Opportunities for Better Understanding the Mechanical Behaviors of Polycrystalline Solids

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Support from:

DEPARTMENT OF THE NAVY ONR Science & Technology

AIR FORCE OFFICE OF SCIENTIFIC RESEARCH UNITED STATES AIR FORCE

Background and Interests

Interests:

- Mechanical performance of engineering alloys
- Microstructure/Property relations -- especially, stiffness and strength
- Plasticity -- including state evolution (texture and dislocation structure)
- Fatigue -- changes over cyclic loading
- Material systems: airframe aluminum alloys, stainless steel alloys, titanium alloys

Approach:

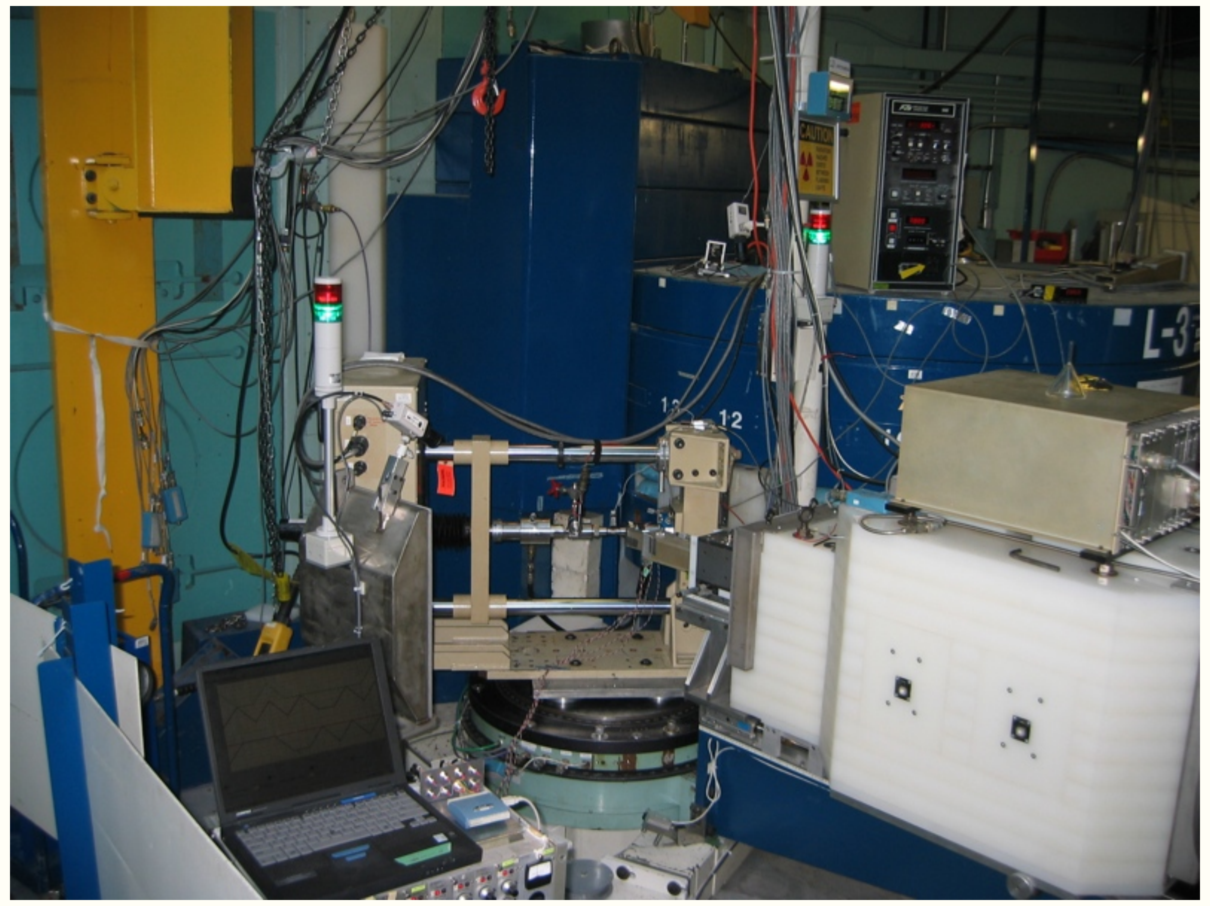
- Coordinated use of numerical simulations and in situ diffraction experiments
- Numerical simulations performed using in-house finite element code developed for this purpose
- Experiments performed with both neutron and x-ray sources

Experiments:

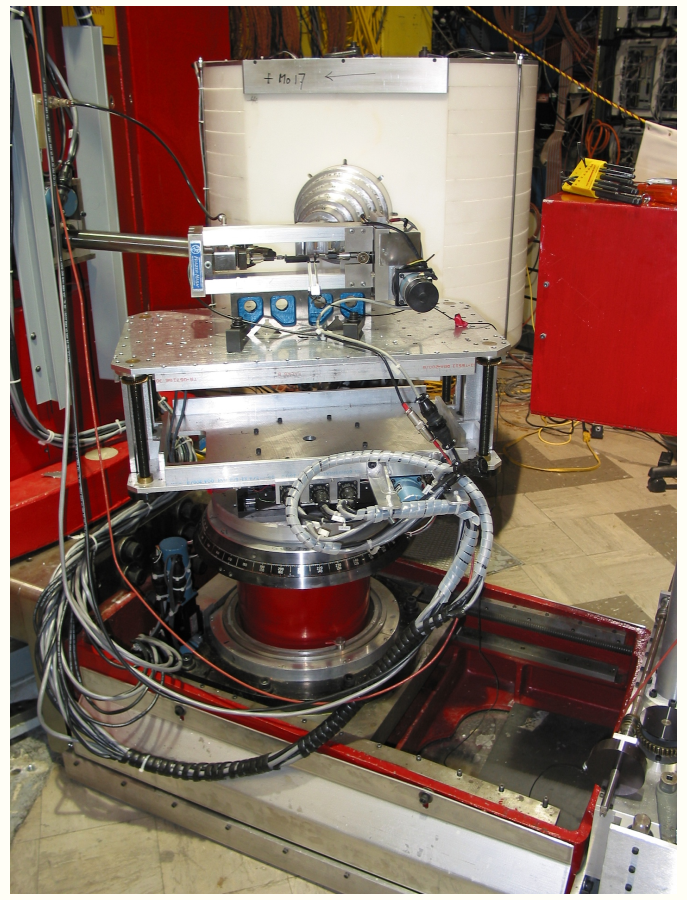
- Monochromatic neutron: Chalk River (Ron Rogge and Mike Gharghouri) and NIST (Thomas Gnaupel-Herold)

and in collaboration with Matt Miller (Cornell):

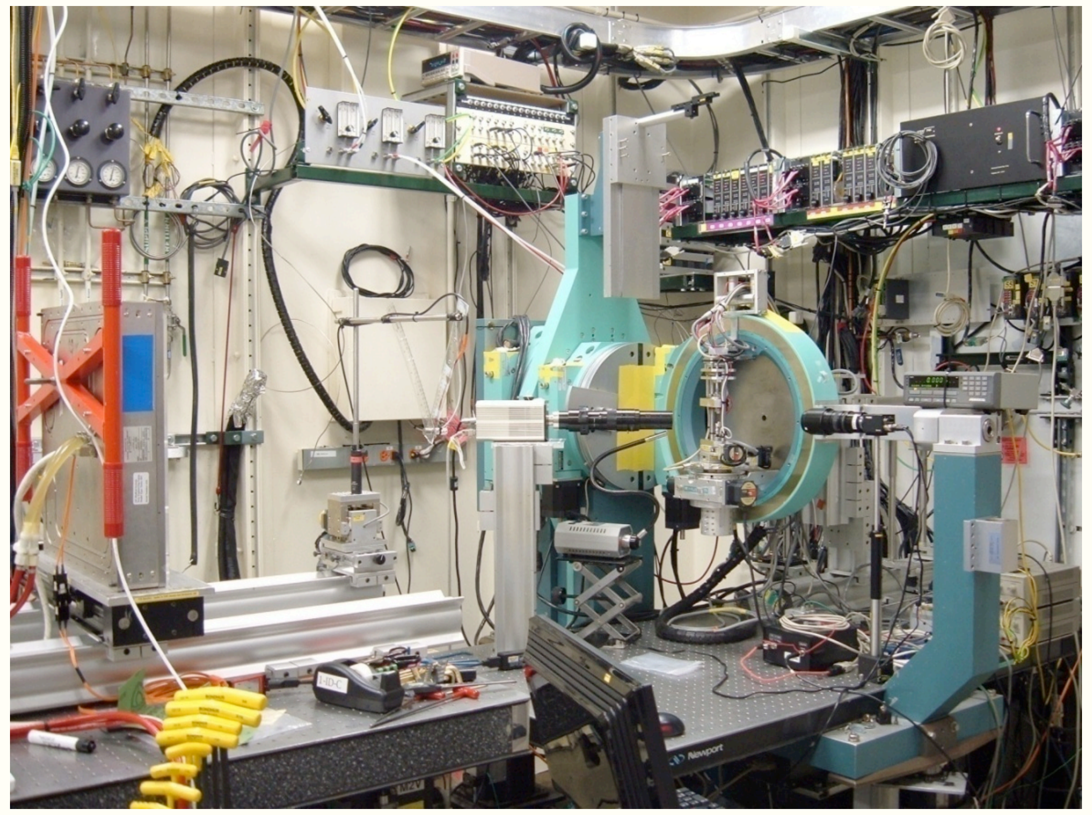
- Time-of-flight neutron: LANSE (Don Brown)
- Monochromatic x-ray: CHESS (Alex Kazimirov) and APS (Ulrich Lienert)
- Polychromatic x-ray: ALS (Martin Kunz)



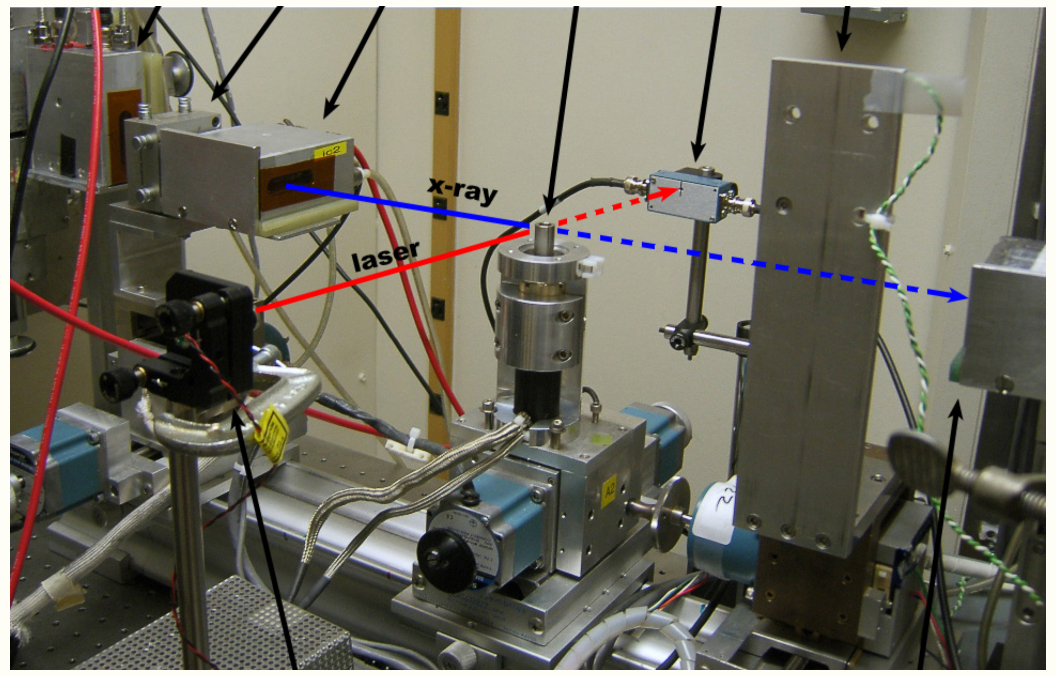
Chalk River



NIST

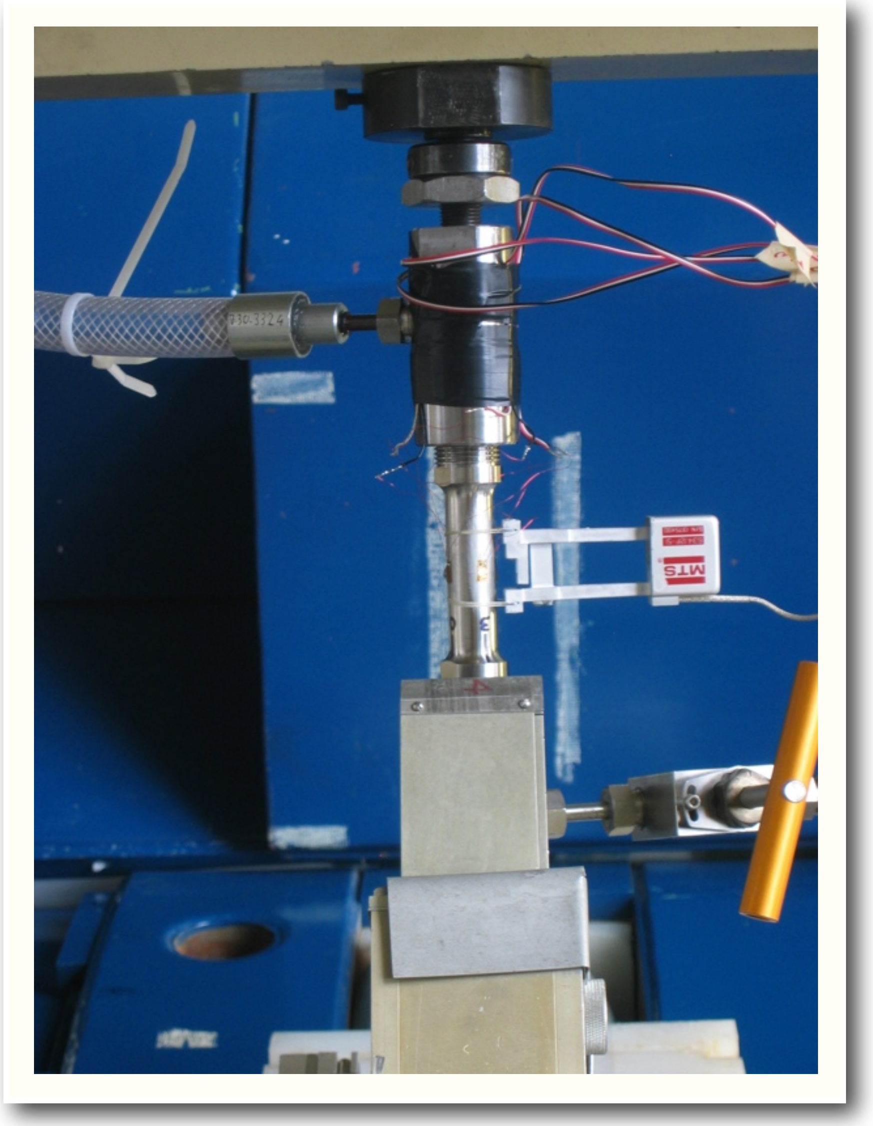


APS



CHESS

Crystal Stress Distributions and Experimental Observations

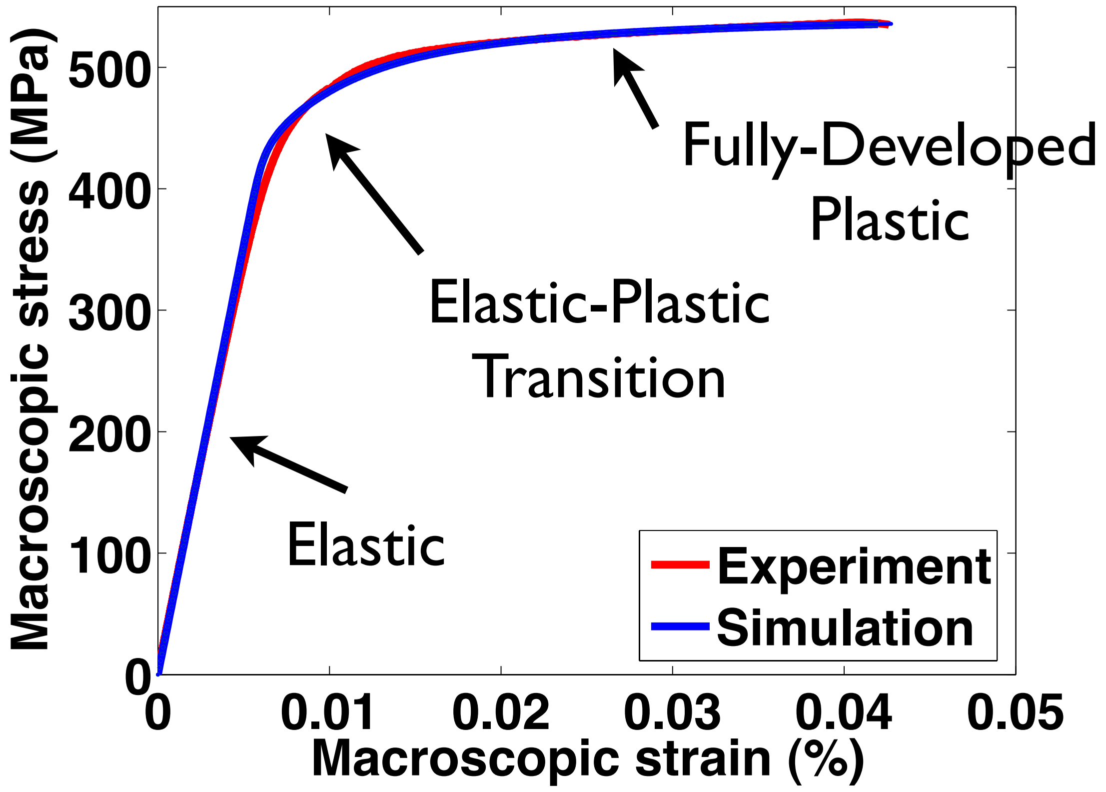


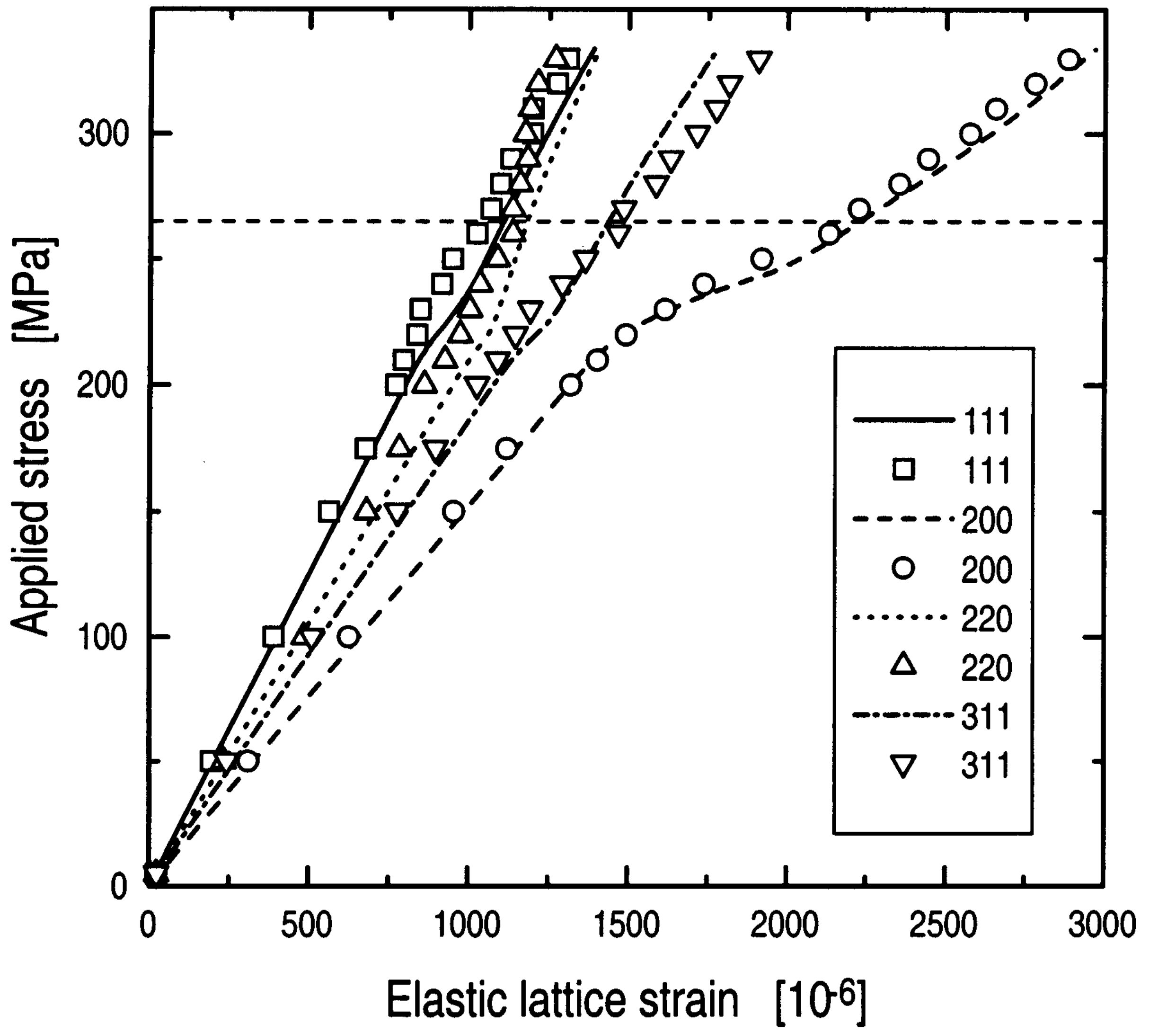
Focus on crystal stresses:

