Using (Neutron) Diffraction Measurements of Strain and Texture to Study Mechanical Behavior of Structural Materials

Los Alamos

Outline

- What Information Can We Get From Diffraction?
  - How Does It Relate to Materials, Especially Polycrystalline Deformation?
- Why Are Stress/Strain and Texture Important, Where Do They Come From?
- How Do We Measure, Interpret, and Visualize Texture?
  - HIPPO diffractometer for measurement of texture.
  - α–β Transformation in Titanium Alloys.
- How Do We Measure and Interpret Lattice Strain?
  - SMARTS diffractometer for measurement of strain.
  - Signatures of Plasiticy:
    - Slip : elasti-plastic transition of uranium.
    - Deformation Twinning :thermo-elastic effect in U6Nb
    - Stress induced phase transformation : pseudo elastic effect in U7Nb
    - Importance of polycrystalline plasticity modeling : anisotropy of high-rate deformed Beryllium
  - If we have time : Residual Stresses in Welds

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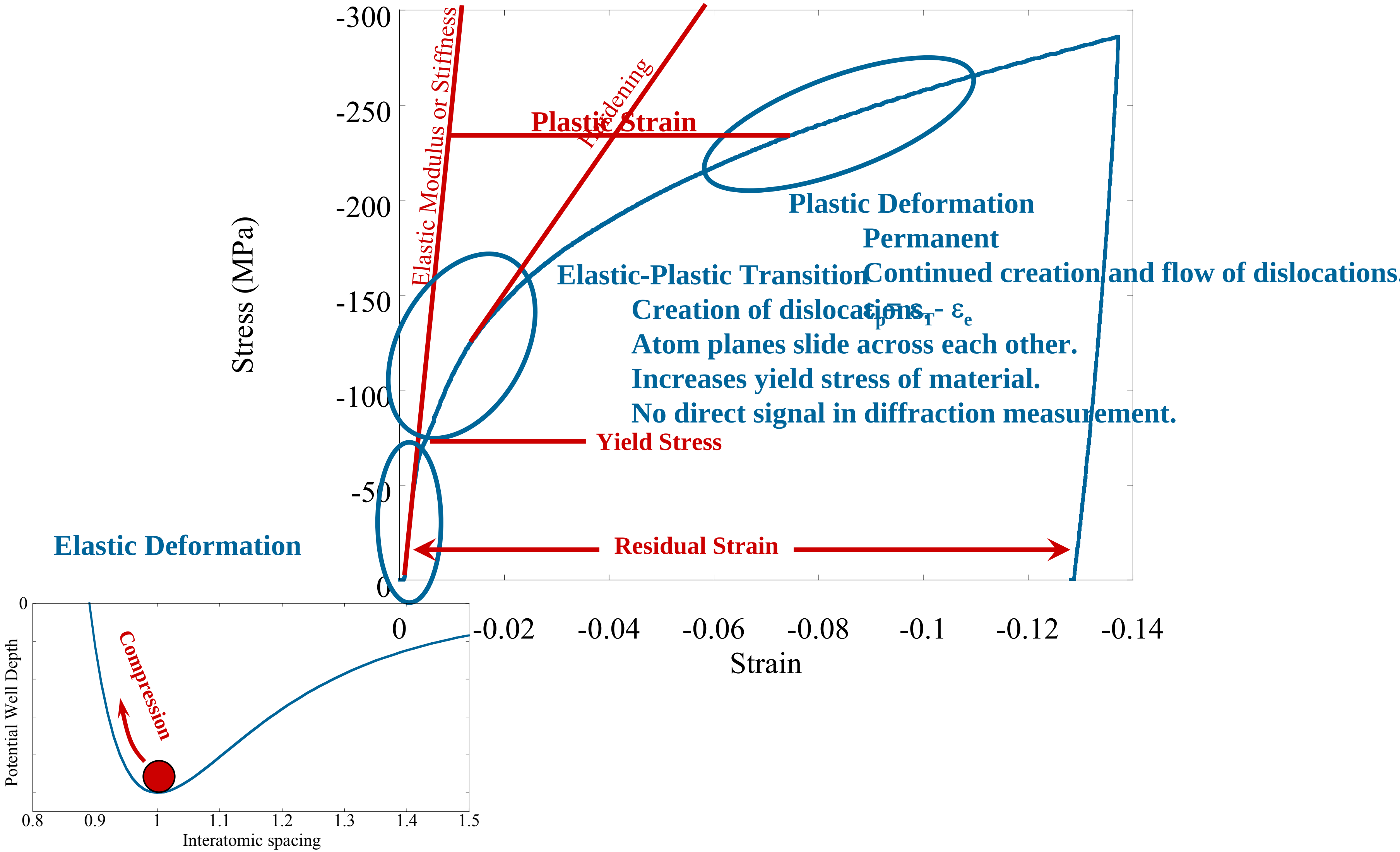
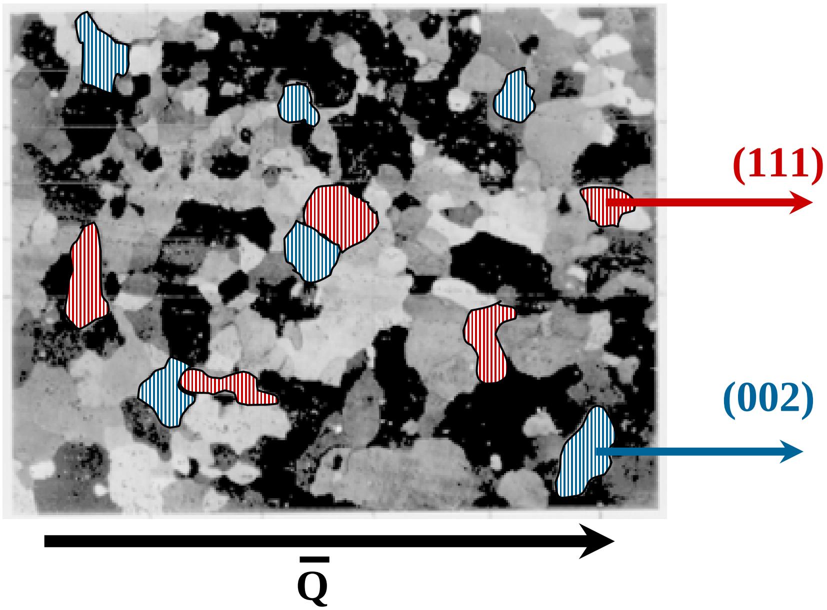
Definitions



