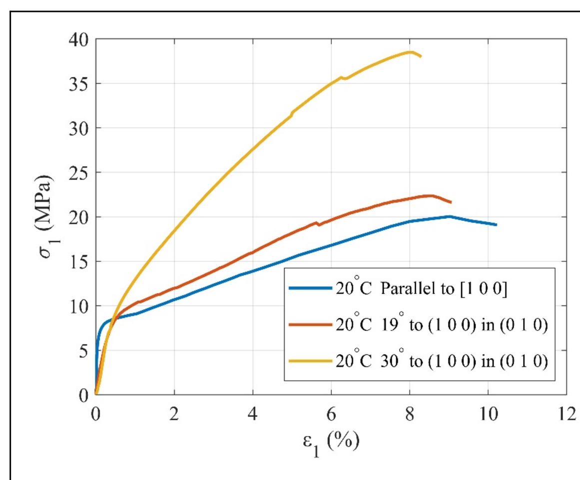
Setup used for Unconfined Compression & Creep Experiments at Room Temperature & Pressures up to 1 MPa



Setup used for Unconfined Compression & Creep Experiments at Elevated Temperatures (up to 150 ℃) & High Pressures (up to 5 MPa)

Experimental Results

Unconfined Compression Experiments

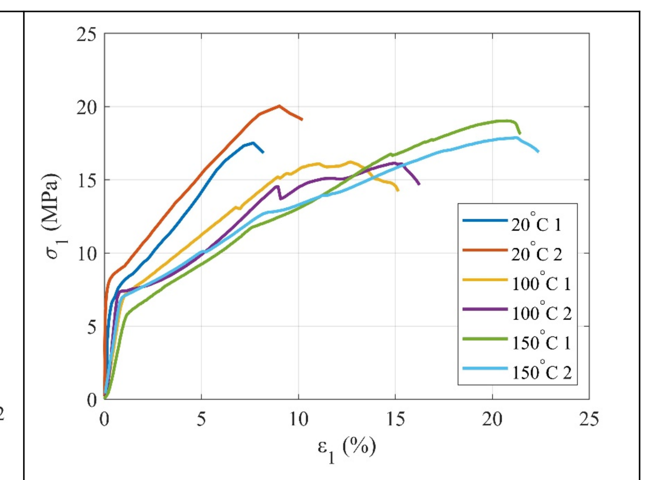


Orientation Effect

T = 20 °C

$\dot{\varepsilon} = 1.7\times10^{-4}/s$

Strain rate was kept constant during the experiments



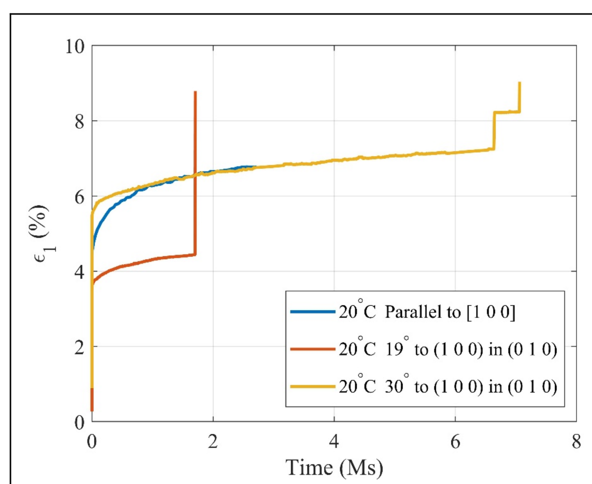
Temperature Effect

T = 20, 100, 150 °C

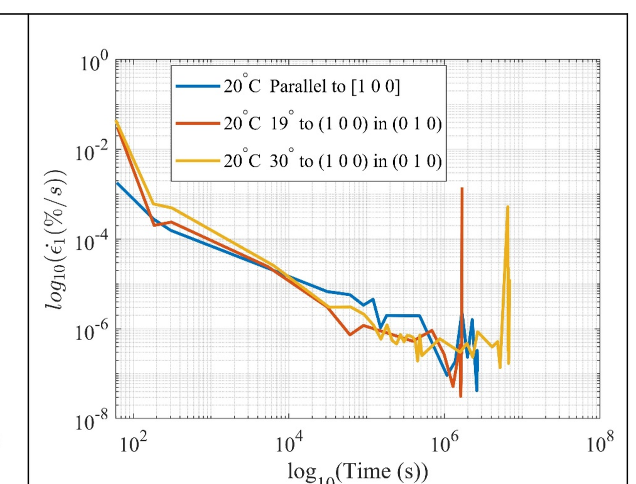
$\dot{\varepsilon} = 1.7\times10^{-4}/s$

Crystals extended parallel to [0 0 1]
Strain rate was kept constant during the experiments

Creep Experiments



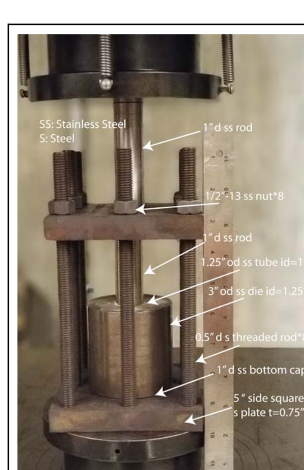
Strain vs. time

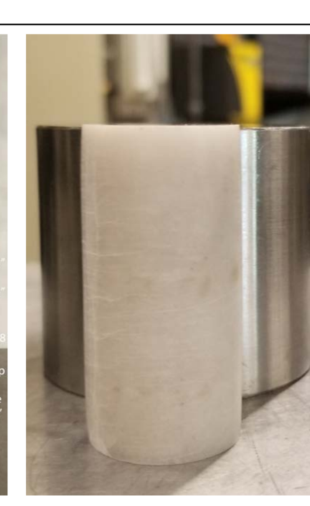


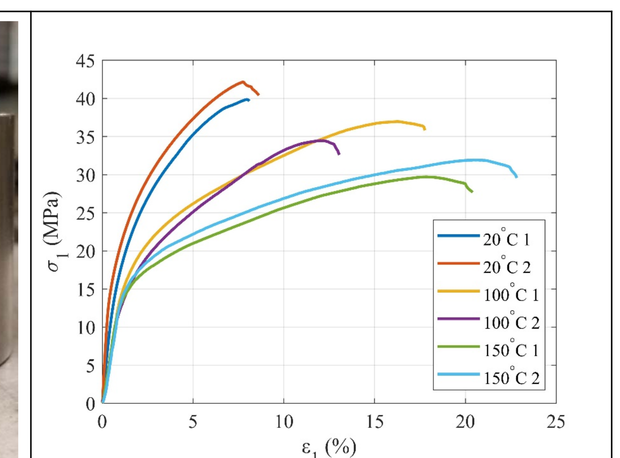
Strain rate vs. time

- Constant deviatoric stress of 13 MPa is applied on the specimens
- Confinement is 0.1 MPa
- Temperature is 20 °C
- Additional tests at higher temperature currently underway

Unconfined Compression of Polycrystalline Specimen







- Made out of dry salt particles smaller than 0.075 mm & salt saturated distilled water
- Pressed at 200 MPa in 3 layers
- Annealed at temperature of 200 °C for 1 week

- T = 20, 100, 150 °C
- $\dot{\varepsilon} = 1.7\times10^{-4}/s$
- Strain rate was kept constant during the experiments

Ongoing Efforts

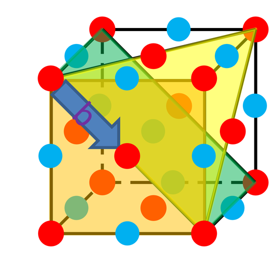
1. Performing tensile fracture tests on single and bi-crystal specimens
2. Calibrating cohesive zone parameters for several distinct failure planes relative to the atomic lattice planes
3. Rigorously compare natural/artificial datasets, experimental/modeling measures of plasticity and fracture anisotropy