- Stress drives mechanical responses: deformation, damage, failure
- Quantifying the crystal stresses is central to making the connection between microstructure and properties
- Exploit neutron and x-ray diffraction because they offer the means to observe the behaviors at the scale of crystals

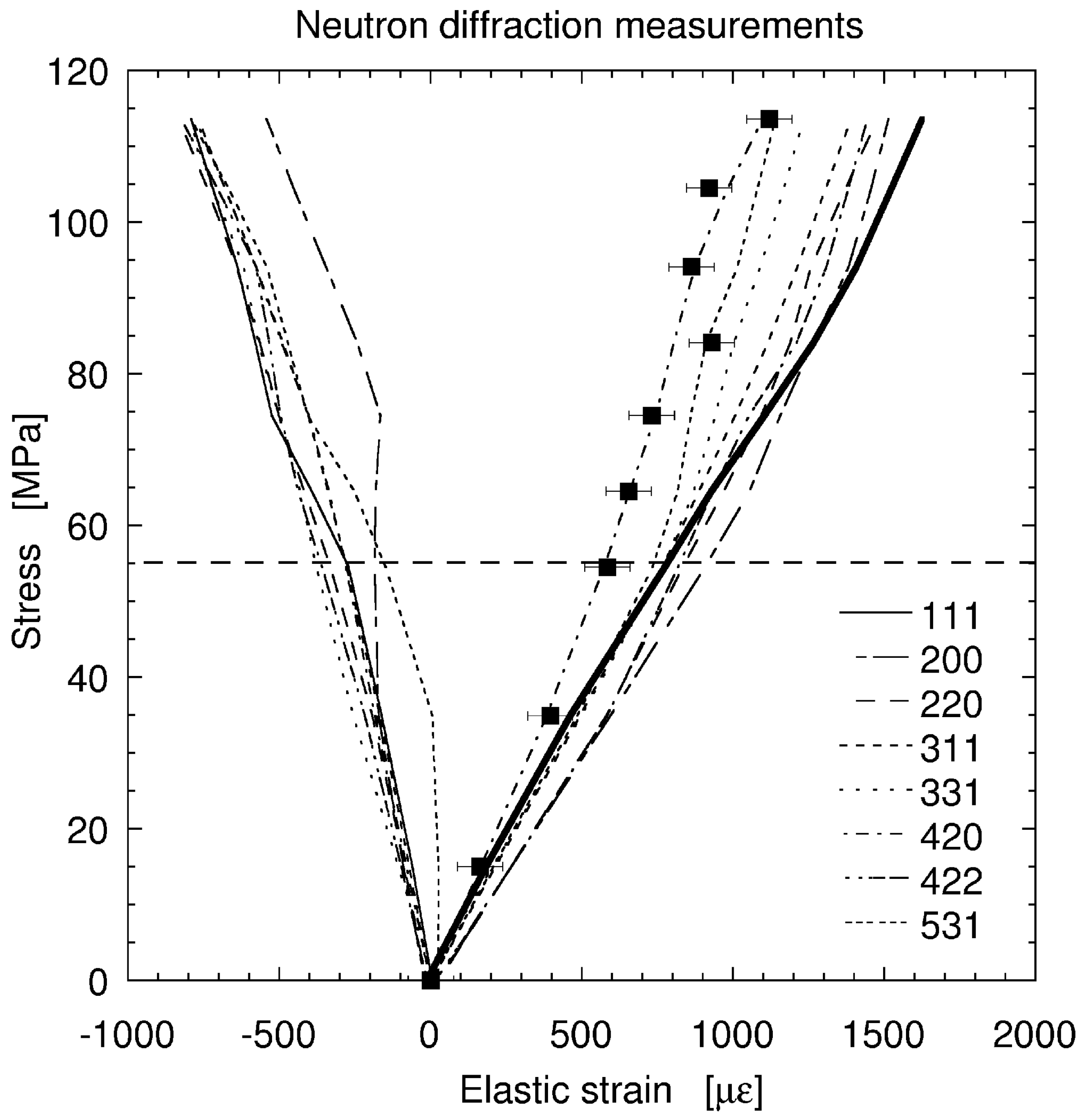
Diffraction measurements:

- Measure lattice orientations and lattice distortions
- Depending on the instrument and experiment, measurements might represent a single value or distribution of values related to distortions
- But …
  - ➛ stress is not observed directly
  - ➛ to determine the stress a model must be invoked
- Recognize that the stress is evolving over the course of a deformation
  - Elastic Regime
  - Elastoplastic transition
  - Fully developed plastic regime
- Need to consider several factors:
  - Elastic anisotropy
  - Yield surface topology
  - Relative strength-to-stiffness among crystals (and/or phases)





Stainless steel
Clausen, Lorentzen, Bourke and Daymond, MSE-A, 1999



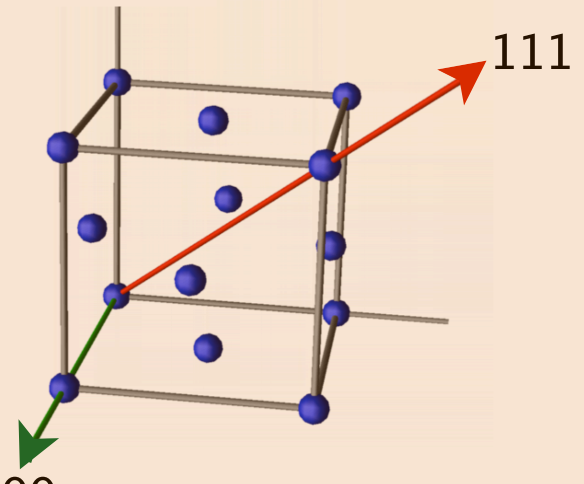
Aluminum alloy
Clausen and Bourke, Met Trans, 2001

Single Crystal Behavior

Elasticity

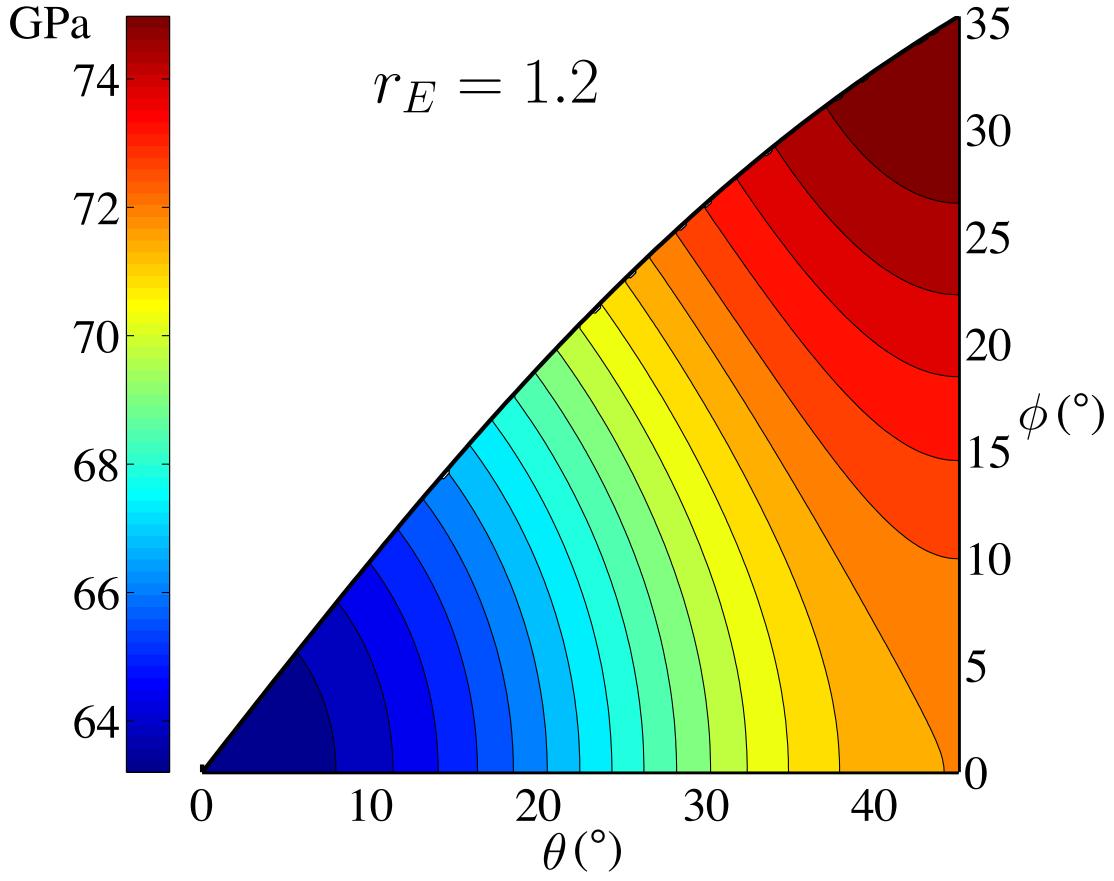
Hooke's Law

$$\boldsymbol{\sigma} = \mathcal{C}\epsilon$$



Face-centered cubic crystal structure

Directional modulus



Elastic anisotropy ratio:

$$r_E = \frac{E_{111}}{E_{100}}$$

Elastic stiffness in 111 direction

Elastic stiffness in 100 direction

Restricted Slip Plasticity

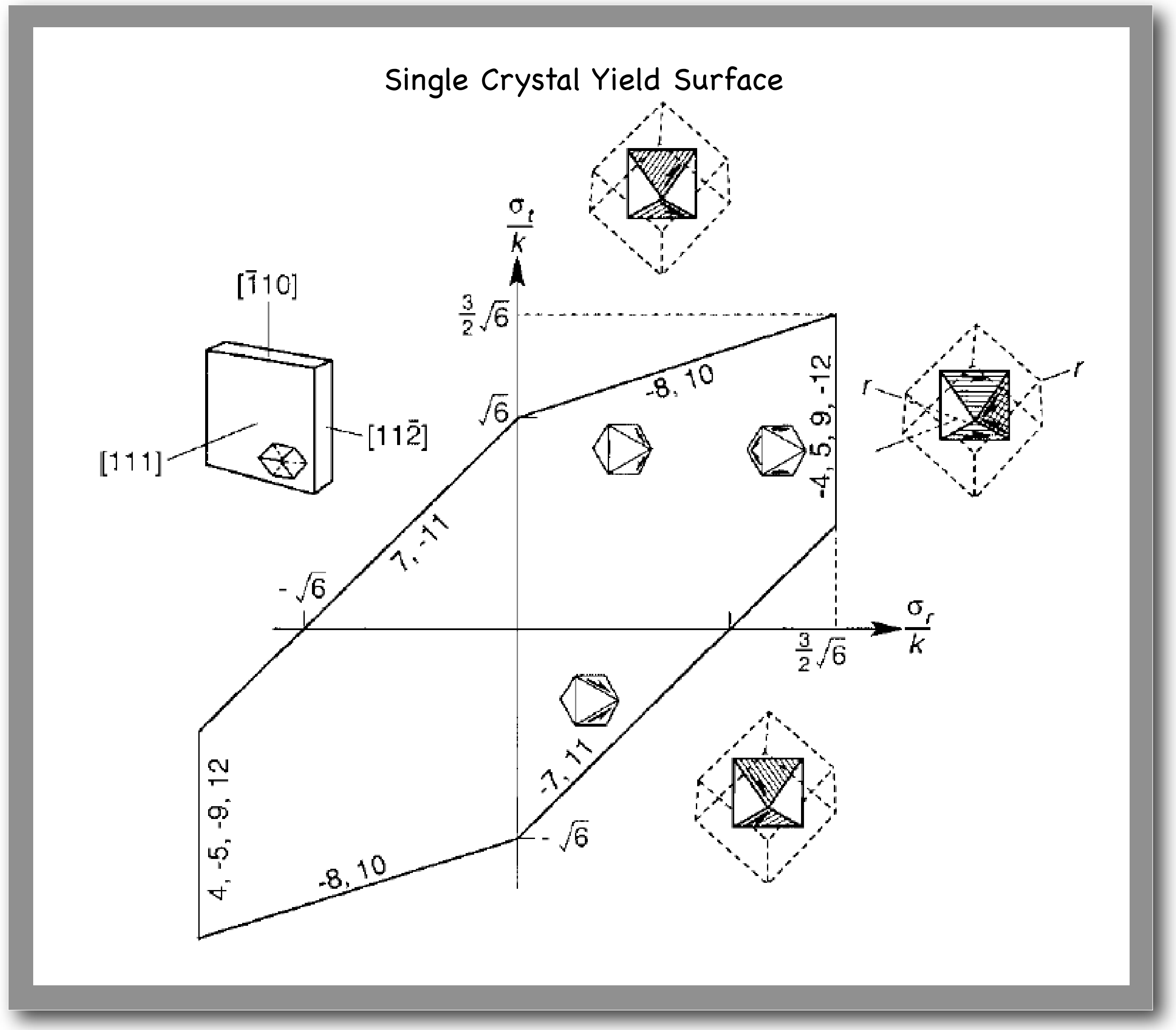
Slip occurs on close-packed planes in close-packed directions

Each slip system defines a plane of the Single Crystal Yield Surface

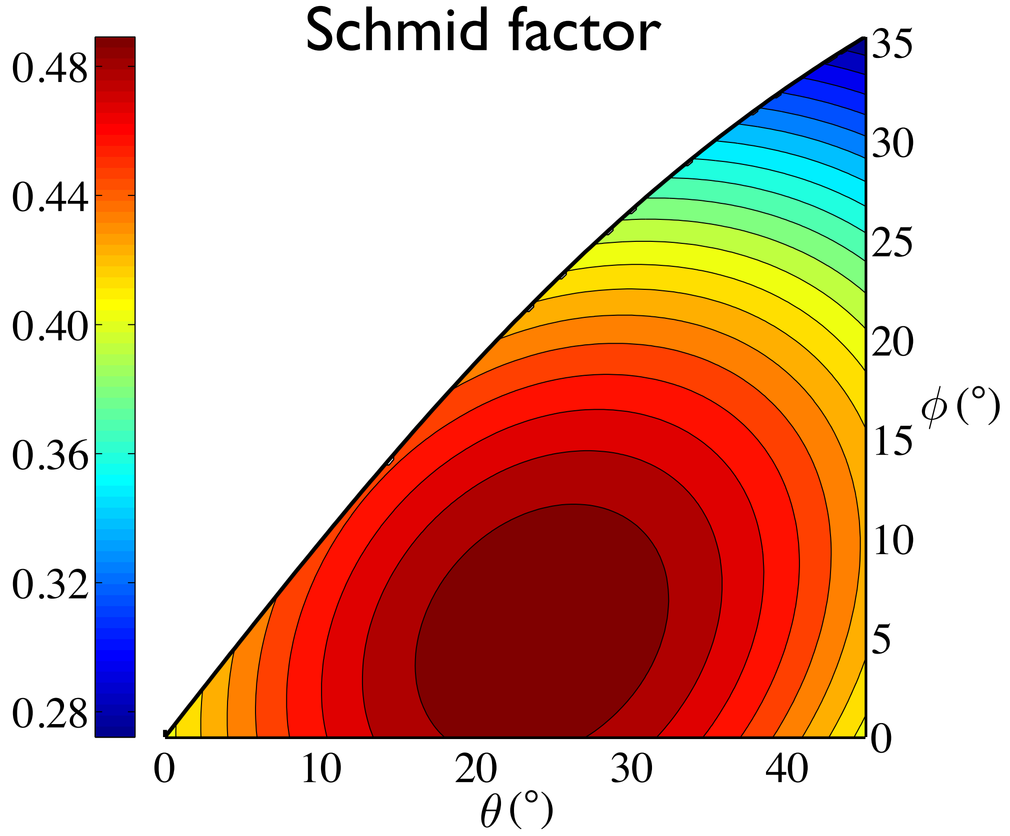
SCYS: inner envelope of planes; intersections: edges and vertices

Polyslip means that: Crystal stress ≈ vertex stress

Backofen, Deformation Processing, 1972

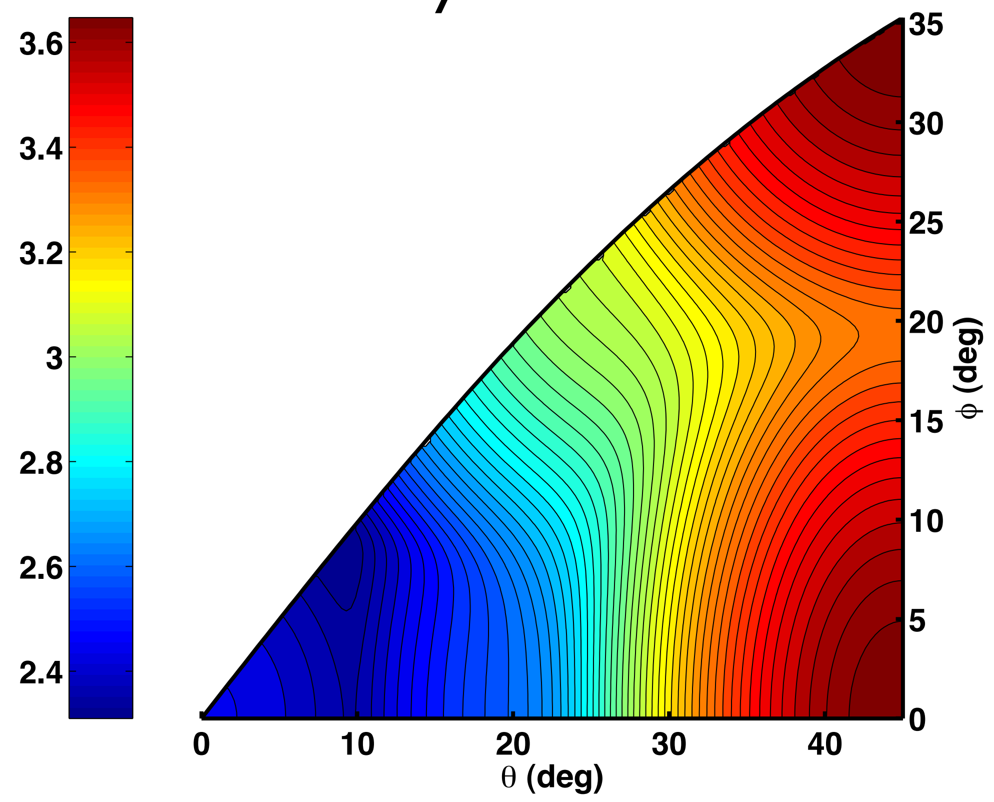


Schmid factor



Ratio of the RSS to the axial stress in tension (single slip)