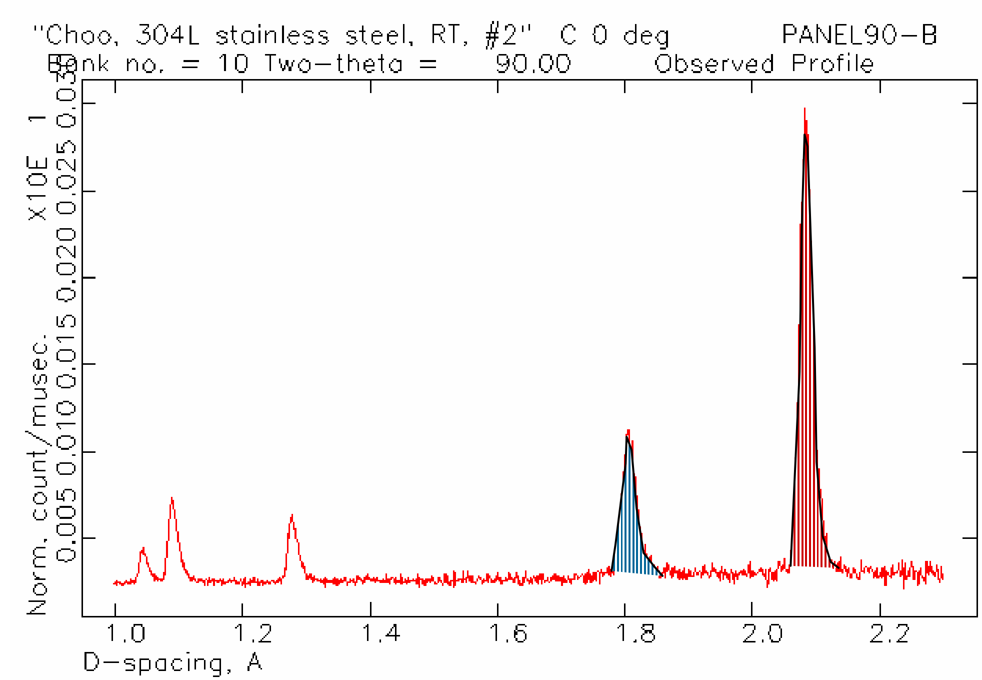
Atoms forced closer together during elastic deformation.
This is what we measure with diffraction.

Neutron Diffraction Separates Response of Grain Orientations

Polycrystalline Aggregate



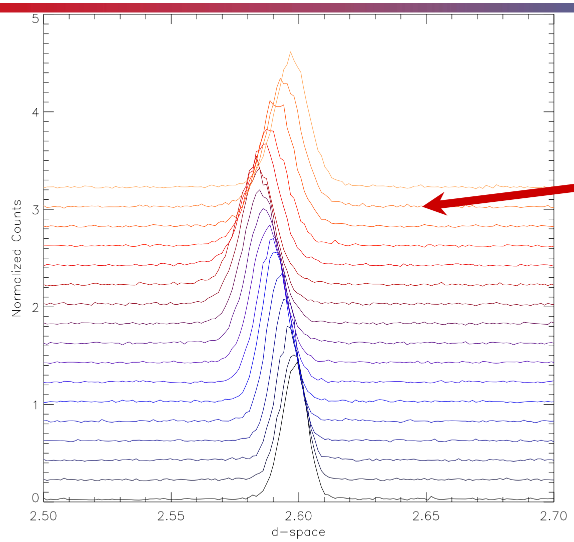
Stainless Steel



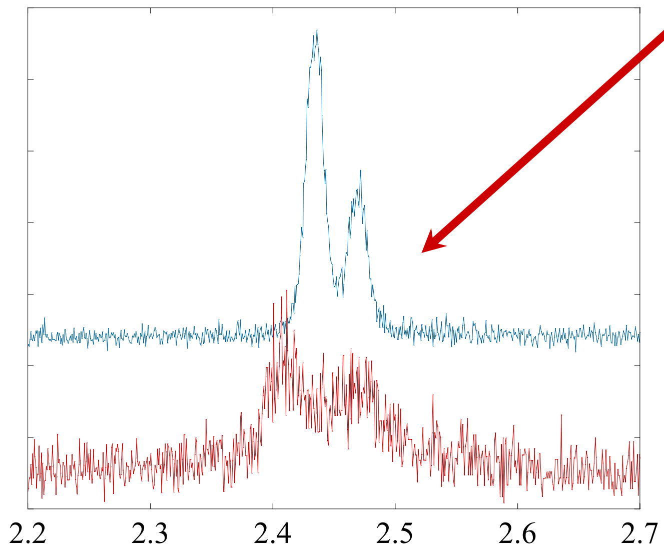
• Grains with plane normals parallel to the diffraction vector defined by the instrument geometry diffract into a detector.