Principal Contributions

1. New measurements of high purity natural rocksalt under high temperature and various loading conditions
2. Dislocation density-based crystal plasticity model captures major contributors to halite's anisotropic plastic response
3. Ductility and creep life affected mostly by temperature
4. Orientation of loading impacts mostly yield and ultimate strength

Computational Procedures

Dislocation Slip Systems



Three slip system families with possibly different critical resolved shear stress and hardening rates:

{ 0 0 1 } < 1 -1 0 > (6 systems)
{ 1 1 0 } < 1 -1 0 > (6 systems)
{ 1 1 1 } < 1 -1 0 > (typical 12 FCC systems)

Loading direction	{1 1 0} <1 -1 0>	{1 0 0} <0 1 -1>	{1 1 1} <1 -1 0>
parallel to [0 0 1]	4 with 0.50	6 with 0.00	8 with 0.41
30° to (1 0 0) in (0 -1 1)	4 with 0.07	2 with 0.47, 1 with 0.43	2 with 0.34
45° to [0 0 1] in (0 1 0)	4 with 0.25	4 with 0.35	4 with 0.41

Dislocation Creep Model

Dislocation density based creep model, *T* and $\dot{\varepsilon}$ sensitive: Ma, Roters, Raabe. (2006)

Model is modified from pure aluminum; deformation mechanisms expected to fall between glide, power-law creep, and diffusional creep

Shear strain rate:

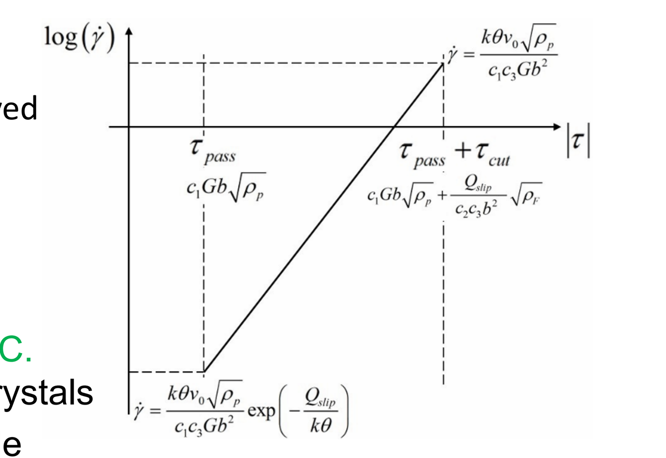
$$\dot{\gamma}^\alpha = \begin{cases} \dot{\gamma}_0^\alpha \exp\left[-\frac{Q_{\mathrm{slip}}}{k_B\theta}\left(1-\frac{|\tau^\alpha|-\tau^\alpha_{\mathrm{pass}}}{\tau^\alpha_{\mathrm{cut}}}\right)\right]\mathrm{sign}(\tau^\alpha), & |\tau^\alpha| > \tau^\alpha_{\mathrm{pass}}, \\ 0, & |\tau^\alpha| \leqslant \tau^\alpha_{\mathrm{pass}} \end{cases}$$

Hardening:

$$\dot{\rho}^\alpha_{\mathrm{SSD}} = c_4\sqrt{\rho^\alpha_F}\dot{\gamma}^\alpha + c_6 d^\alpha_{\mathrm{dipole}}\rho^\alpha_M\dot{\gamma}^\alpha - c_5\rho^\alpha_{\mathrm{SSD}}\dot{\gamma}^\alpha - c_7\exp\left(-\frac{Q_{\mathrm{bulk}}}{k_B\theta}\right)\frac{|\tau^\alpha|}{k_B\theta}(\rho^\alpha_{\mathrm{SSD}})^2\dot{\gamma}^{c_8}$$

Calibration Procedure:

(1) extract shear strain rate and resolved shear stress from experiment;
(2) estimate dislocation density;
(3) linear curve fit;
(4) moderate adjust.