Taylor factor



Ratio of the axial stress to the RSS to invoke uniaxial extension (polyslip)

The Elastic Regime

Important factors:

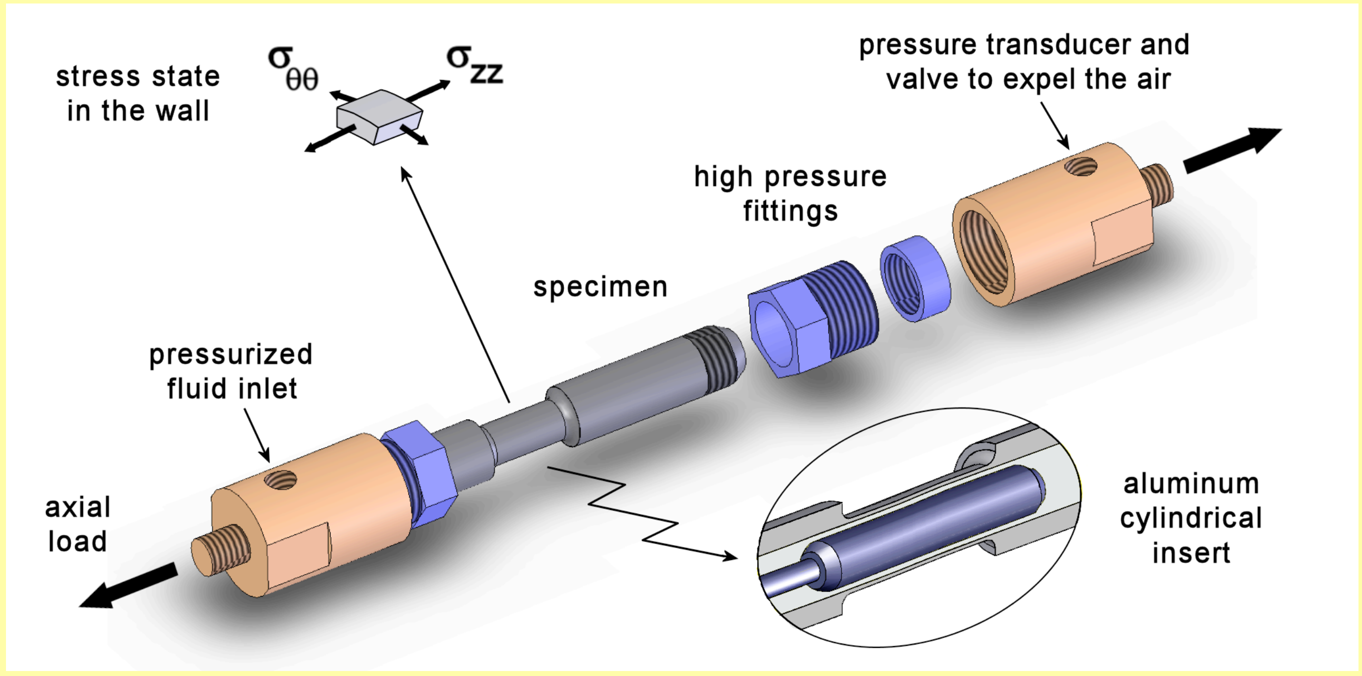
* Level of elastic anisotropy at the crystal level
* Content of the stress

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}' + \sigma_m \boldsymbol{\delta}$$

$$\boldsymbol{\sigma}' = \tilde{\boldsymbol{C}} \boldsymbol{\epsilon}'$$

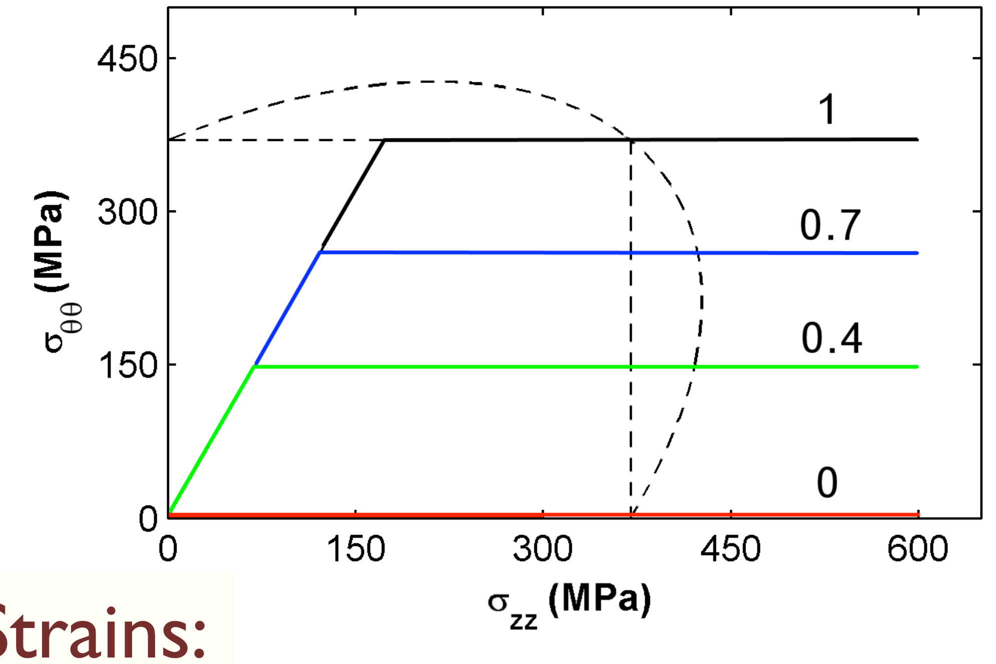
$$\sigma_m = K \epsilon_m$$

Thin Tube Subjected to Internal Pressure plus Axial Load

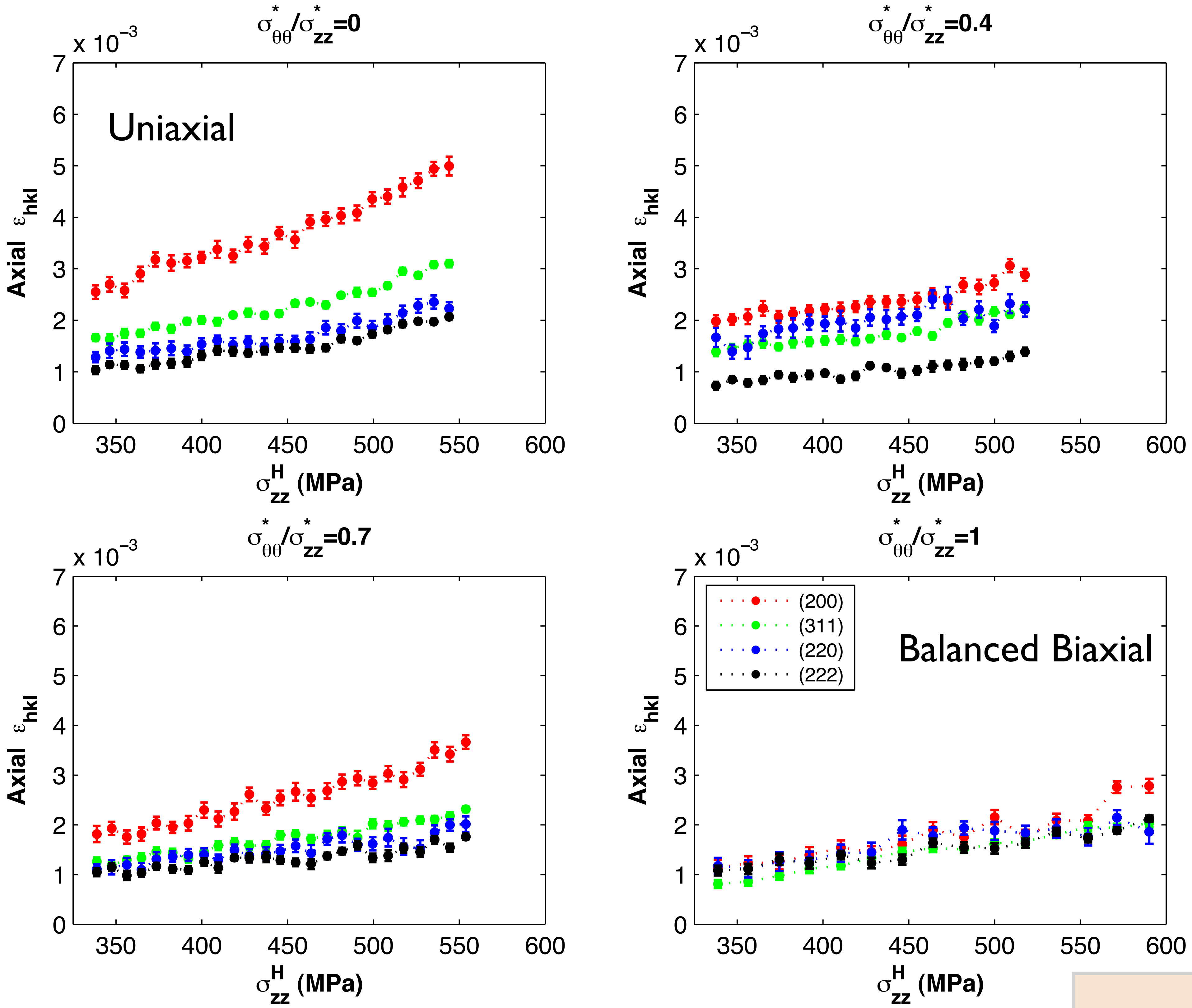


Principal stress directions do not change with level of biaxiality

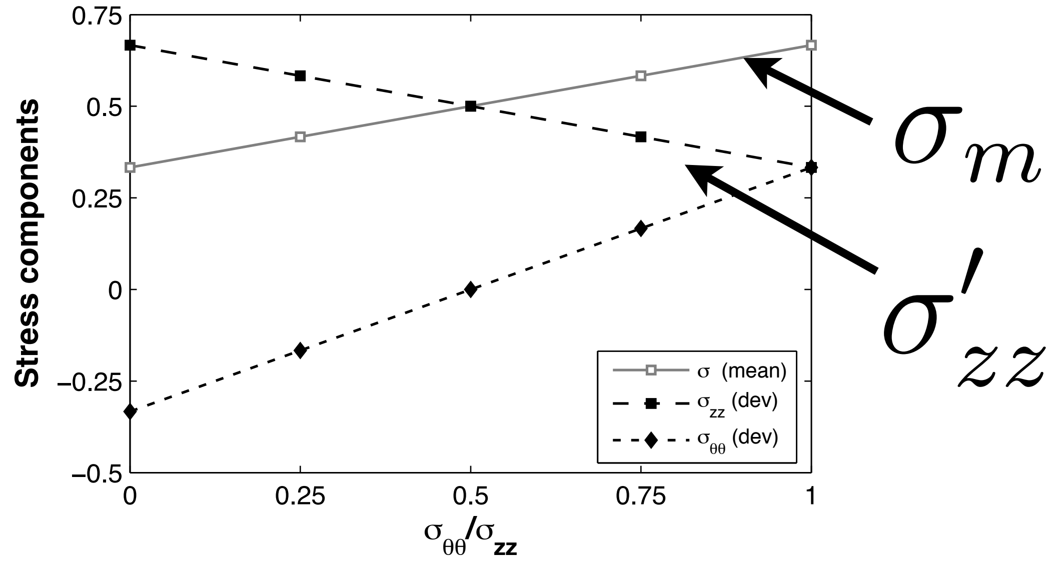
Applied Loading:



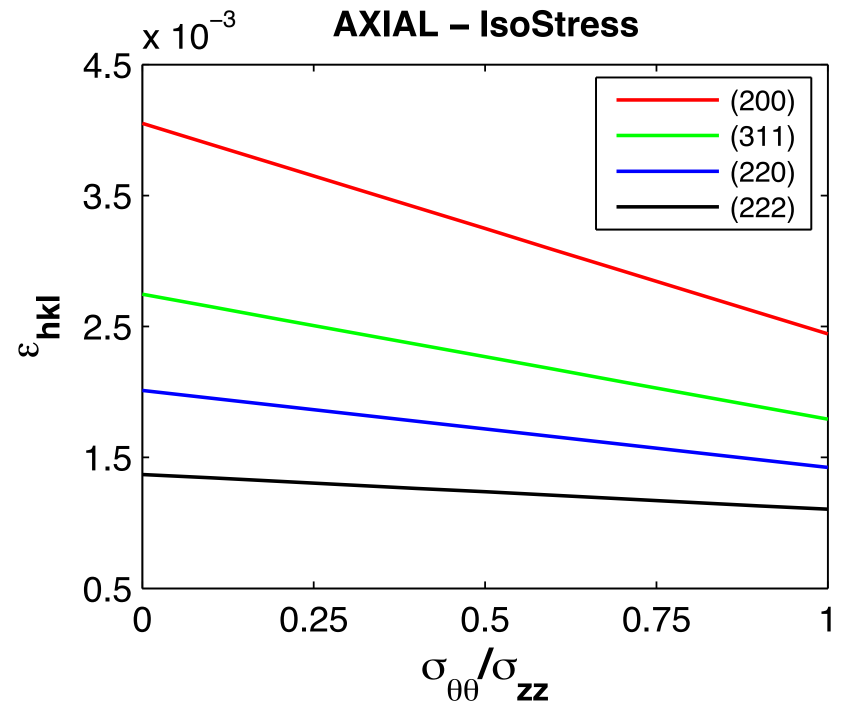
Measured Lattice Strains:

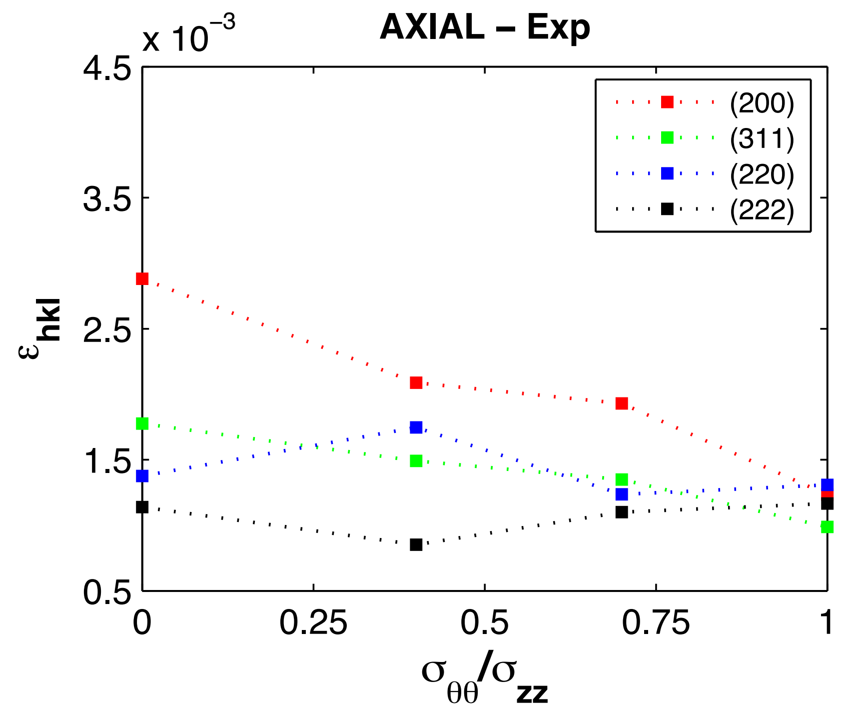


Stress Components:



Uniaxial → Balanced Biaxial



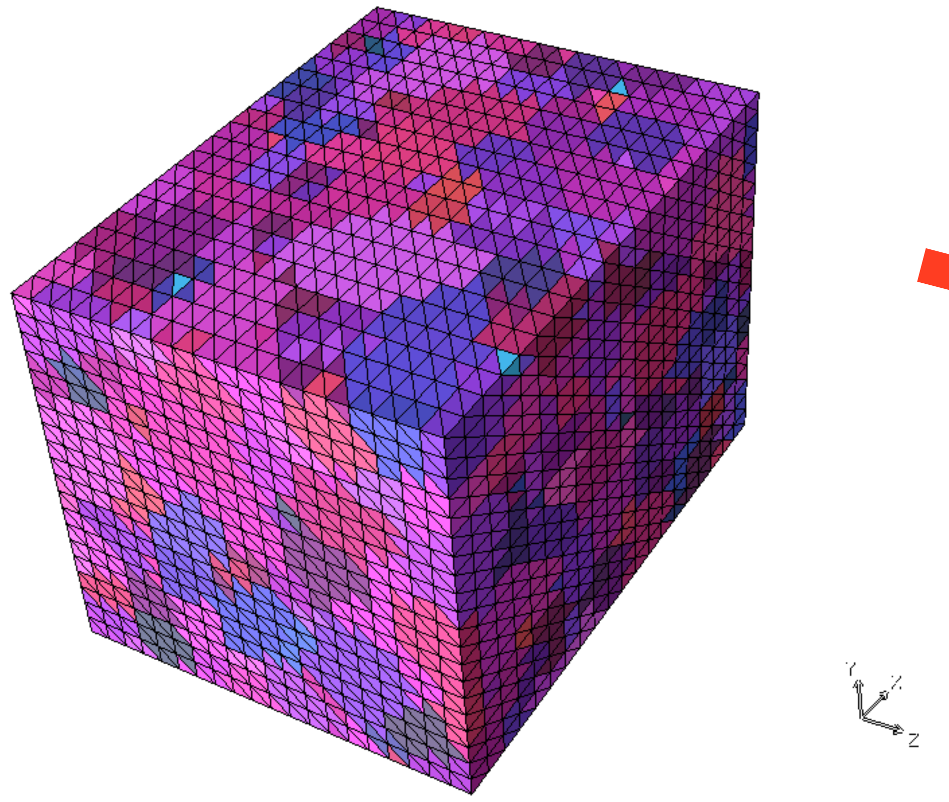


HKL trends in lattice strains:

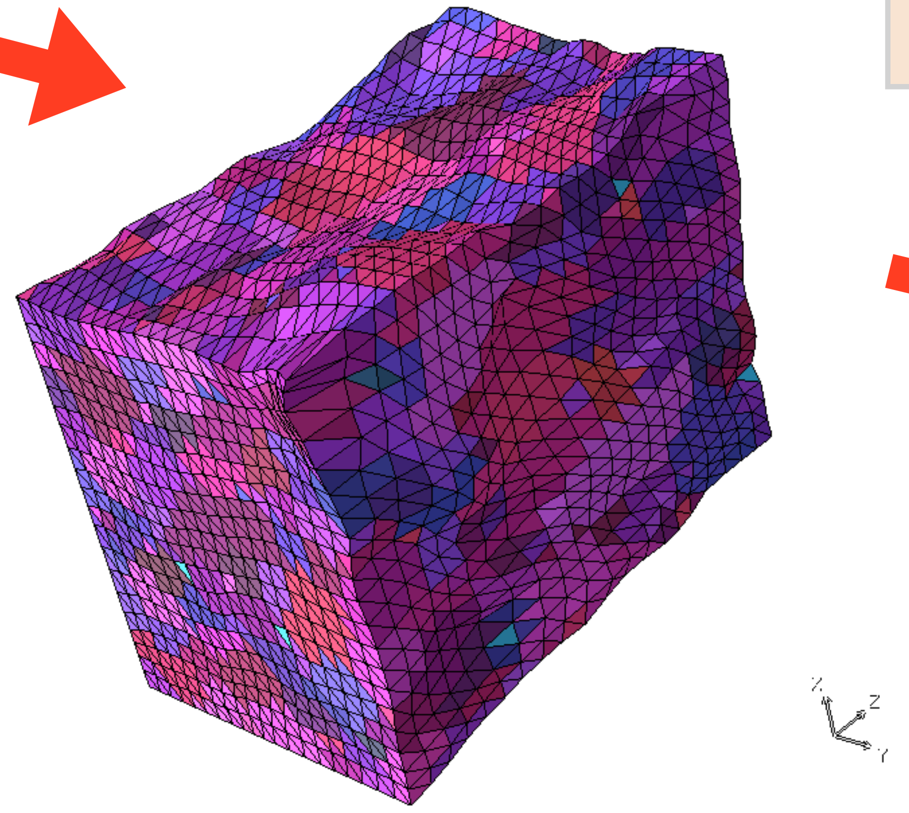
- Greater contrast with stronger elastic anisotropy
- Reduced contrast with higher ratio of $\frac{\sigma_m}{\sigma'}$

See ☞ T. Marin, P. R. Dawson, M. A. Gharghouri, and R. B. Rogge. Diffraction measurements of elastic strains in stainless steel subjected to in situ biaxial loading. Acta Materialia, 56:4183–4199, 2008.