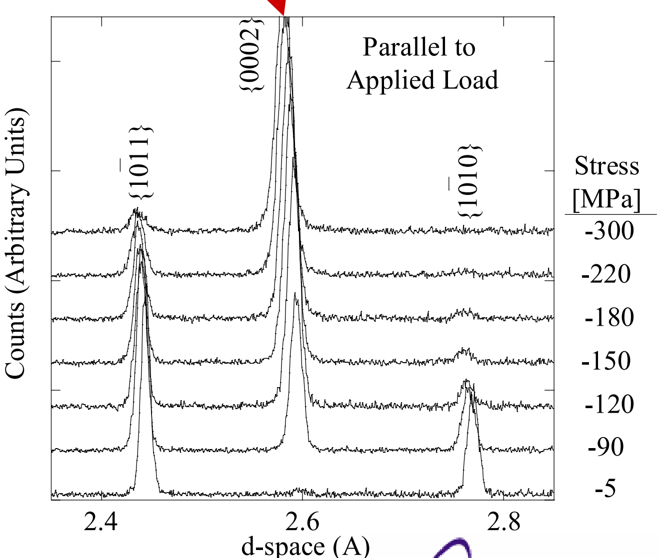
• Each grain orientation (hkl) contributes to a distinct peak, given by the interplanar spacing.

What Information is Contained in a Diffraction Pattern



- Peak Position
- Peak Width
- Peak Intensity





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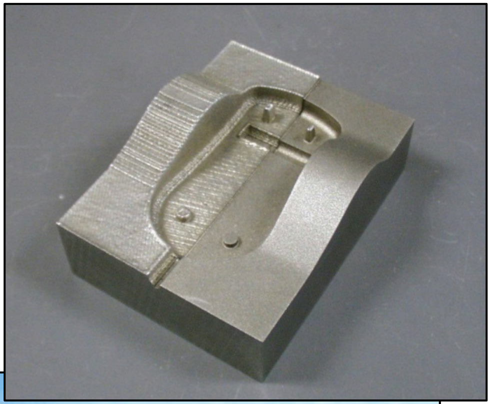
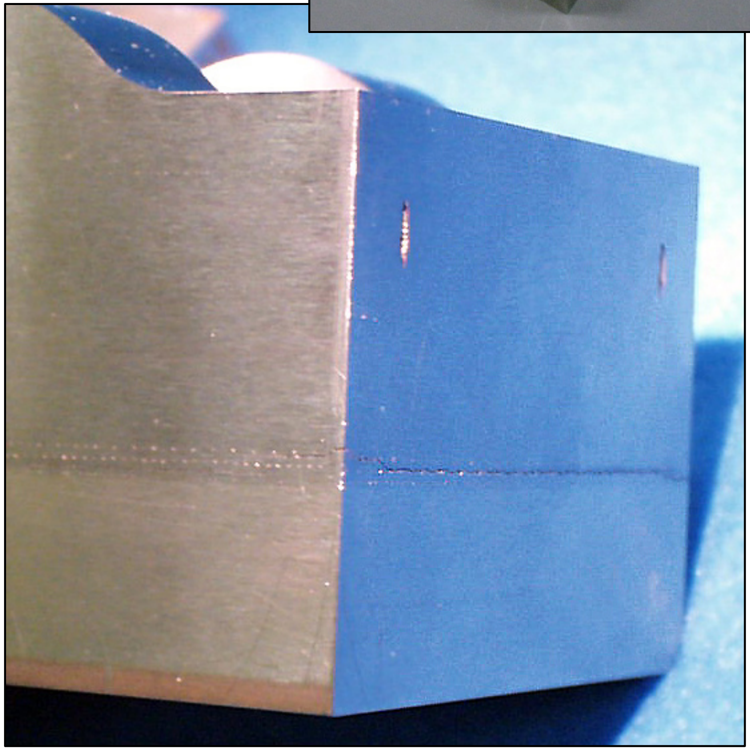
Why Do We Care About Residual Strains/Stresses?

- Premature Failure.
  - Accelerate Fatigue.
  - Crack Growth.
  - Stress Corrosion
- Distortion of Parts During Manufacture.
  - Results in Scrap.
- Tailor Residual Stresses to be Beneficial.
- Residual Stresses Are Often Output from FEM’s.
  - Measuring Them is an Important Validation Tool.





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Where Do Strains/Stress Come From ?