Target dataset: (N. L. Carter and H. C. Heard, 1970), artificial melt-grown crystals

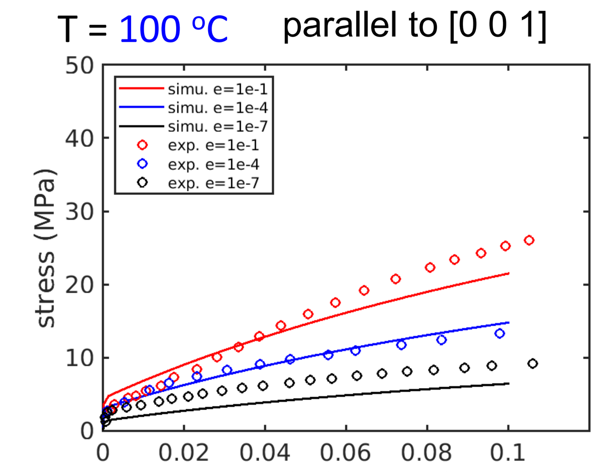
Chosen for calibration purposes while awaiting high temperature results, and to compare versus natural rocksalt

	{ 0 0 1 } < 1 -1 0 >	{ 1 1 0 } < 1 -1 0 >	{ 1 1 1 } < 1 -1 0 >
c_1	0.20	0.20	0.20
c_2	0.07	0.05	0.05
c_3	0.07	0.06	0.06
c_4	0.0025	0.0270	0.0155
c_5	20.0	200.0	135.0
Q_{slip}	2.6×10^{-19}	2.6×10^{-19}	2.6×10^{-19}

Computational Results

Strain Rate Effect

T = 100 °C parallel to [0 0 1]



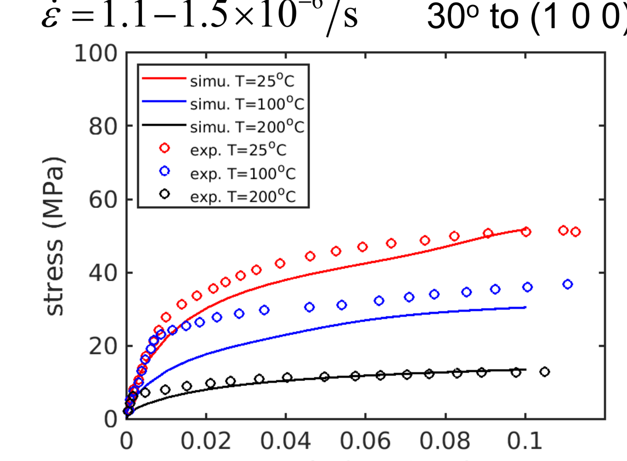
$\dot{\varepsilon} = 1.1-1.4\times10^{-1}/s$

$\dot{\varepsilon} = 1.1-1.5\times10^{-4}/s$

$\dot{\varepsilon} = 1.1-1.5\times10^{-7}/s$

Temperature Effect

$\dot{\varepsilon} = 1.1-1.5\times10^{-6}/s$ 30° to (1 0 0)



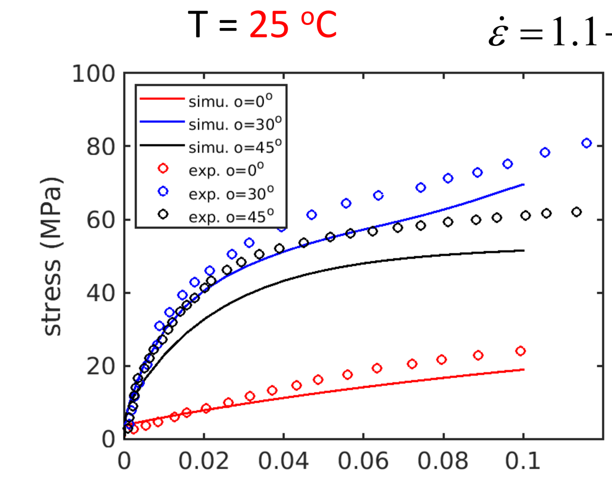
T = 25 °C, 100 °C, 200 °C

Observation: { 1 1 0 } < 1 -1 0 > exhibits most plastic anisotropy; rate sensitivity is lower compared to temperature