Simulating the Diffraction Experiments

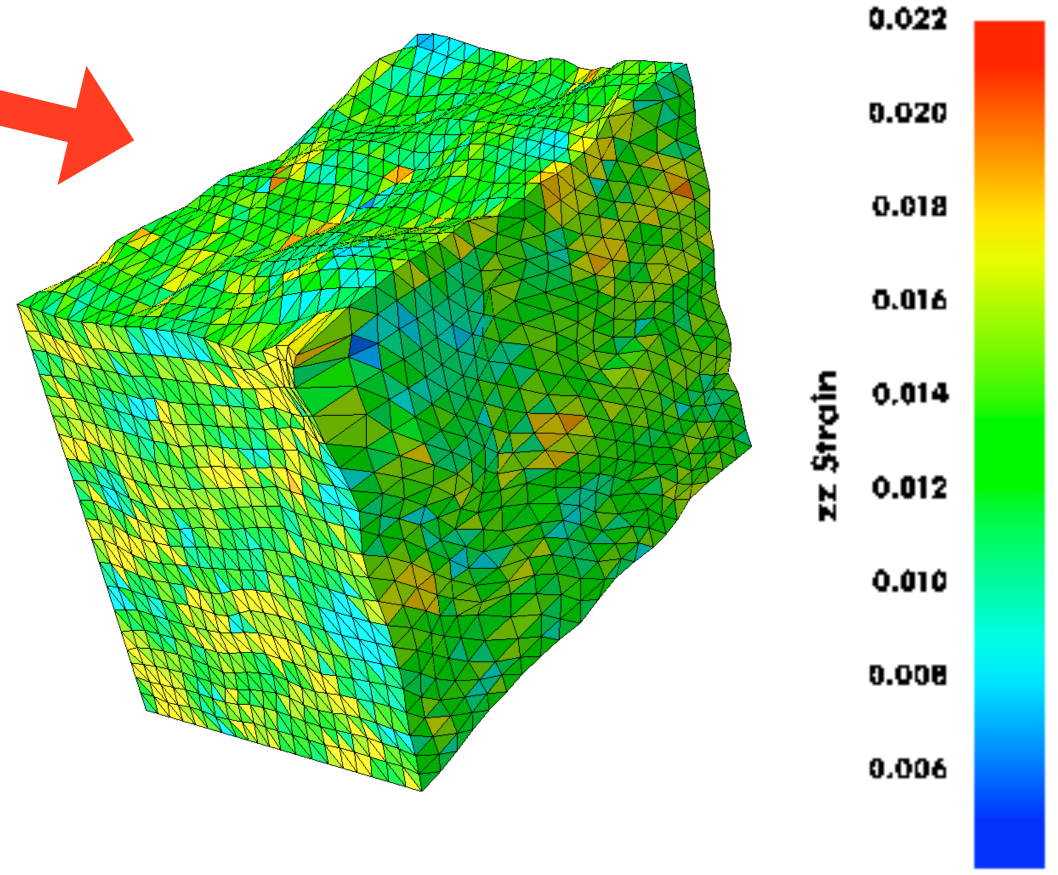


Instantiate Virtual Specimens:
- define domain dimensions
- lay out geometric features
- assign attributes

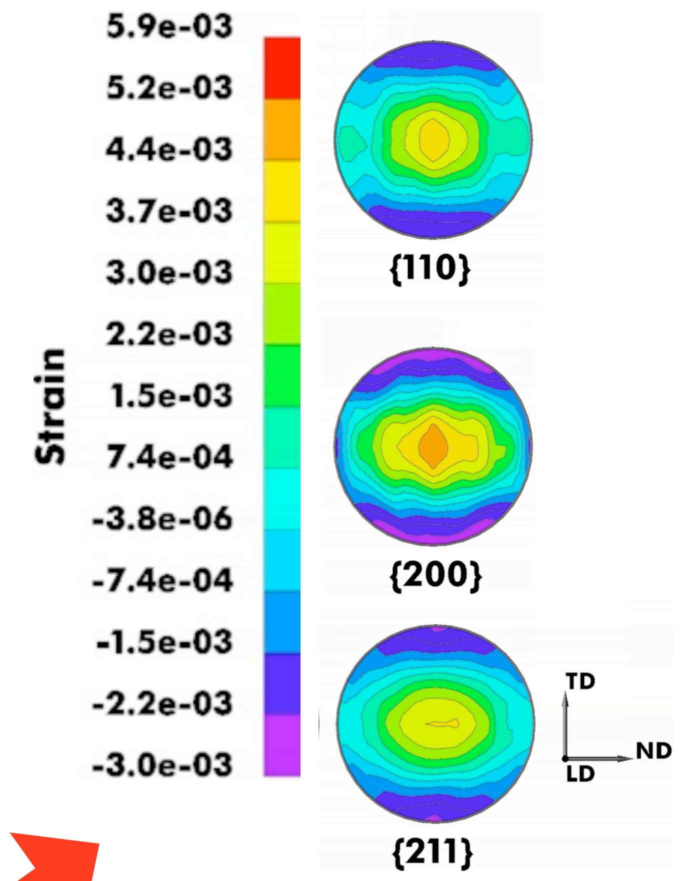


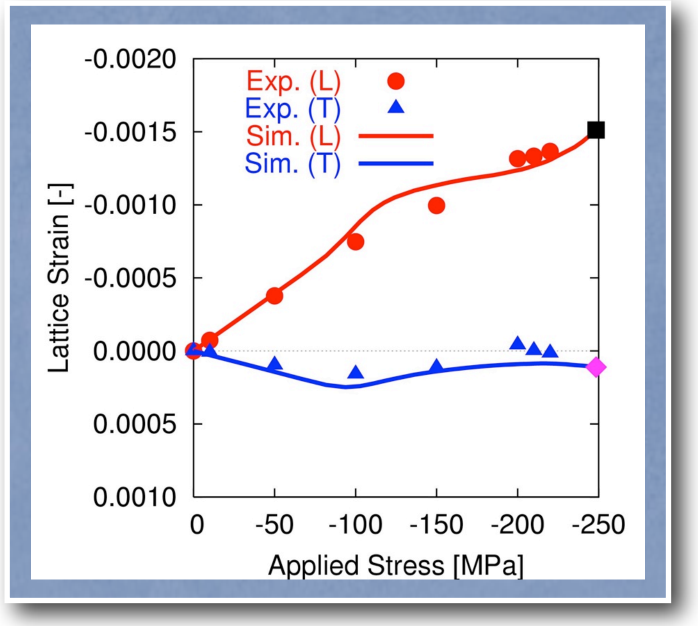
Load Specimens:
- apply boundary conditions
- execute simulations
- record results

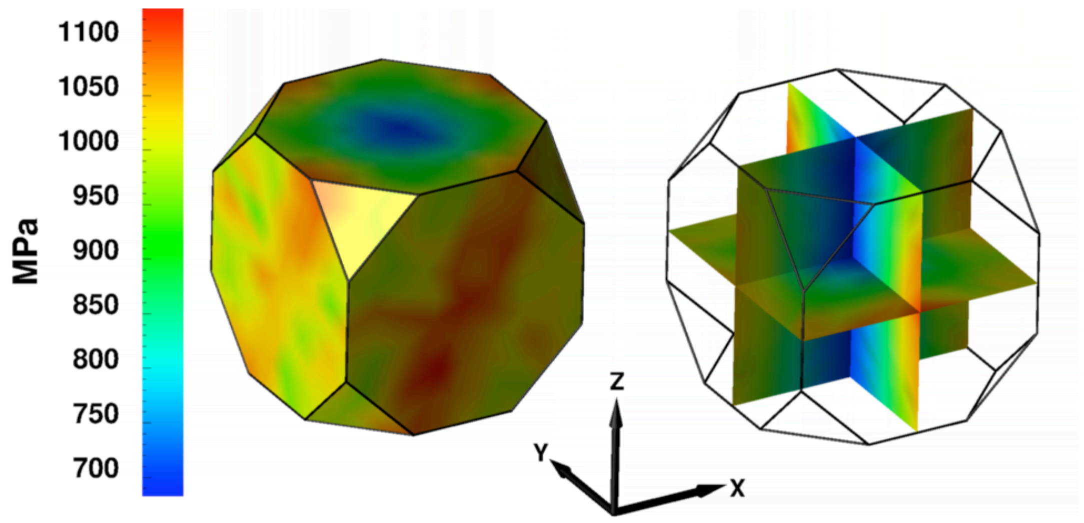
Modeling the Crystals
within the
Diffraction Volume



Monitor Responses:
- invoke digital probes for:
  stress, lattice strain, texture







Abstract Results:
- evaluate properties
- define State-X attributes
- assess fidelity

Draws on microstructural characterization data to initialize specimens

Utilizes large strain, crystal-scale finite element code

- Quasi-static, cyclic or dynamic loading
- Large strain kinematics
- Elastoplastic behaviors of polycrystals
- Plastic deformation by slip and/or twinning
- Anisotropic elasticity

Utilizes post-processing scripts to extract and reduce results

Draws on experimental data for comparisons to mechanical performance and state evolution

See ☞

P. R. Dawson, M. P. Miller, T.-S. Han, and J. Bernier. An accelerated methodology for the evaluation of critical properties in polyphase alloys. Metallurgical and Materials Transactions, 36A:1627–1641, 2005.

D. E. Boyce, P. R. Dawson, and M. P. Miller. The design of a software environment for organizing, sharing and archiving materials data. Materials Science and Engineering A, 40:2301–2318, 2009.

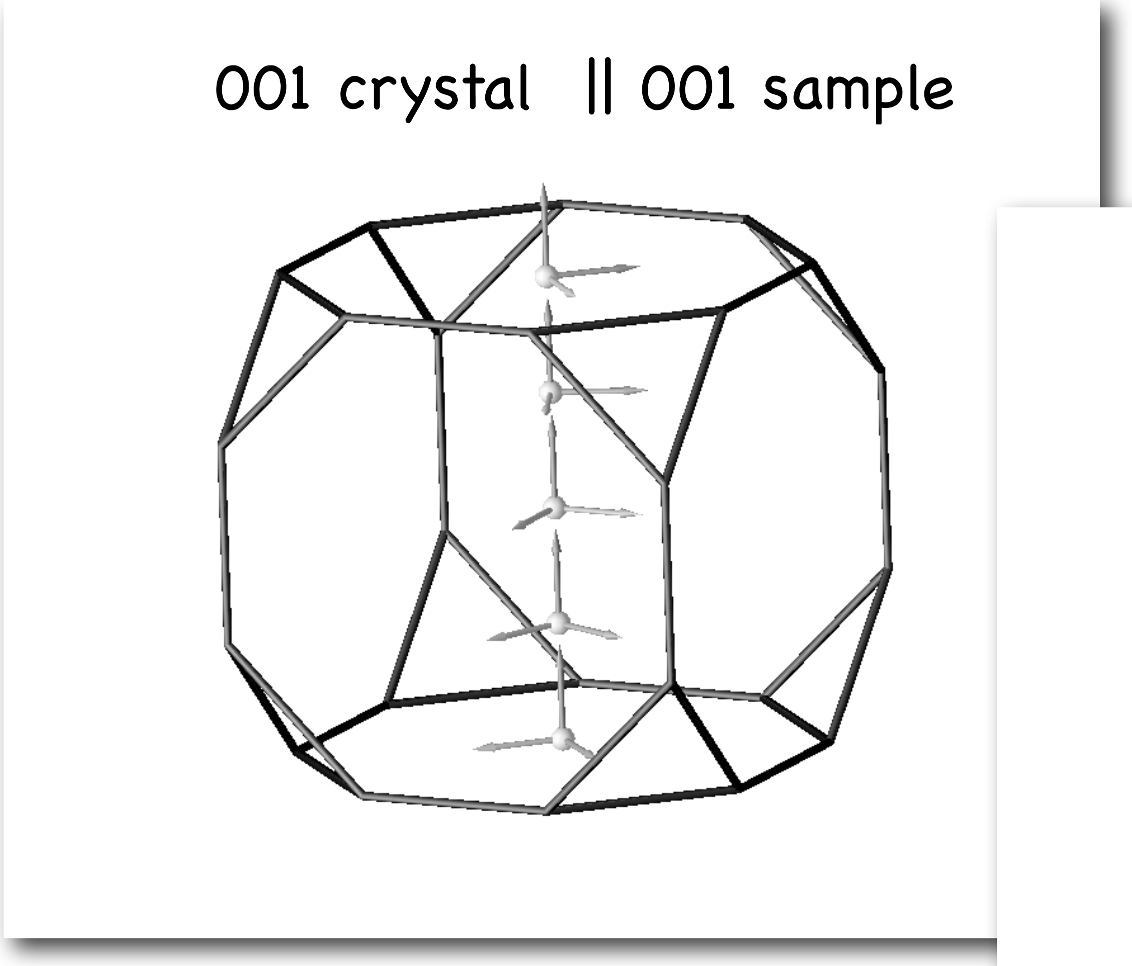
Orientations and Fibers

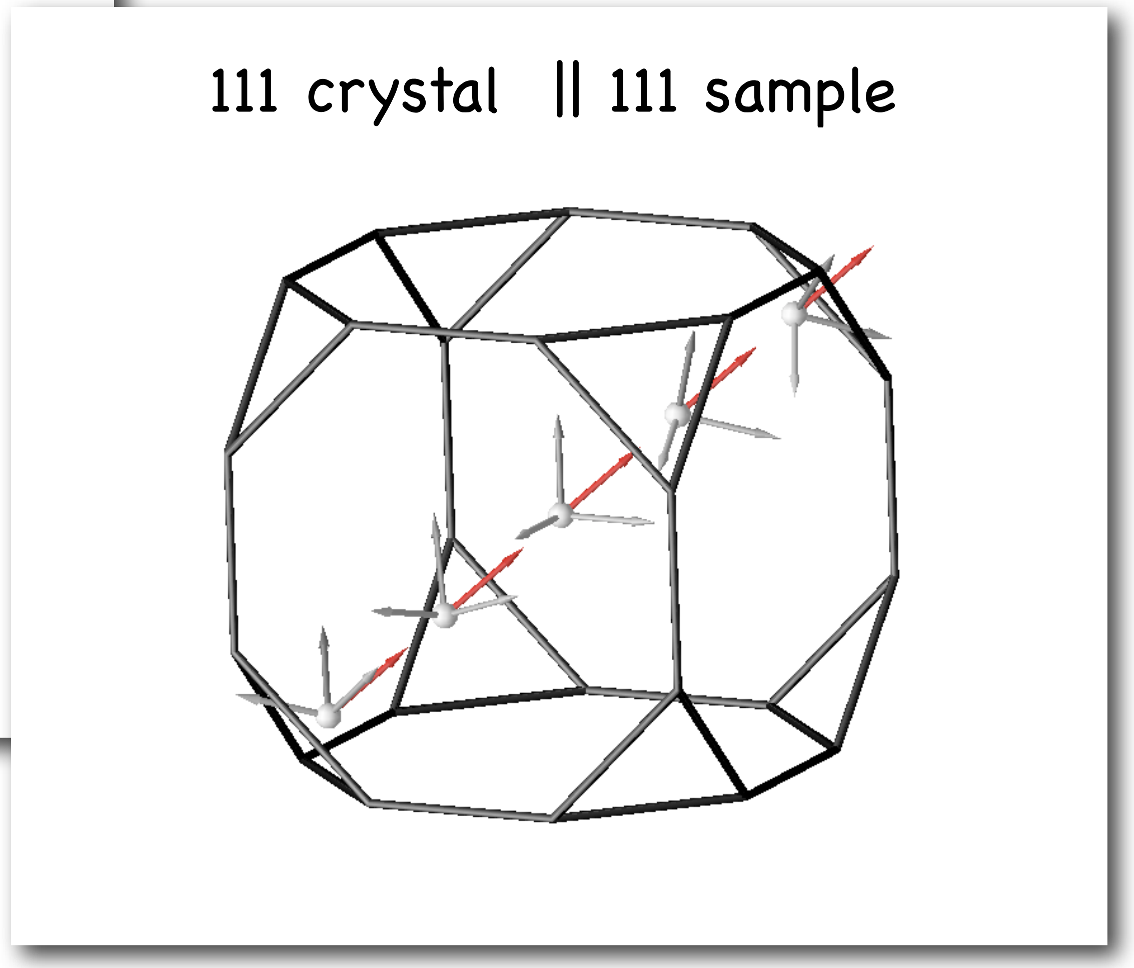
Rodrigues vector

- Crystal orientation prescribed by $\boldsymbol{r} = \boldsymbol{n} \tan \frac{\phi}{2}$
- Fundamental region defined by symmetries

Crystallographic fibers

- Fibers are straight lines connecting orientations that differ by rotation about one axis





See ☞

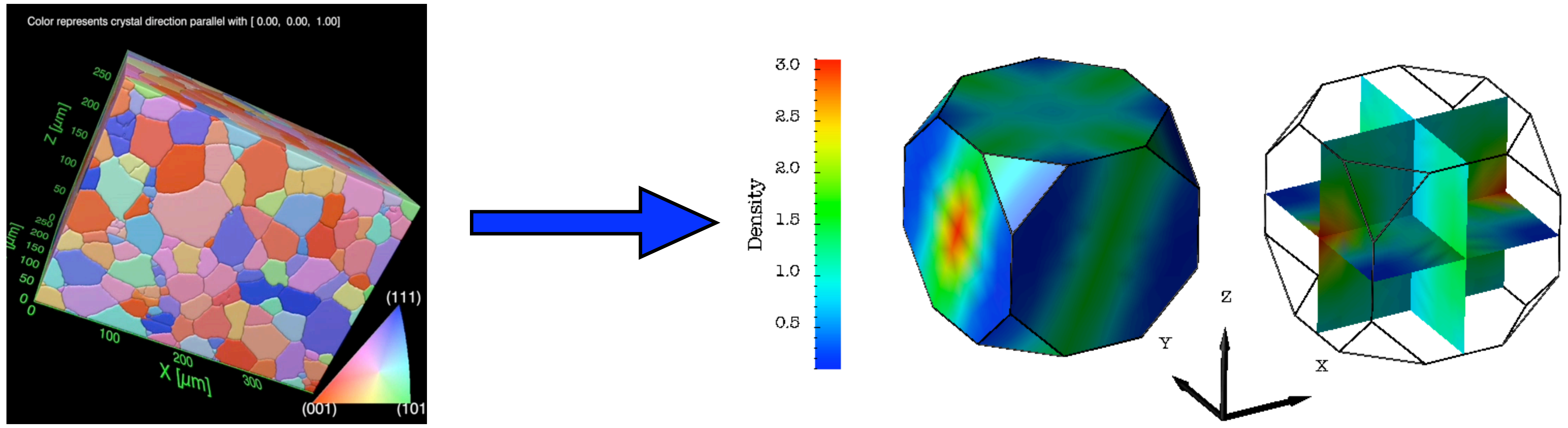
A. Kumar and P. R. Dawson. Computational modeling of FCC deformation textures over Rodrigues space. Acta Materialia, 48:2719–2736, 2000.

N. R. Barton, D. E. Boyce, and P. R. Dawson. Pole figure inversion using finite elements over Rodrigues space. Textures and Microstructures, 35(2):113–144, 2002.