- Applied Load.
- Thermal Gradients :
  - Quenching, Tempering : Beneficial
  - Welding : Derogatory
- 2 Phase Materials : CTE Mismatch
  - Superalloys : γ,γ'
  - Composites
- Mechanical Treatments
  - Peening : Beneficial Residual Stress
  - Rolling
- Chemical Changes
  - Carburizing : Beneficial Residual Stress
  - Solutionizing During Welding

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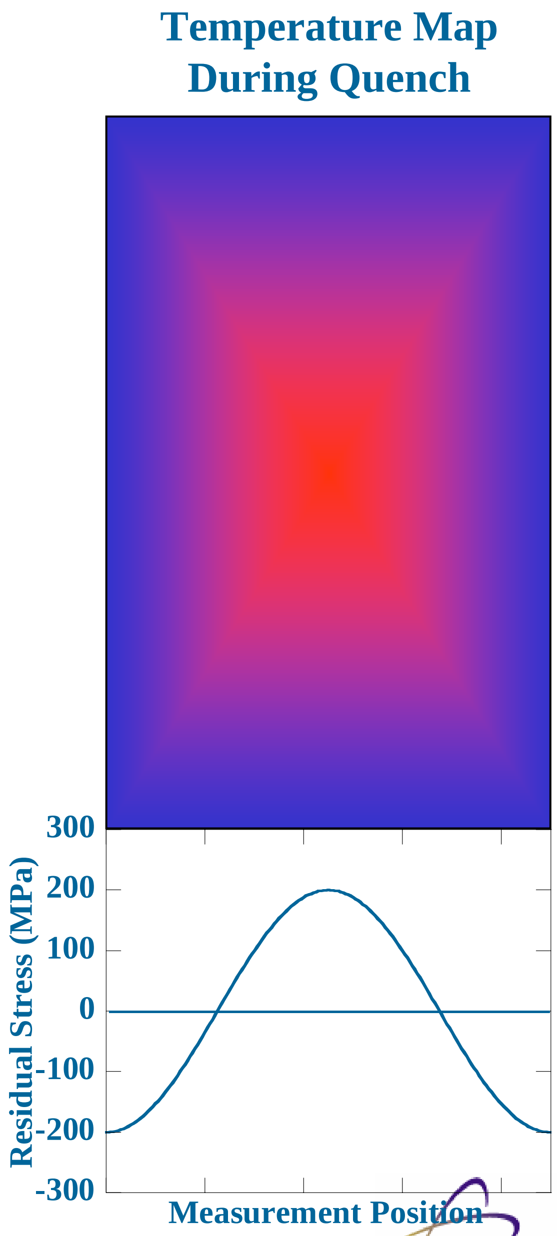

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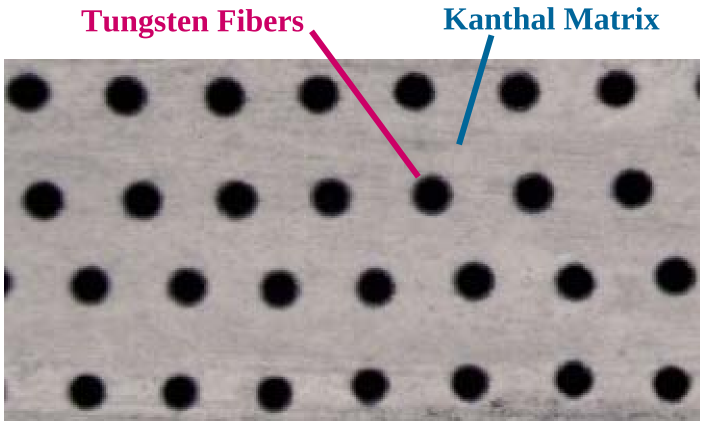

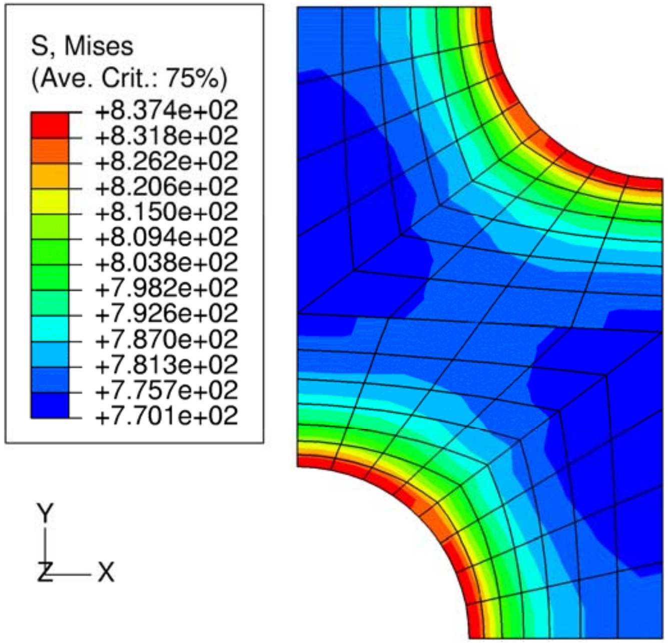

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Residual Stresses in a Shot-Peened Plate

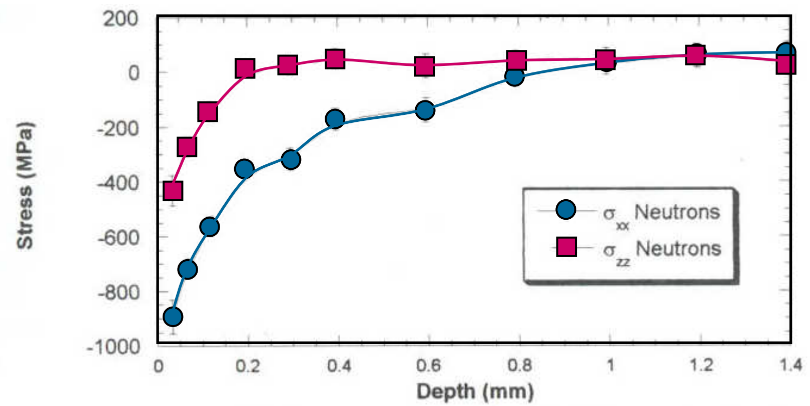

Figure 4 : Residual stresses determined by Neutron diffraction for the 100% coverage sample

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Fig. 1. Near surface microstructure (Nital etch) the light region near the surface results from the high volume fraction of retained austenite.