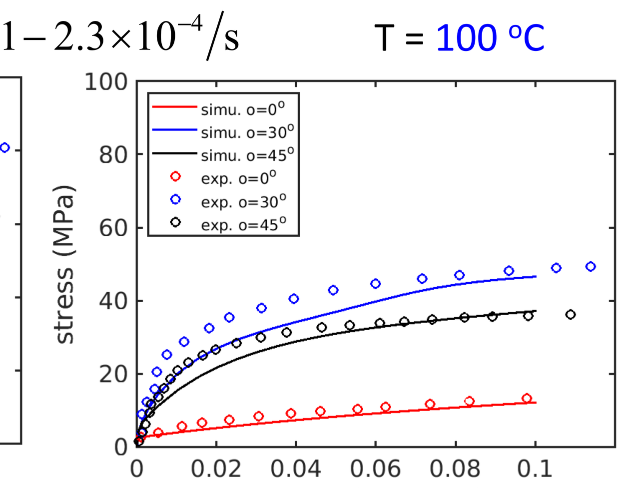
Orientation Effect

$\dot{\varepsilon} = 1.1-2.3\times10^{-4}/s$

T = 25 °C



T = 100 °C

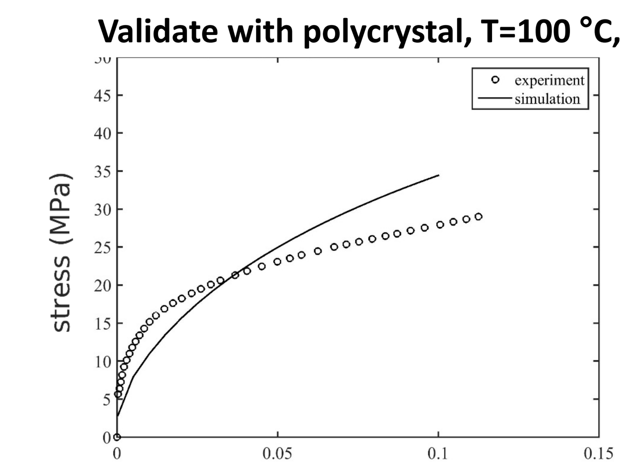


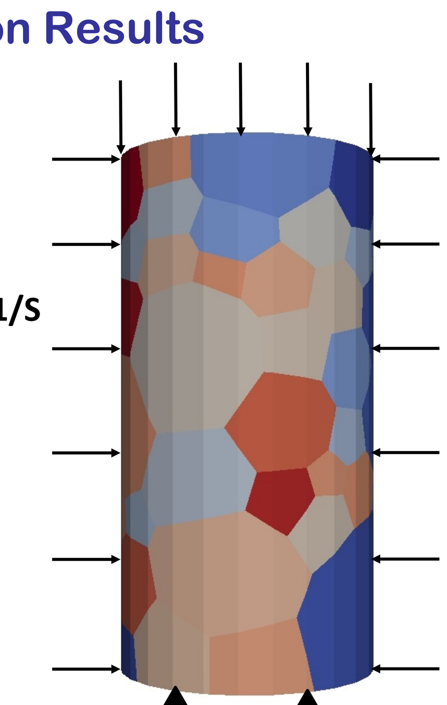
Polycrystalline Simulation Results

Avery Island Mine

- NaCl content: 99 %.
- Grain size: 2.5 to 15 mm
- Grains shape: polygonized
- Average subgrain size: 0.17 mm
- Free-dislocation density is 10^6 to 10^7 cm^{-2}

Validate with polycrystal, T=100 °C, rate=1e-4 1/S





Handin, J., et al. (2013). Experimental Deformation of Rocksalt. Mineral and Rock Deformation: Laboratory Studies: The Paterson Volume, American Geophysical Union: 117-160.

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