Orientation-dependent distributions

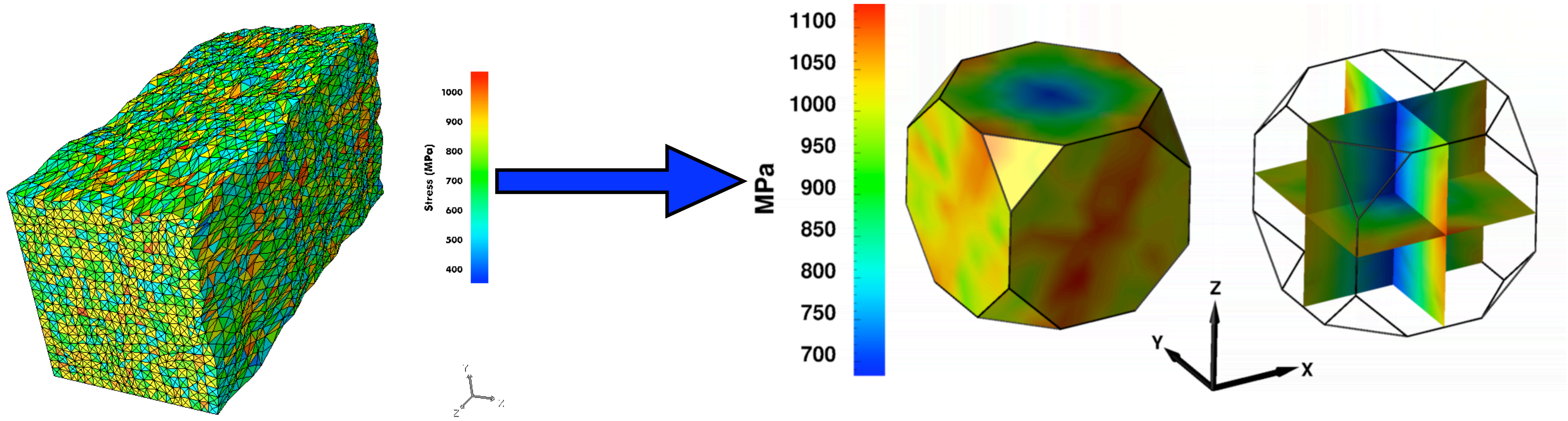
- Plot various quantities over fundamental region
- Shows how that quantity depends on orientation of the crystal lattice

Crystallographic texture:



β21S lattice orientations from serial section (NRL)

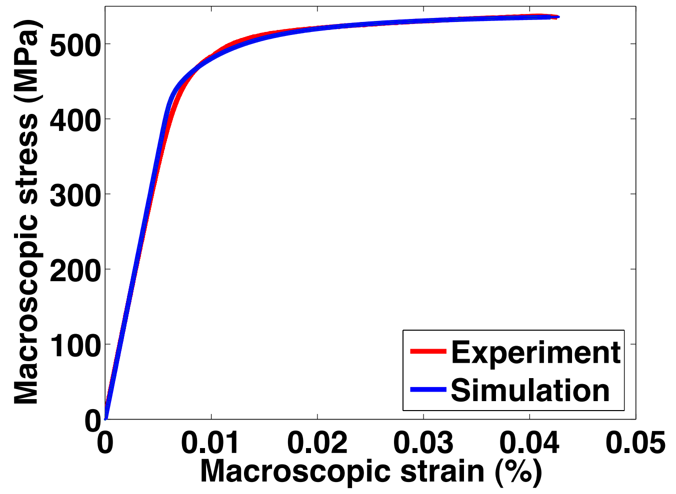
Crystal stresses:



Crystal stresses from FEM/PX Simulation

Cornell University

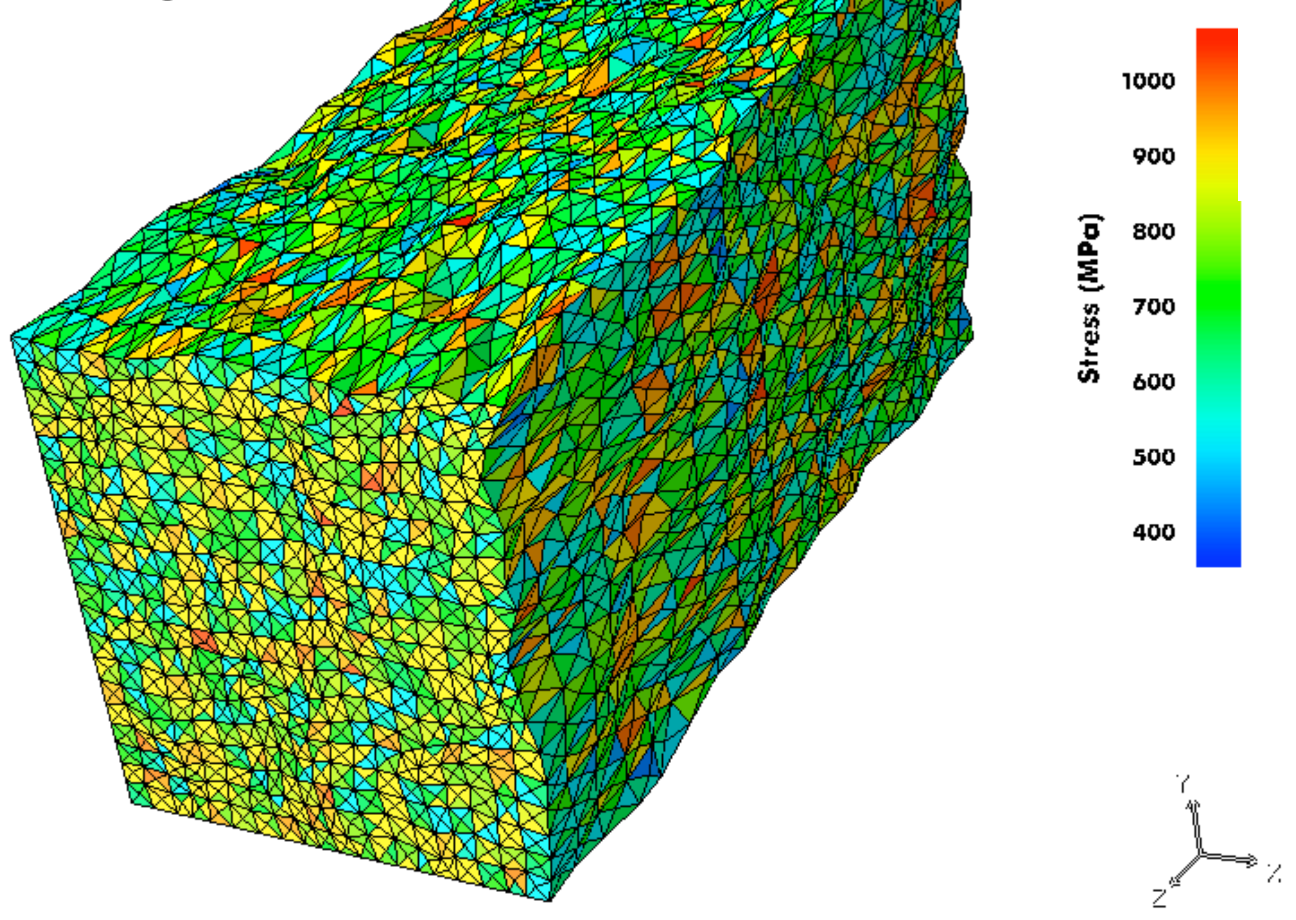
Fully-Developed Plastic Flow



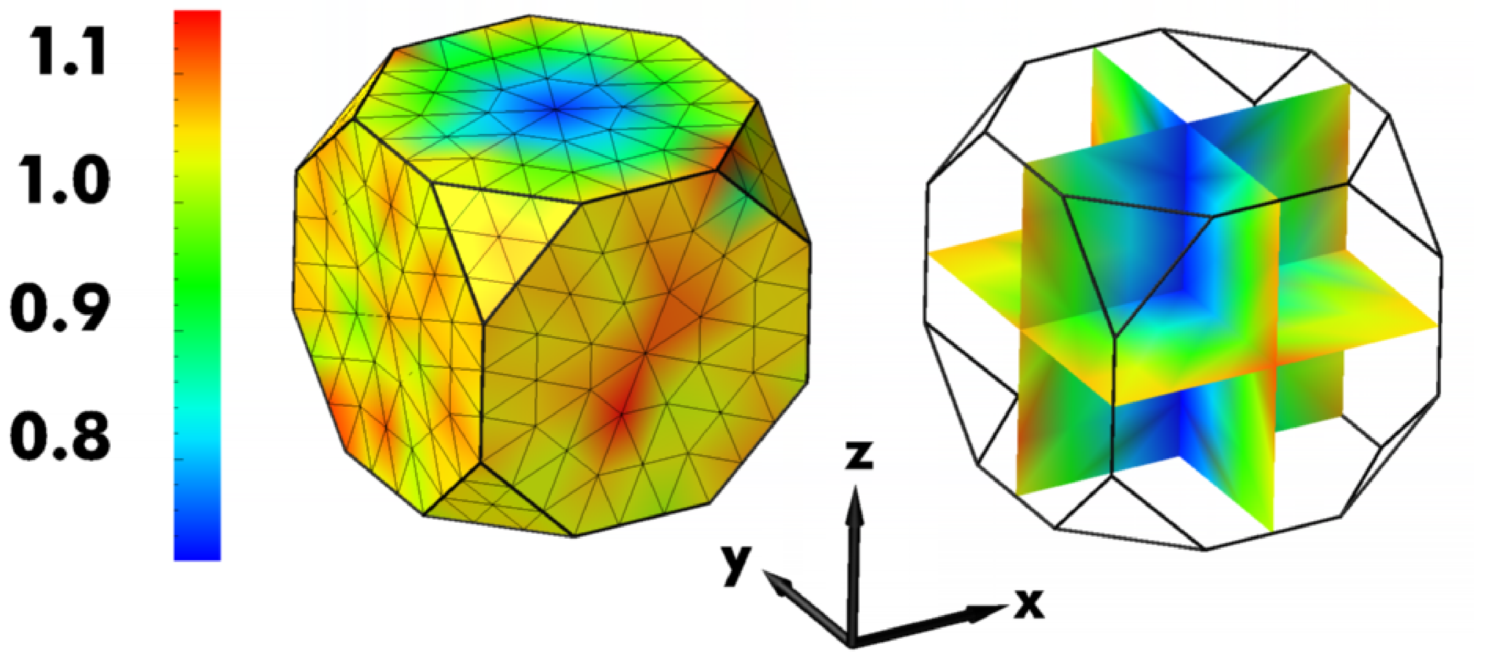
Stress is Spatially Heterogeneous:

- ✲ depends on the crystal's lattice orientation
- ✲ depends on orientations of neighboring grains

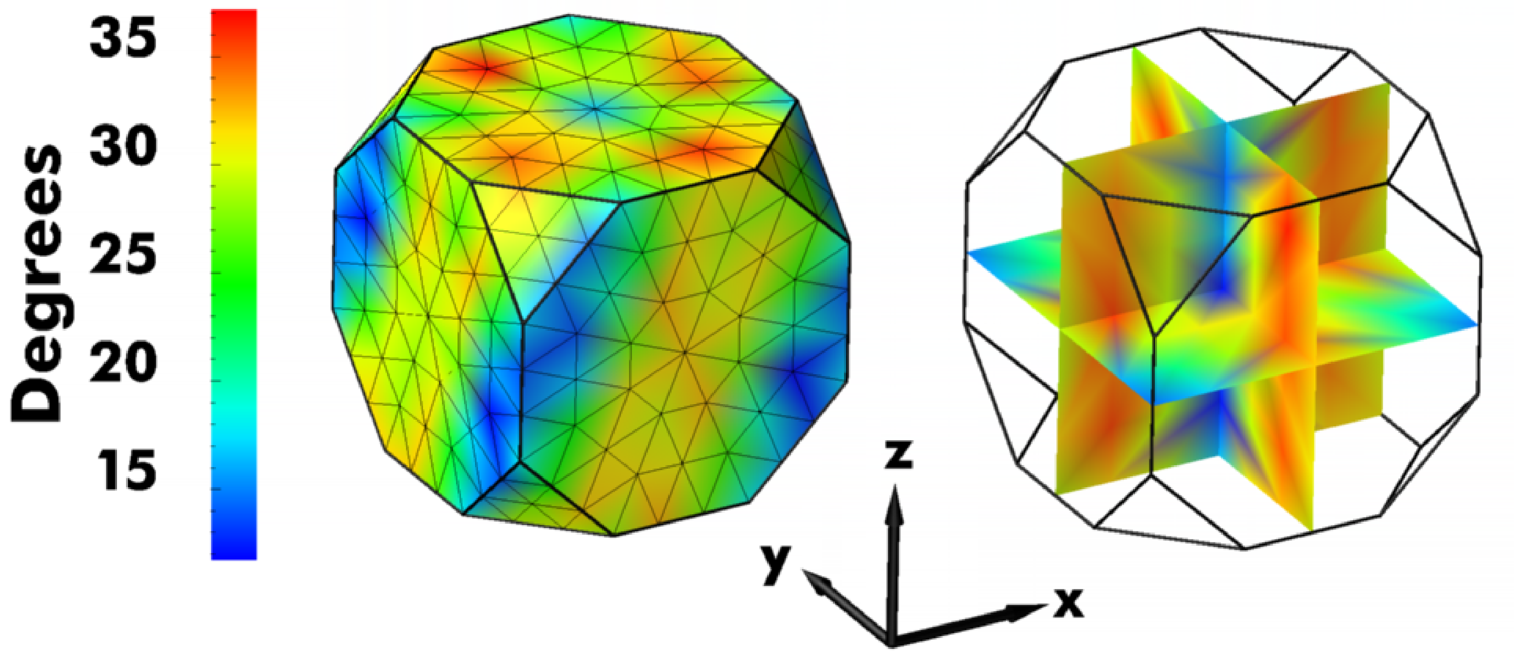
Stress Magnitude



Stress Magnitude (normalized)



Stress Direction (tilt of principal axes)

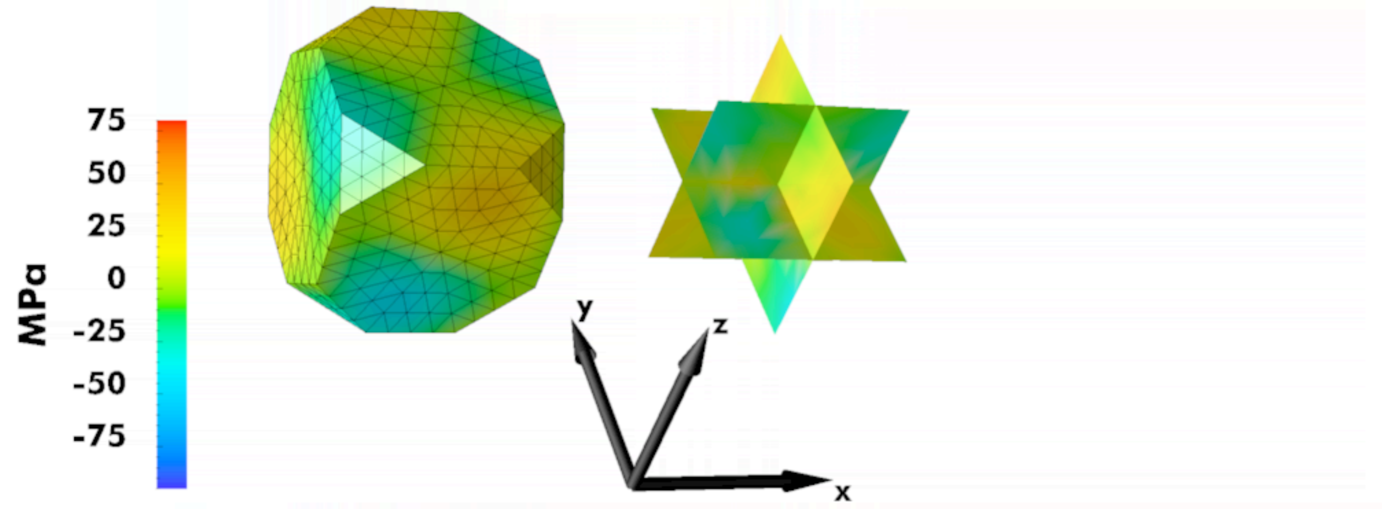


Comparison to experiment:

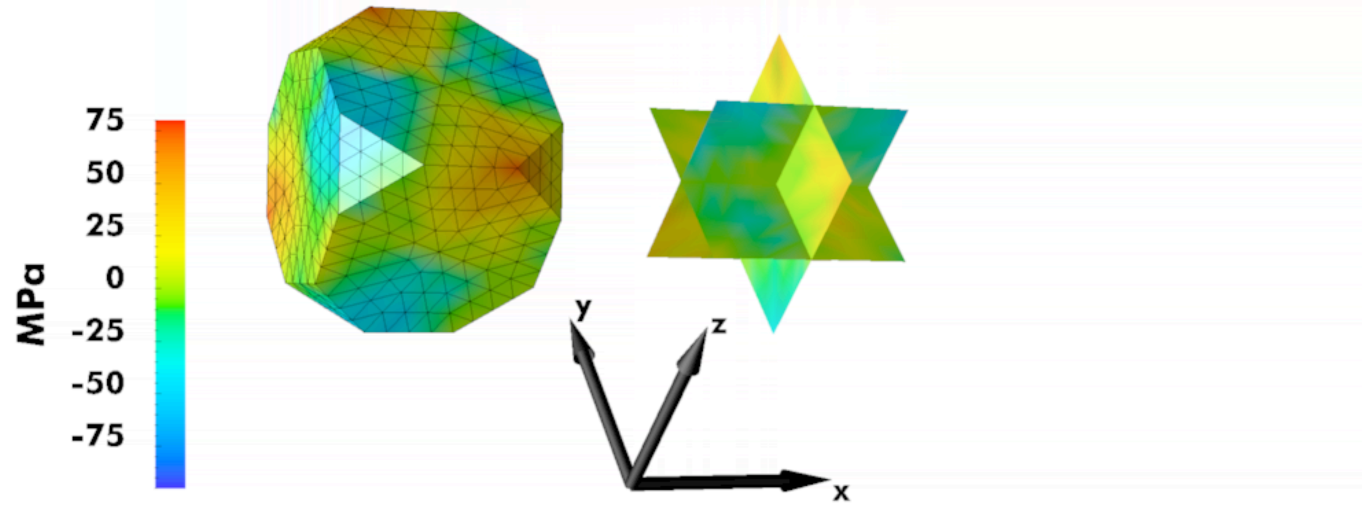
- ✲ X-ray diffraction w/broad strain pole figure coverage
- ✲ Tensile loading of pure copper (nominally 200MPa)
- ✲ Shear stress in the transverse plane (nominally zero)

See ☞ M.P. Miller, J.-S. Park, P. R. Dawson, and T.-S. Han. Measuring and modeling distributions of stress state in deforming polycrystals. Acta Materialia, 56:3927–3939, 2008.