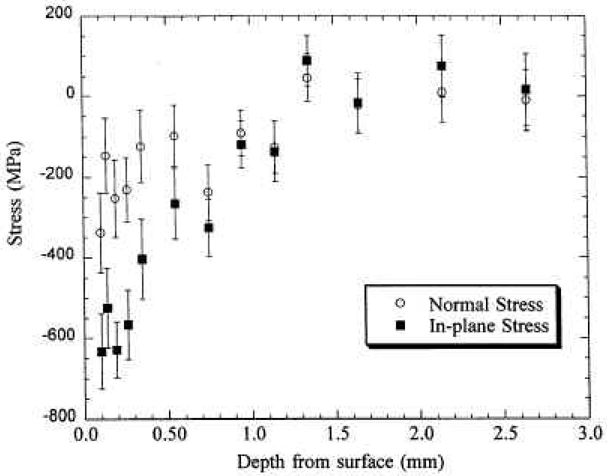

Fig. 10. Stresses determined from the strains in Fig. 9 with the assumption that the in-plane stresses are isotropic.

Bourke, M.A.M., Rangaswamy, P., Holden, T.M., and Leachman, R., *Mat Sci Eng A*, 1998, **257**(#2), p. 333-340.

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Where does Crystallographic Texture (Preferred Orientation) Come From?

- Directional Growth of polycrystal:
  - Dendritic formation in cast metals.
  - Chemical Vapor Deposition.
  - Epataxial growth.
- Thermal Gradients during solidification:
  - Vacuum Arc Remelting.
- Processing :
  - Rolling
  - Swaging
  - Extruding
- Deformation :
  - Uniaxial loading
  - Geological flow

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Why is Texture Important ?

- Mechanical properties of crystals are dependent on crystallographic direction.
  - Stiffness.
  - Critical Resolved Shear Stress.
  - Coefficient of thermal expansion.
- Subsequently, macroscopic material properties of bulk polycrystalline samples are dependent on the texture.
  - Yield Stress.
  - Speed of sound.
- Can use texture to learn about the history of a sample.
  - Formation of minerals from deep in the earth's crust.
  - Phase transformations
  - Fossils.
  - Metal pieces from past civilizations.
  - Post-mortem analysis of failed parts.

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Why is Texture Important ?

*(soda can example)

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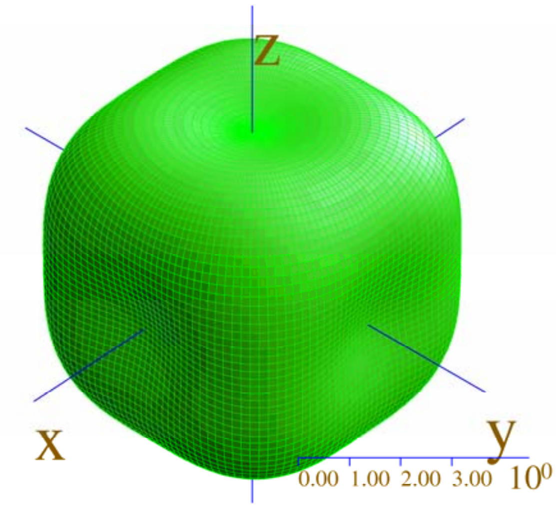

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*(book demo)

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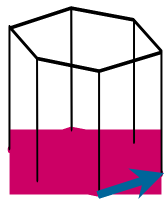
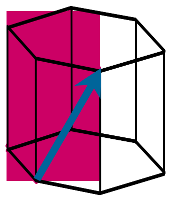
Hexagonal Beryllium



$(0001)\langle 11\bar{2}0\rangle$

Basal slip

τ_C~5MPa



$(11\bar{2}2)\langle 11\bar{2}3\rangle$

Pyramidal slip

τ_C~2000MPa

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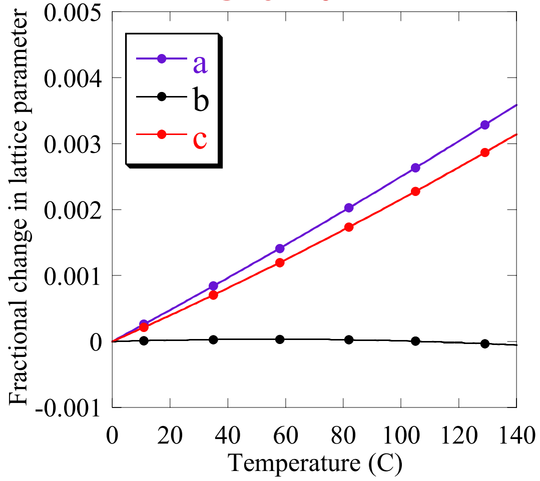
Orthorhombic Uranium