Experiment σ_{12}



Simulation σ_{12}



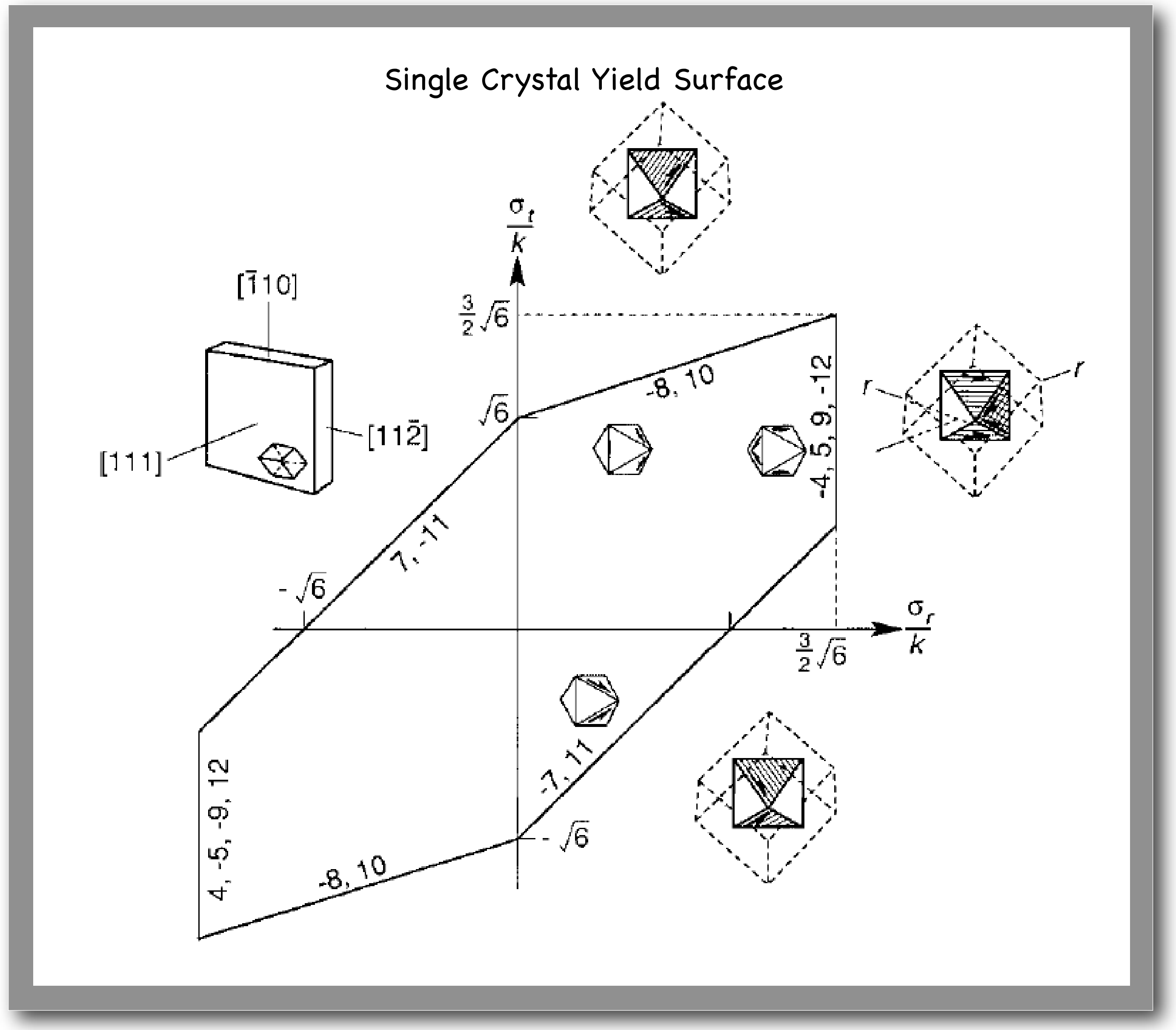
Trends:

- ✲ Both the magnitude and the direction of the stress depend on lattice orientation
- ✲ Holds true over a number of FCC systems

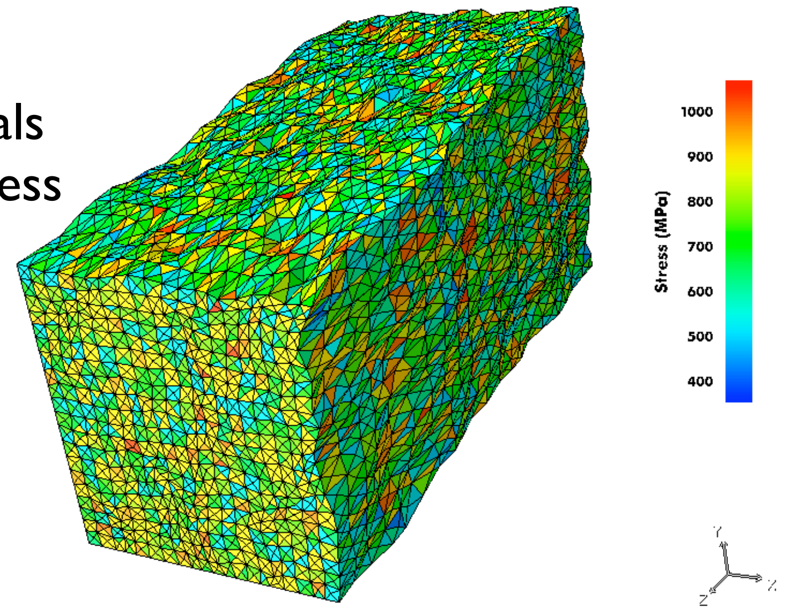
Fully-Developed Plastic Flow

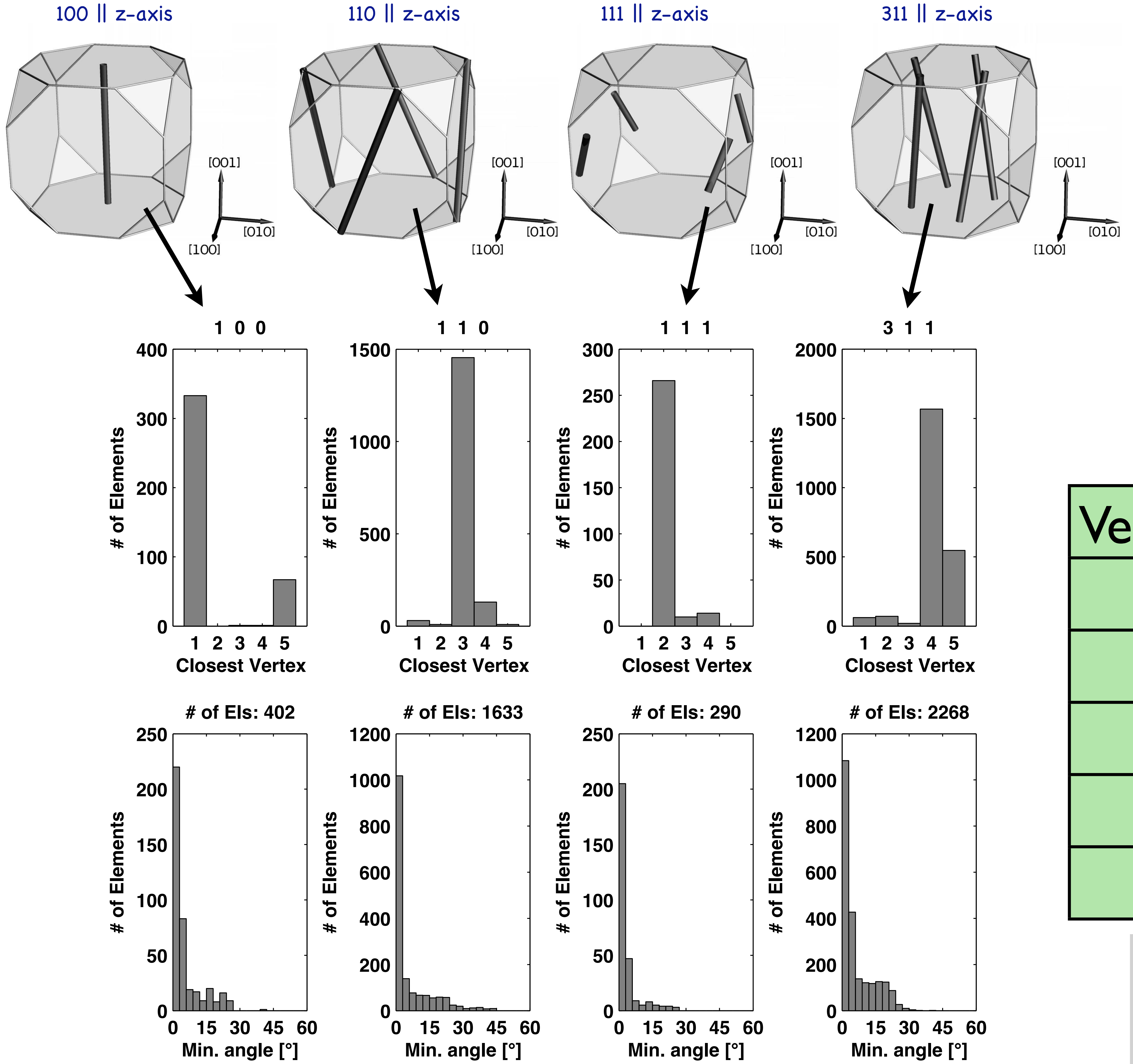
Single crystal yield surface:

- ✲ 12 FCC slips
  - ➔ 56 yield surface vertices
  - ➔ 5 families
- ✲ Families consist of symmetrically equivalent sets of vertices
- ✲ Families associate closely with fibers for tensile stress state

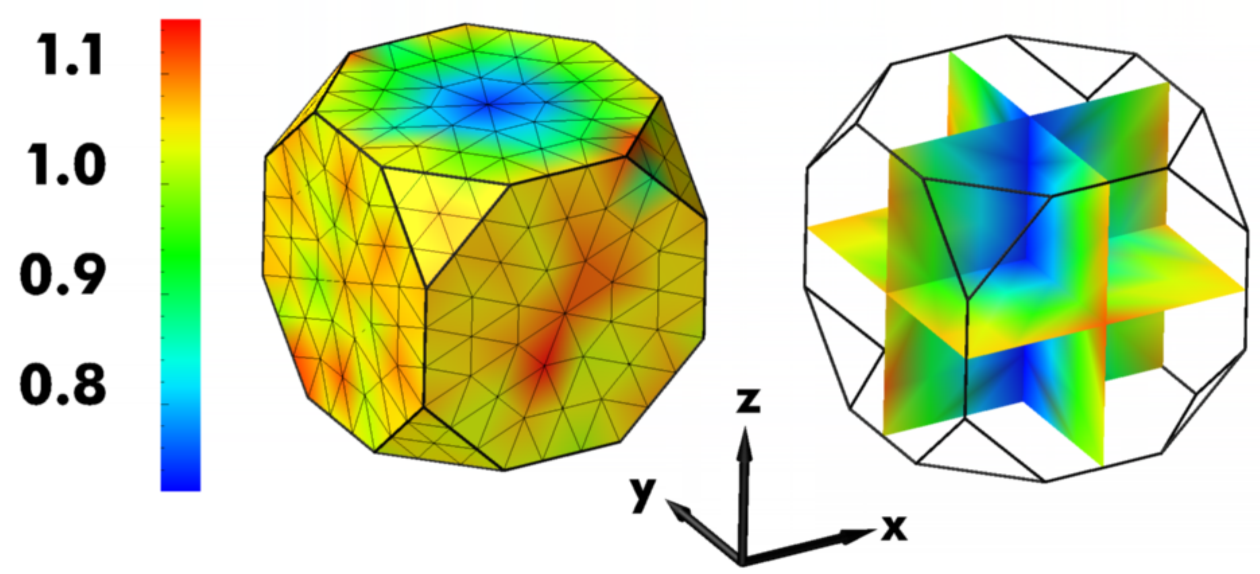


Deformed Polycrystals showing effective stress

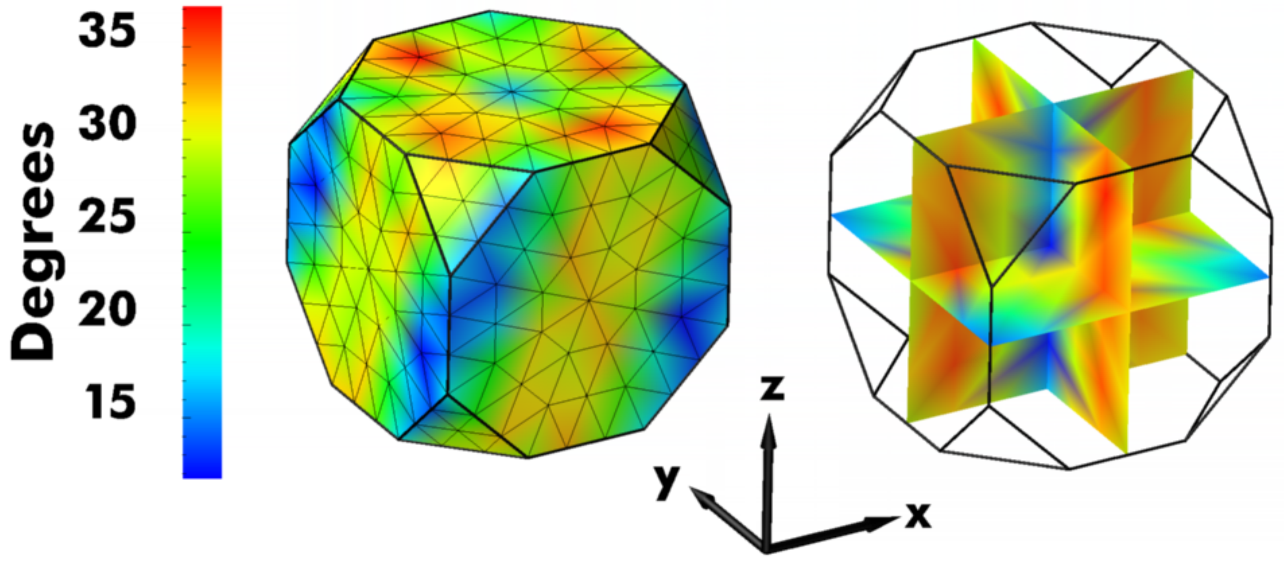




See ☞ H. Ritz, P. R. Dawson, and T. Marin. Analyzing the orientation dependence of stresses in polycrystals using vertices of the single crystal yield surface. Journal of the Mechanics and Physics of Solids, 58:54–72, 2010.



Stress Magnitude (normalized)



Stress Direction (tilt of principal axes)

VertexFamily	Magnitude	Tilt (Deg)
1	1	0
2	1.5	0
3	1.73	30
4	1.33	26
5	1.23	39

Trends:

- ✲ Stress state controlled by the single crystal yield surface once the plastic flow is fully developed

The Elastoplastic Transition

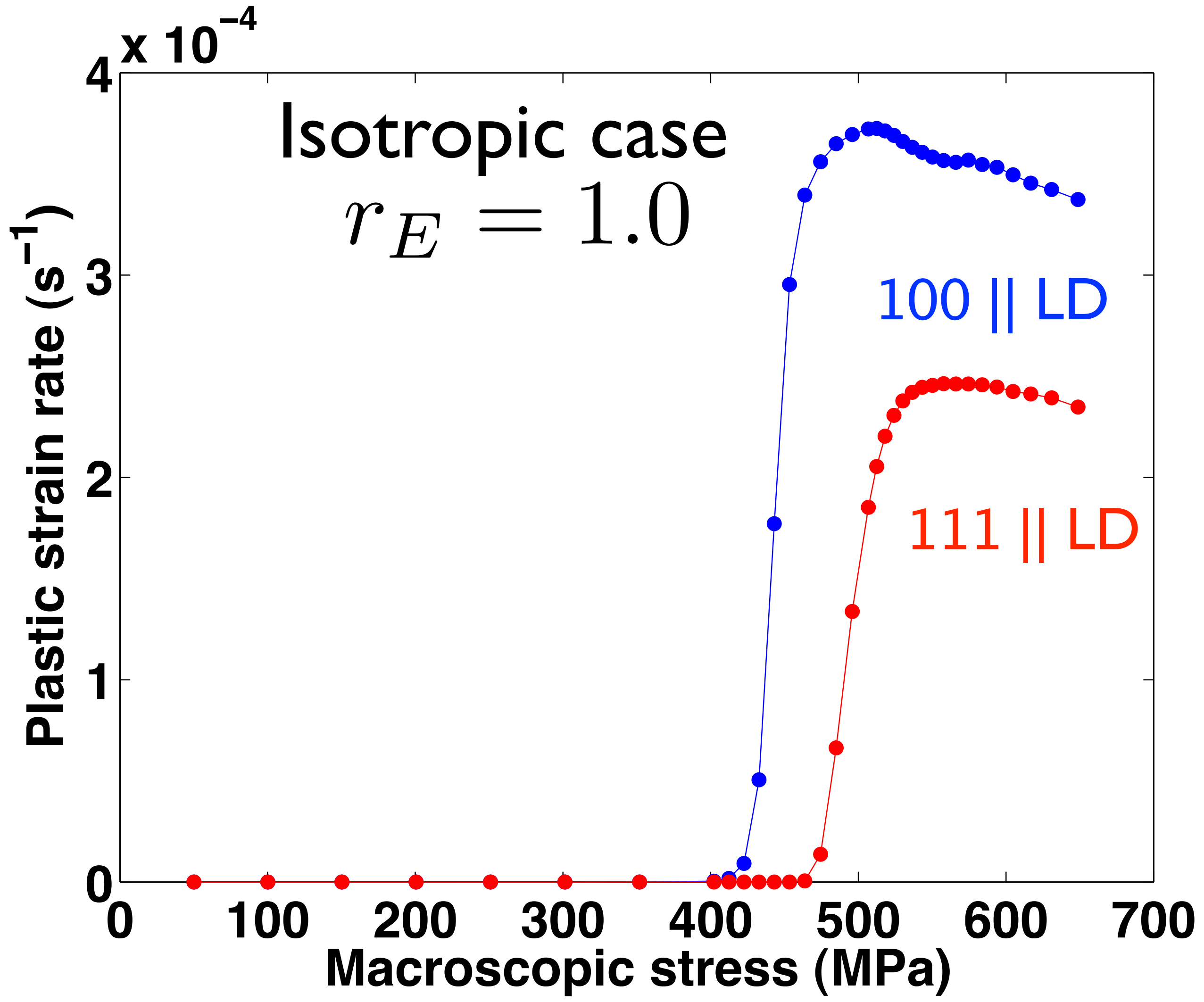
Obvious observations:

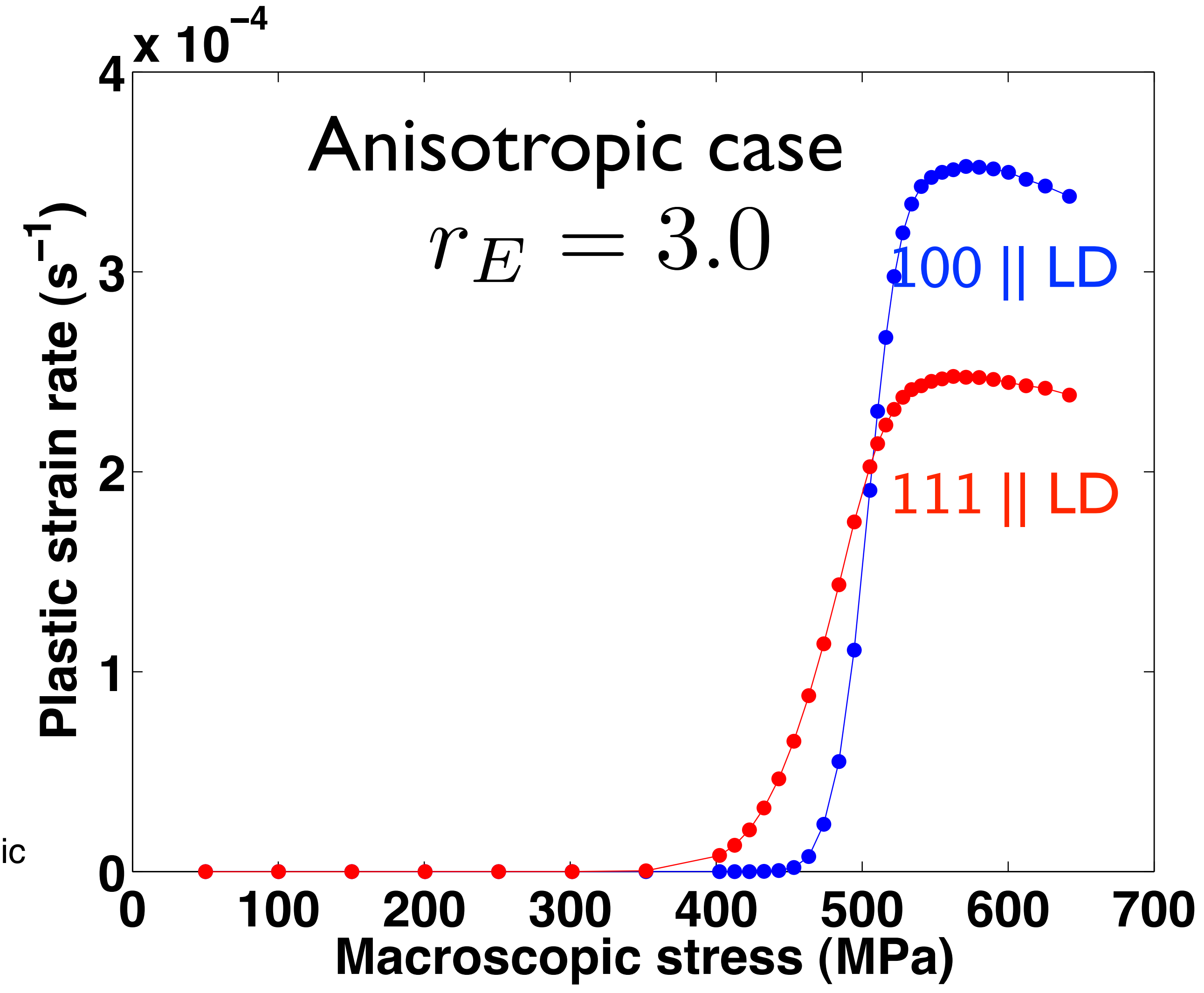
- Stress in the elastic regime is not affected by topology of the yield surface
- Rather, the elastic anisotropy is the determining property
- Some changes have to take place to arrive at the vertex stresses