α_a=25x10^{-6}/C

α_b=-0.3x10^{-6}/C

α_c=22x10^{-6}/C

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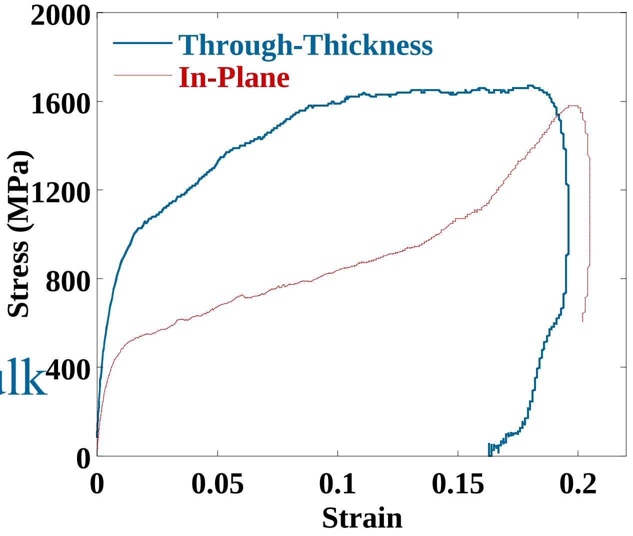

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Neutron Sources Do Not Sit on Desktop's

Los Alamos Neutron Science Center : LANSCE

Lujan Neutron Scattering Center

Weapons Neutron Research Facility

Isotope Production Facility

Proton Radiography

800 MeV Proton Linear Accelerator

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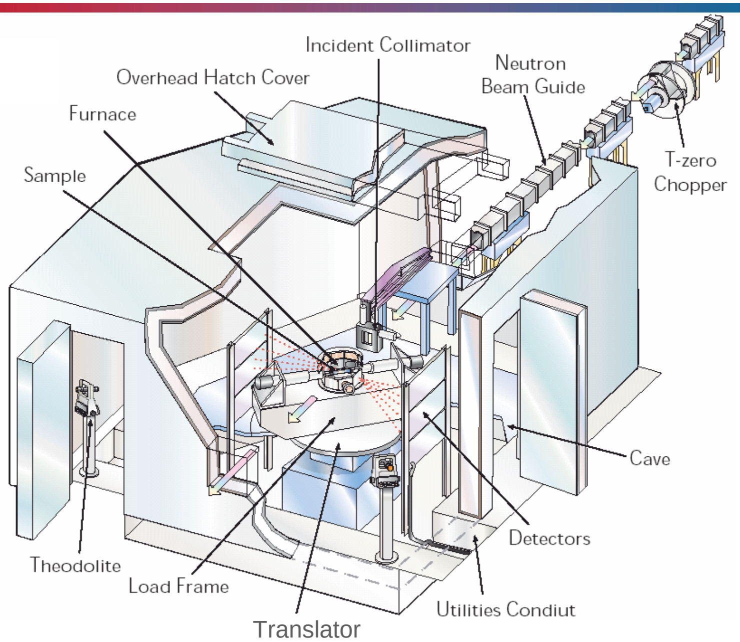
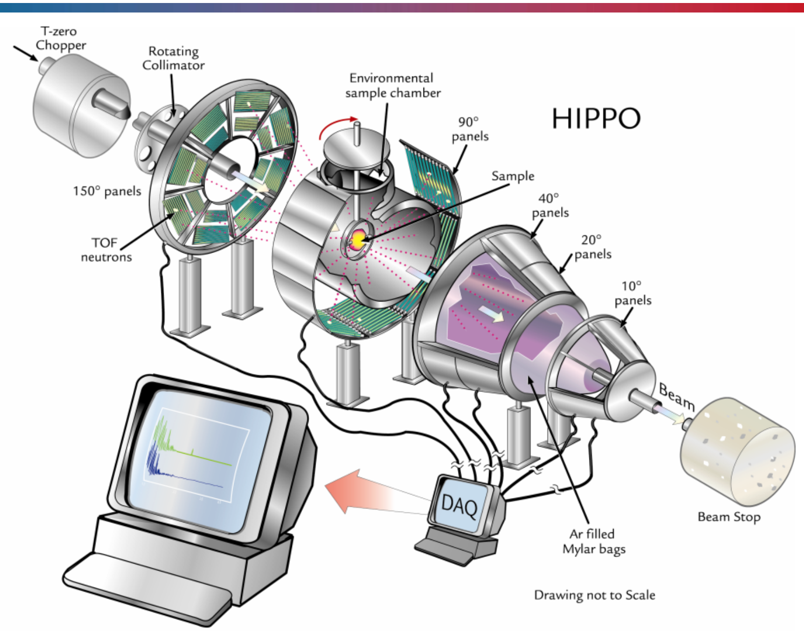
Advanced Diffractometers On-line at LANSCE





- LANSCE : Time-Of-Flight neutron source.
  - Continuous spectrum of incident neutrons.
  - Record entire diffraction pattern simultaneously.
- SMARTS : Optimized for study of lattice parameters in engineering materials.
- HIPPO : Optimized for high pressure and texture measurements.
- Next call for proposals : July 2004.