Stress re-direction:

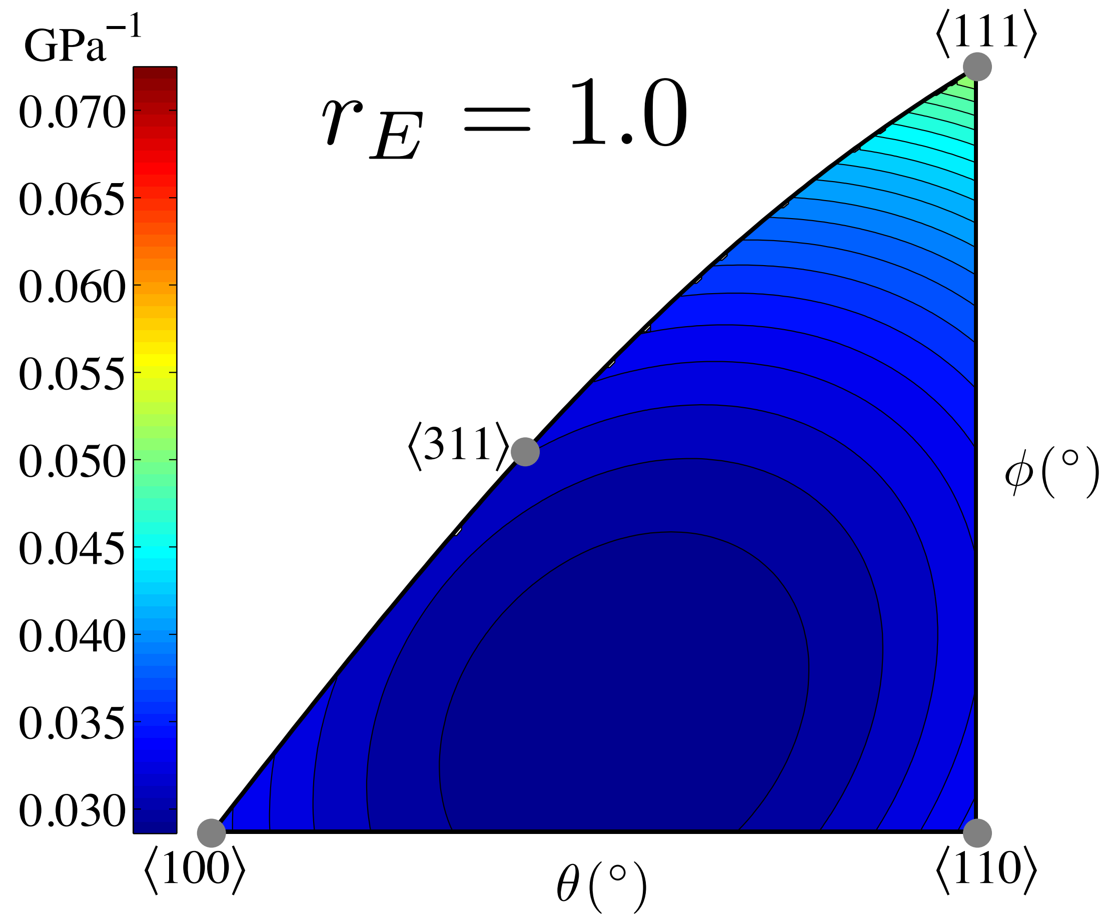
- Response in the elastic-plastic transition involves the re-direction and re-ordering of the stress distribution
- Controlled by combination of the stiffness (elastic) and strength (plastic) ➔ Strength-to-stiffness ratio
- In particular, the relative values of the directional strength-to-stiffness ratios
- Computed by taking ratio of the directional stiffness to directional strength (Schmid factor)

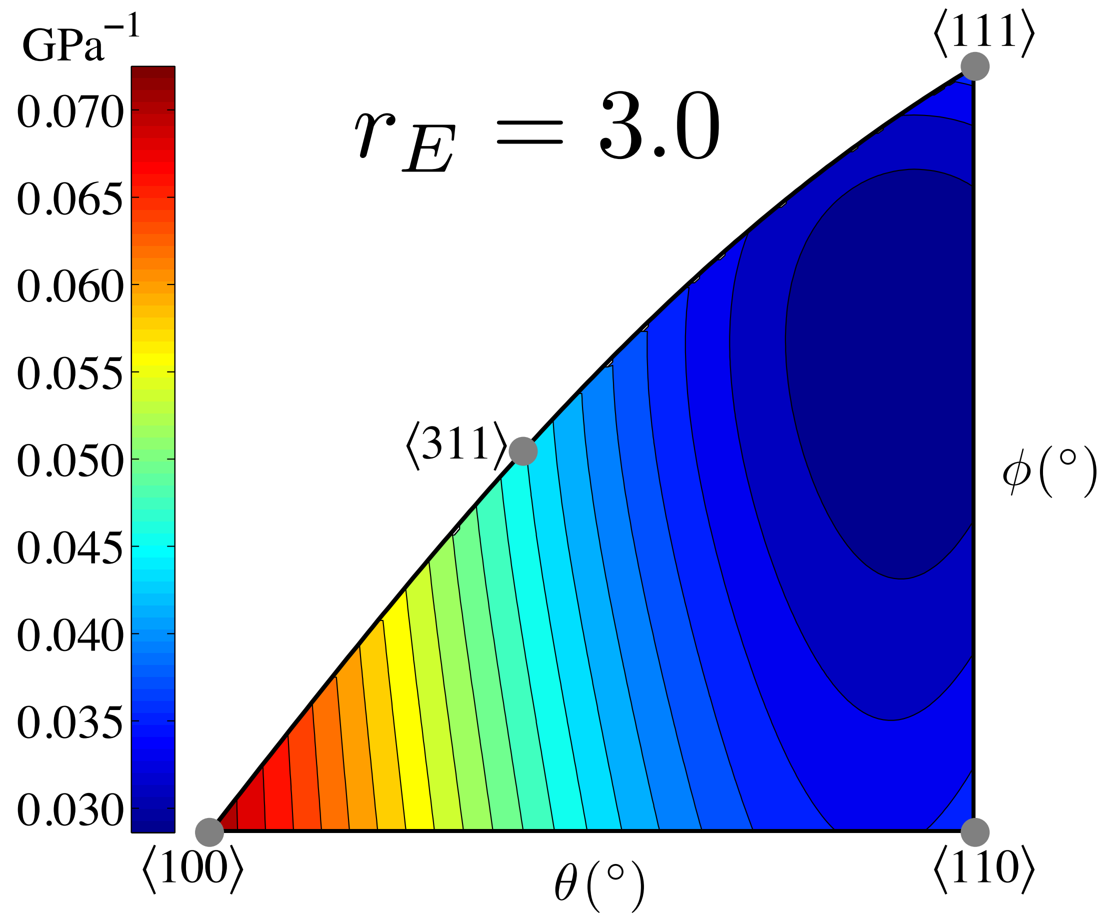
Plastic Strain Rates





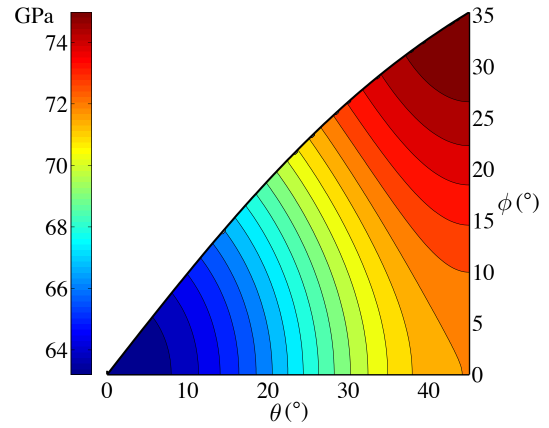
Strength-to-Stiffness Ratio



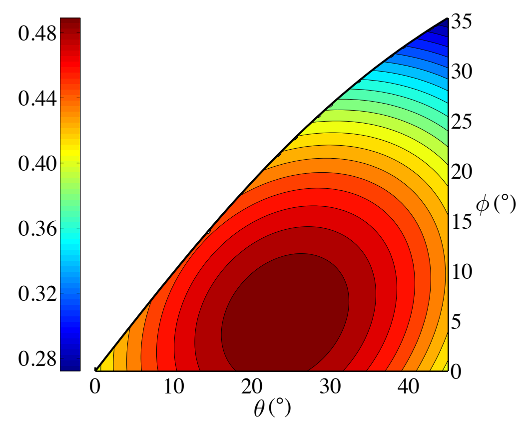


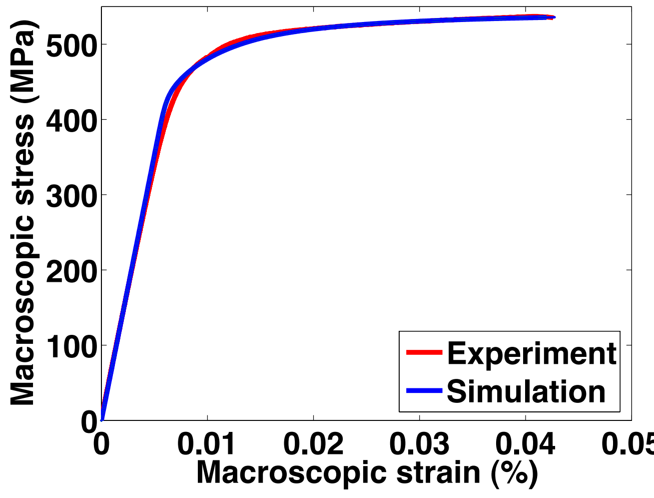
Uniaxial tension loading

Directional stiffness



Directional strength



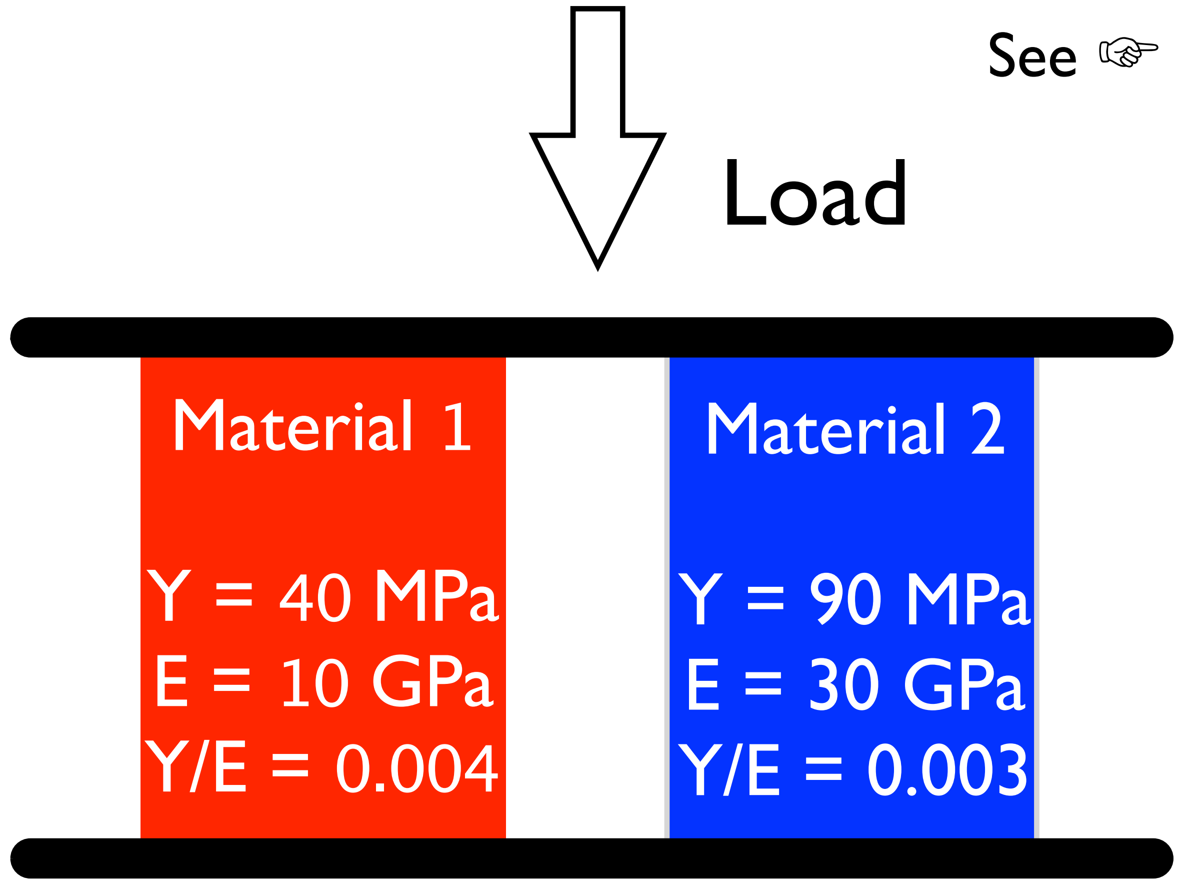


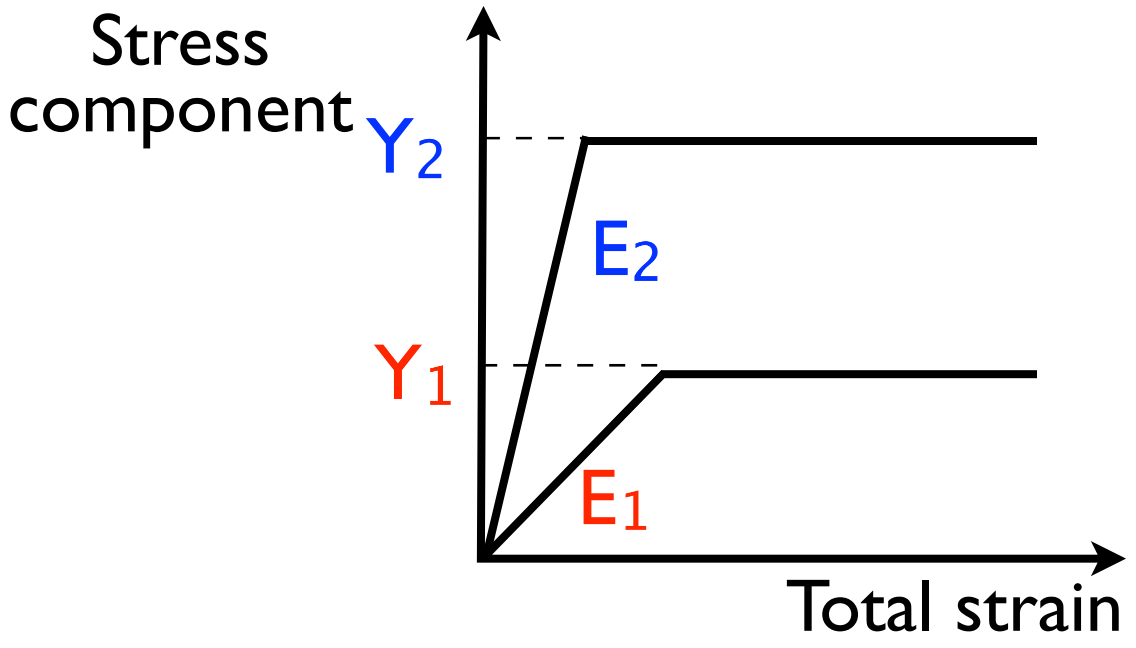
See ☞ S. L. Wong and P. R. Dawson. Influence of directional strength-to-stiffness on the elastic plastic transition of fcc polycrystals under uniaxial loading. Acta Materialia, 58:1658– 1678, 2010.

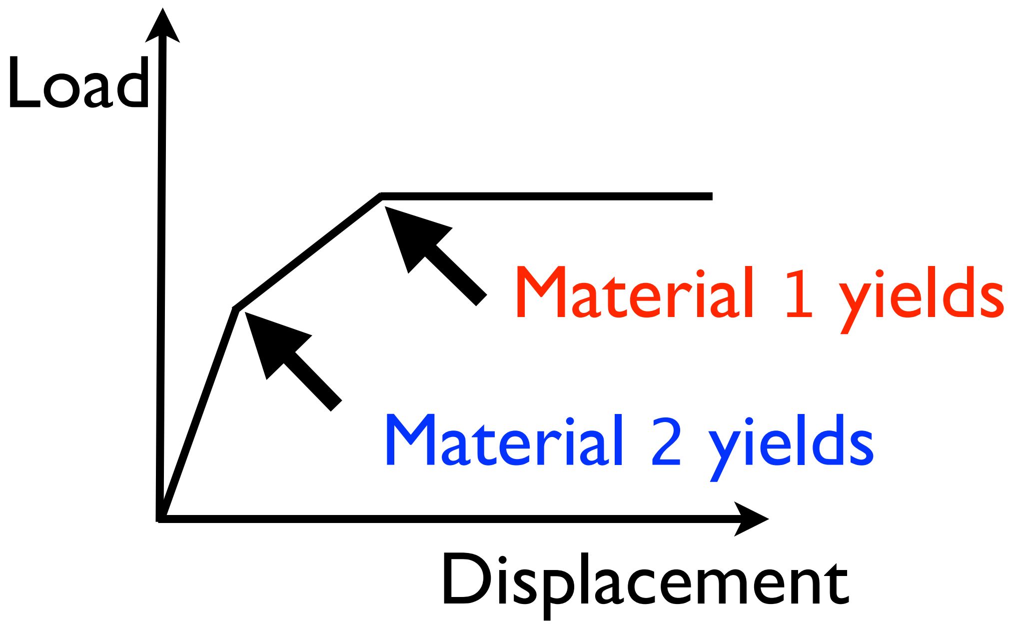
The Elastoplastic Transition

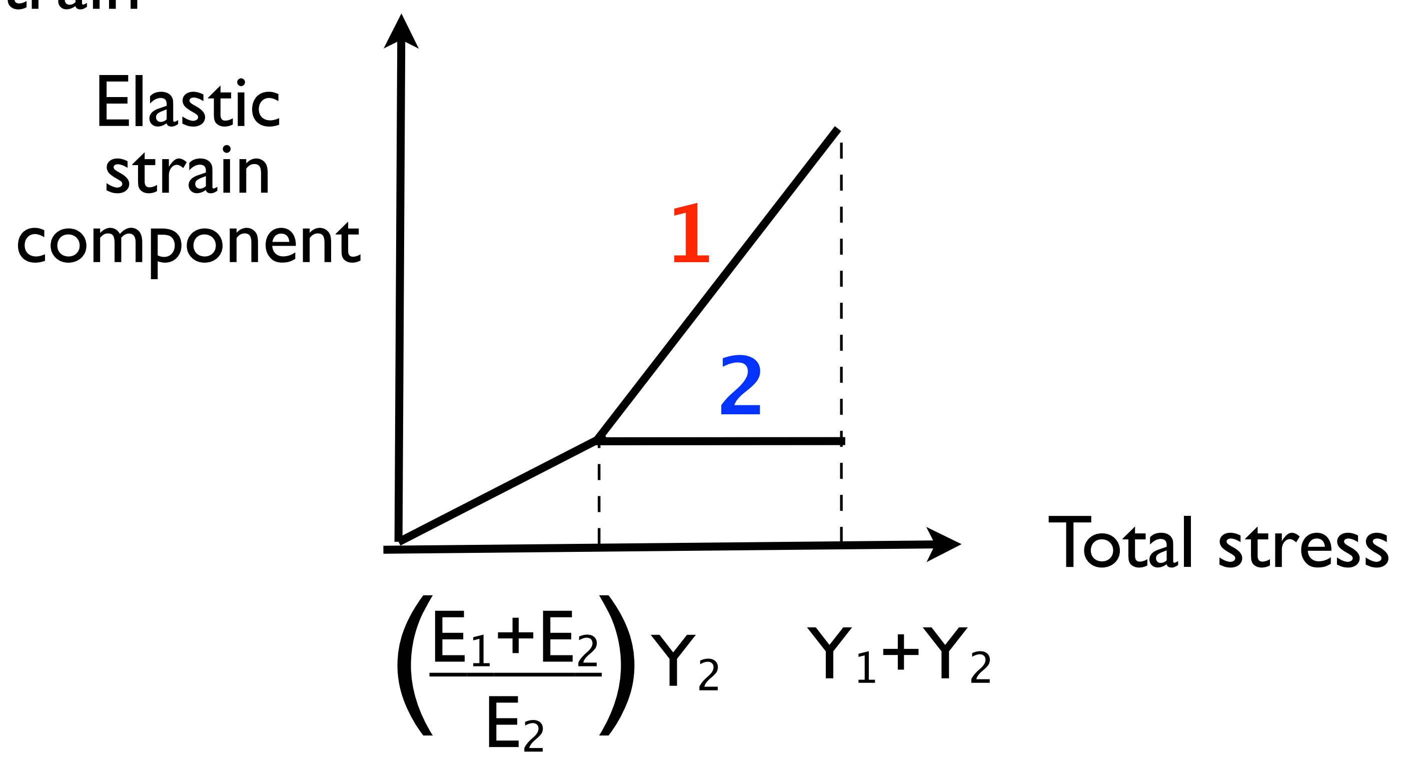
Influence of relative strength-to-stiffness:

See ☞ S. L. Wong and P. R. Dawson. Influence of directional strength-to-stiffness on the elastic plastic transition of fcc polycrystals under uniaxial loading. Acta Materialia, 58:1658– 1678, 2010.