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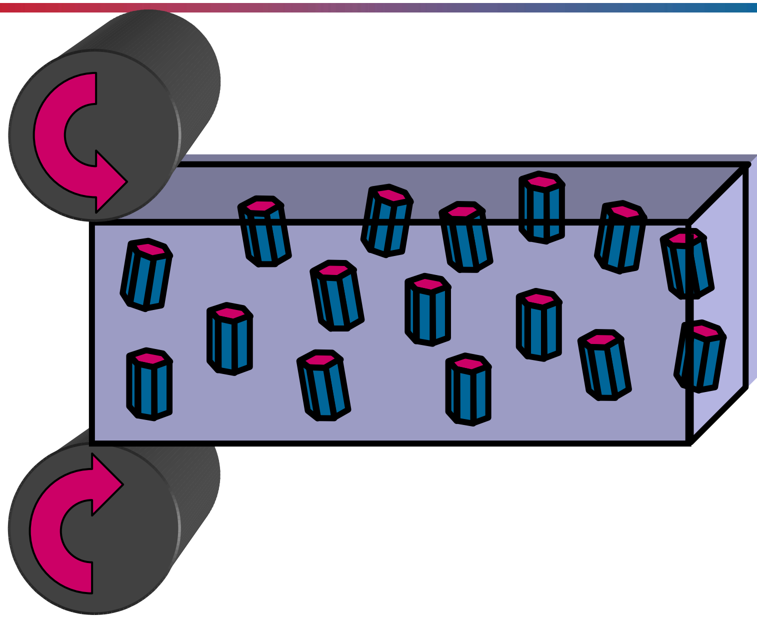
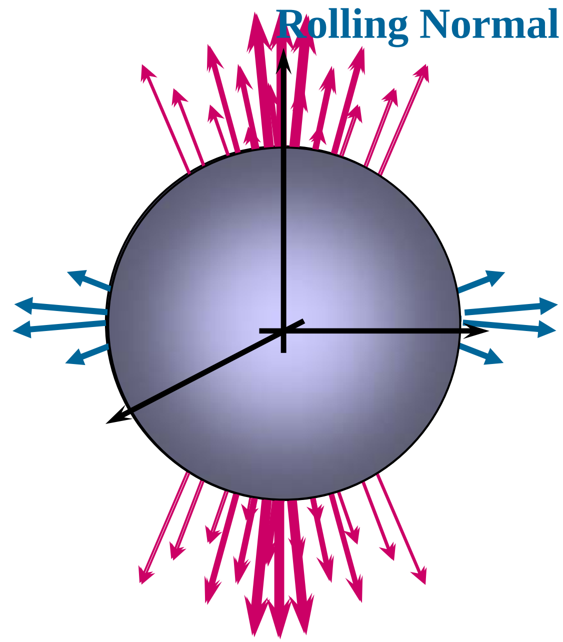
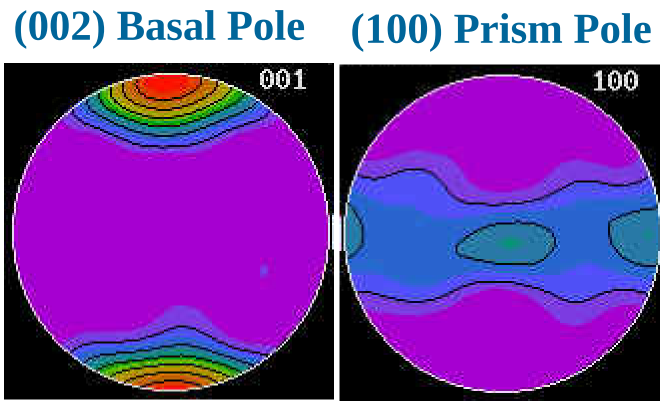
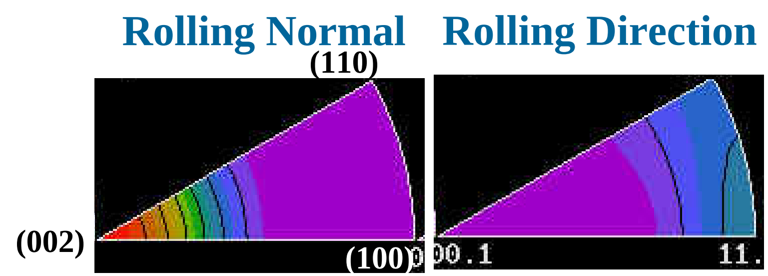
Representation of Crystallographic Texture : Pole Figures and Inverse Pole Figures