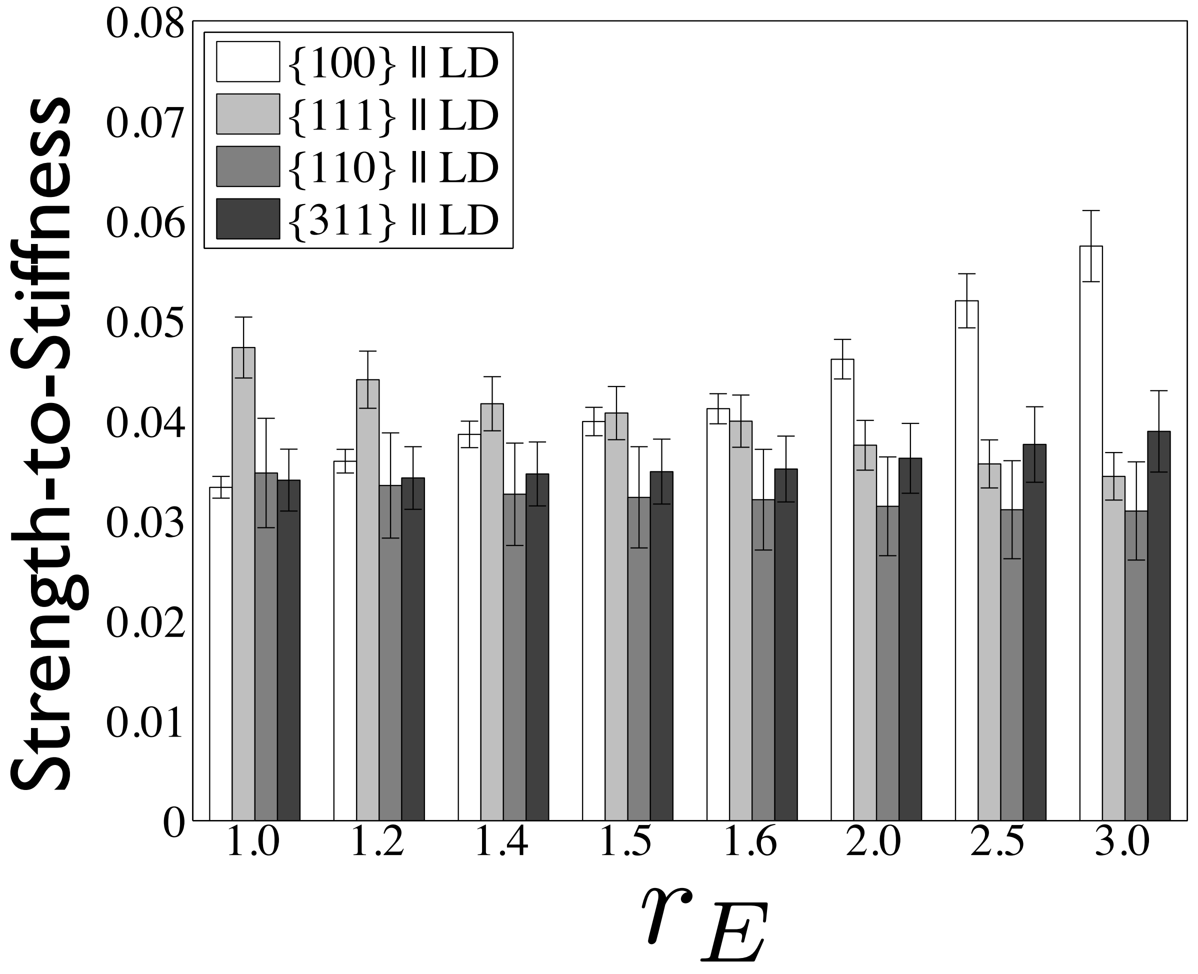






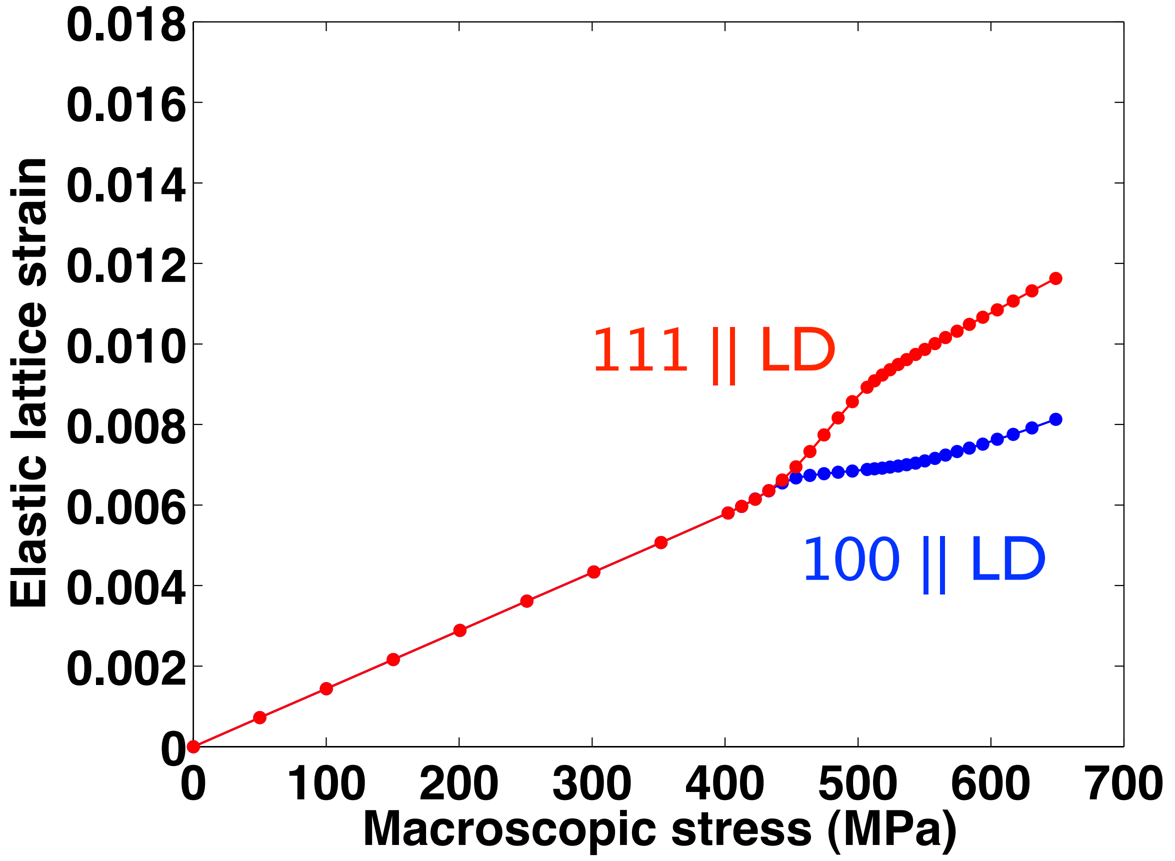


Fiber Strength-to-Stiffness Ratio

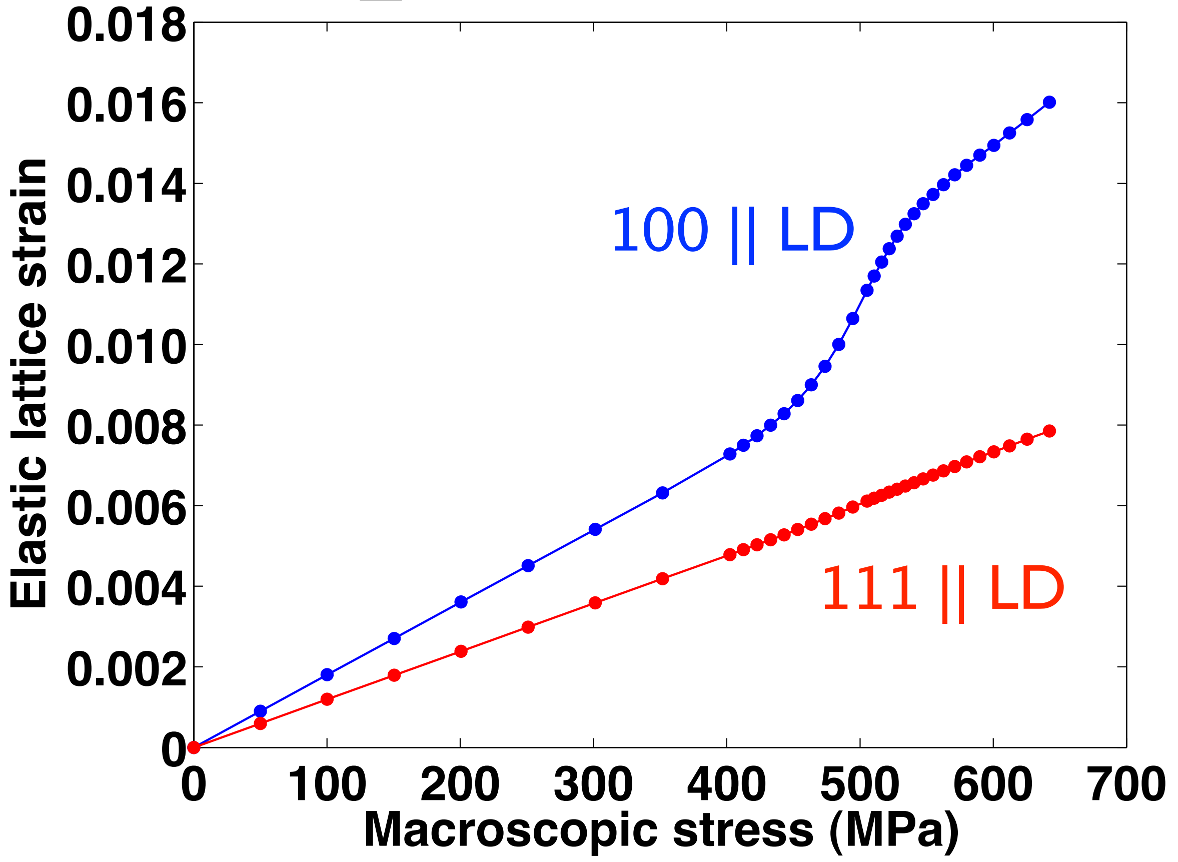


Computed Lattice Strains

Isotropic case $r_E = 1.0$



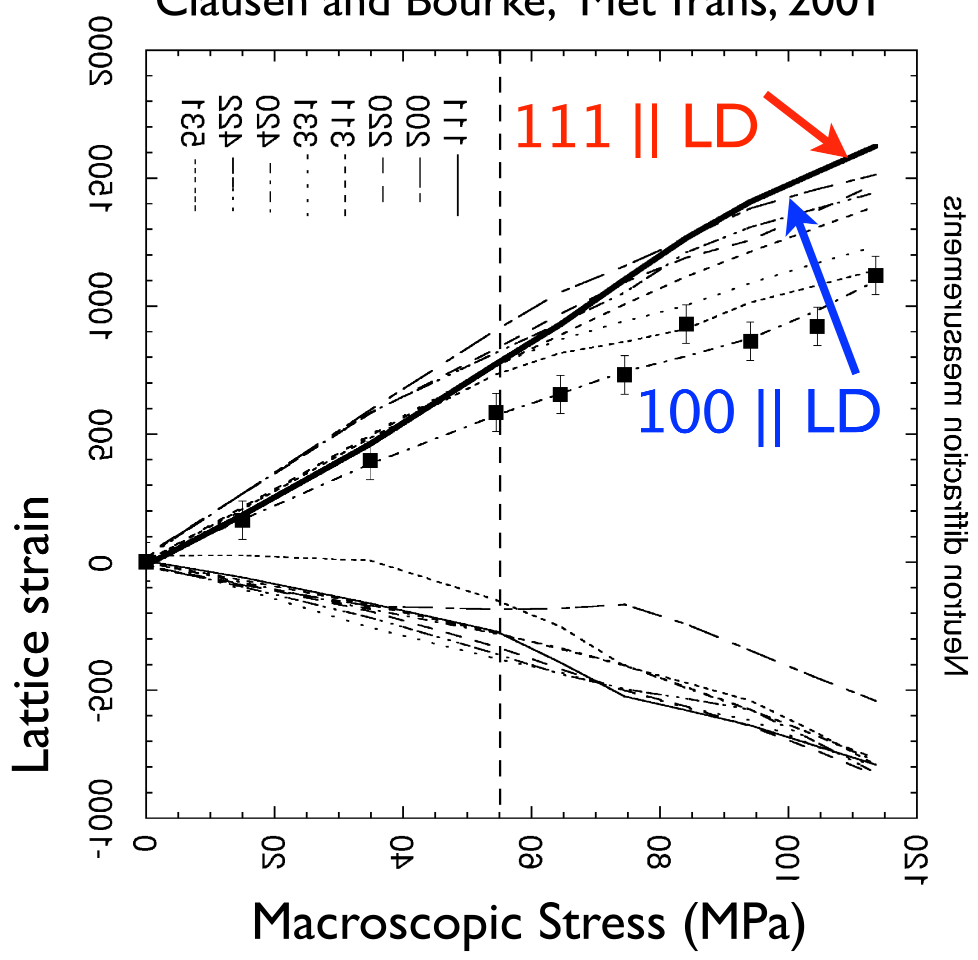
Anisotropic case $r_E = 3.0$



'Measured' Lattice Strains

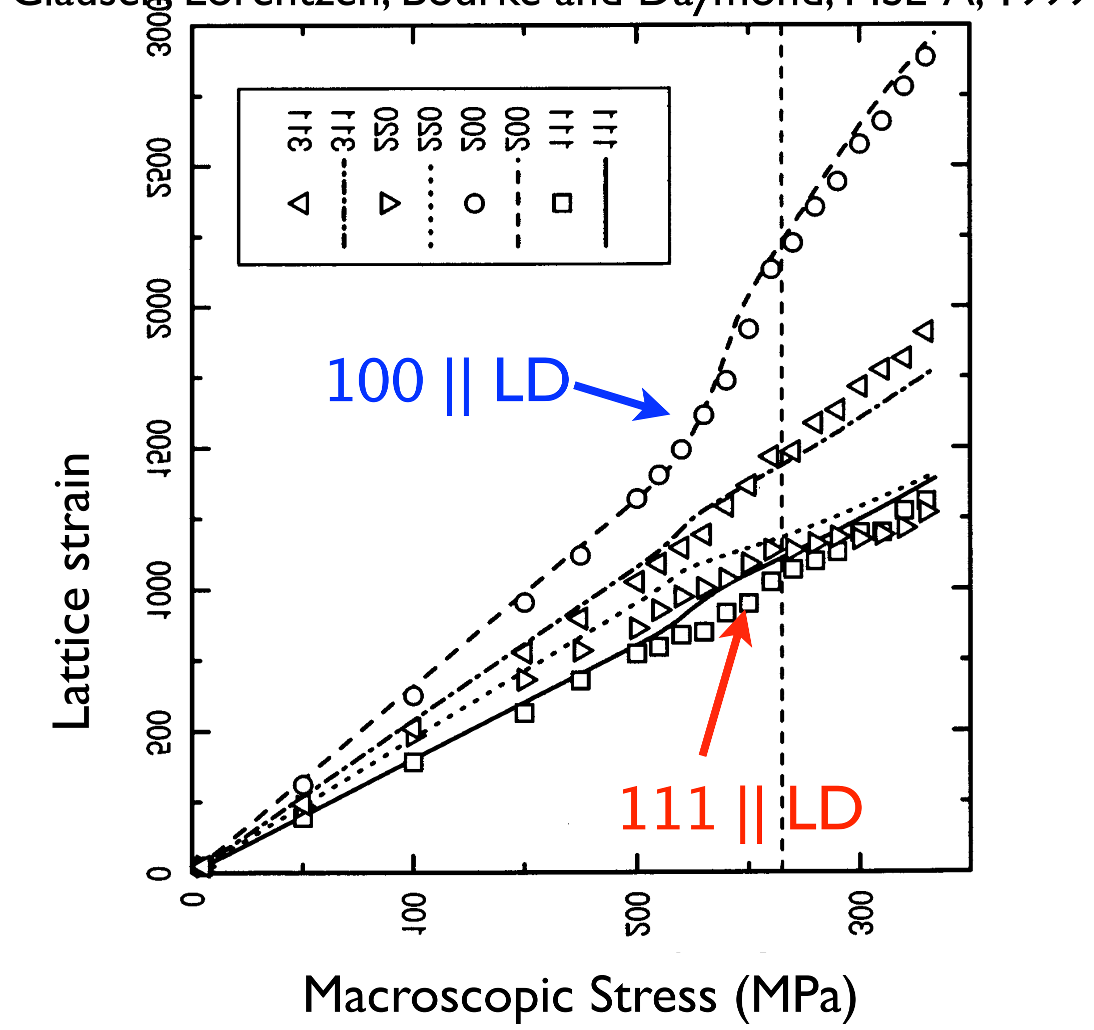
Aluminum alloy

Clausen and Bourke, Met Trans, 2001



Stainless alloy

Clausen, Lorentzen, Bourke and Daymond, MSE-A, 1999



Concluding Comments

Relevance of stress distributions

Stress is ubiquitous as a driving or contributing factor of materials processes

Crystal stresses are quite heterogeneous and evolve in magnitude and direction during deformation

Their relation to observed lattice strains depends on a number of factors: s/x anisotropy, loading mode, stress level

Analysis tools that accommodate the spatial heterogeneity of stress are essential to interpret the data fully

Exciting Challenges

Design investigations that intimately integrate experiments and simulations.

Understanding stress evolution during transformations (recrystallization, twinning, …).

Understanding the origins of failure in polyphase alloys.

Determining if dislocation structure is smoke or fire.

Collaborative Environments

Approaches using coordinated experiment and simulation best exploit the strengths of both

More rigorous and systematic archiving of data (experimental and numerical) is overdue.

Linkage of data for characterization and mechanical behavior is critical to enable simulation of experiments