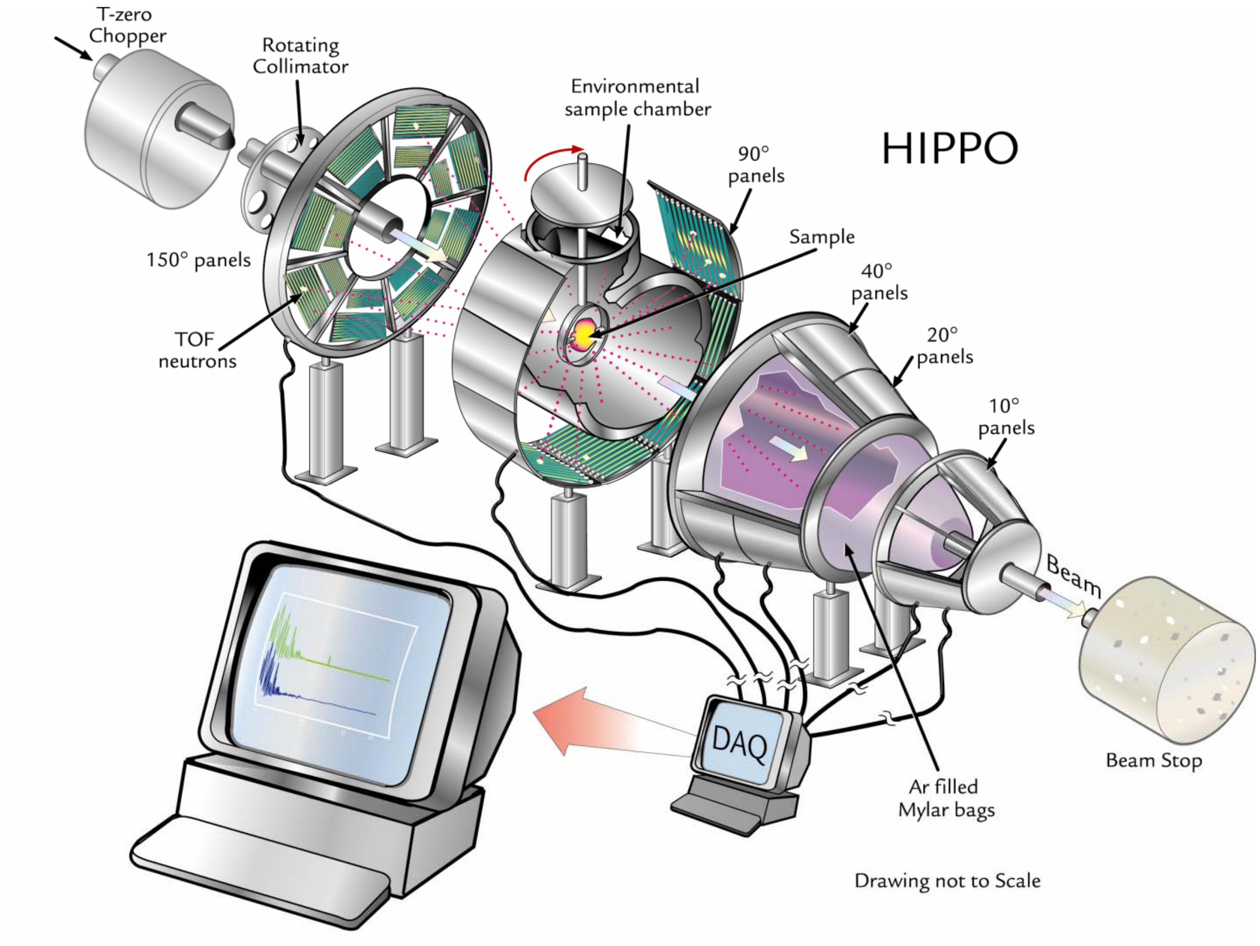






- Pole Figure :Density of a given {hkl} as a function of orientation relative to sample axis.
    - Measured directly with x-ray or monochromatic neutron diffraction.
- Density of all {hkl}'s on stereographic triangle along a given sample axis.
    - Measured directly with TOF neutron diffraction

HIPPO : A Neutron Diffraction Instrument Optimized for Texture Measurement.



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Example 1 : Formation of β phase during transformation in titanium alloy.

- **Question: Does β phase grow from pre-existing β grains or does it nucleate from α grains ?**
- **Ti64 : Titanium - 6% Aluminum - 4% Vanadium**
- **Microstructure at room temperature :**
  - **94-98% hcp (α-phase).**
  - **Remaining small bcc (β-phase) grains.**
  - **Typical hcp rolling texture in α-phase, (001) parallel to rolling normal.**
  - **Not enough β-phase present at RT to determine texture.**
- **Transforms from hcp (α) to bcc (β) crystal-structure at ~980°C**
- **If β phase nucleates from α grains Burgers orientation relationship predicts $(001)_{\alpha}||(110)_{\beta}$.**
- **If β phase grows from pre-existing β grains expect bcc rolling texture, i.e. (111) parallel to rolling normal.**

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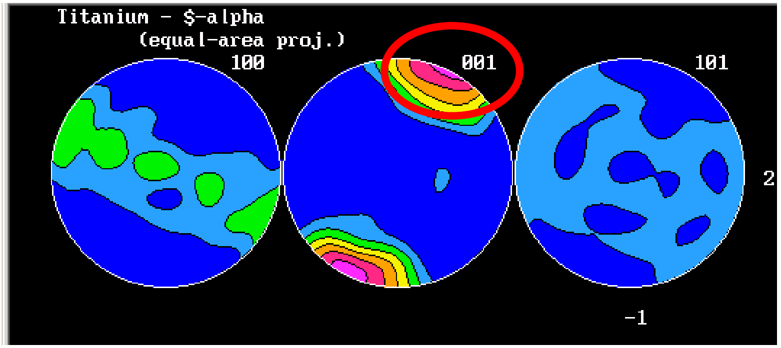
In-situ texture measurements reveal transformation path in Ti64.

α- 500 C

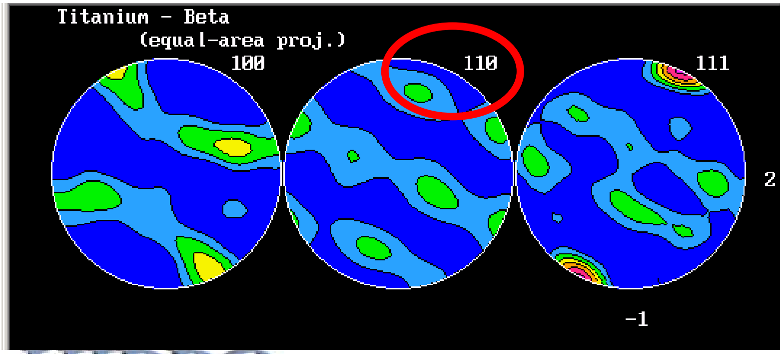


- **α phase below transformation temperature**
- **(001) parallel to rolling normal direction.**
- **Typical titanium rolling texture.**

- **If β phase nucleates from α grains Burgers orientation relationship predicts $(001)_{\alpha}||(110)_{\beta}$.**
- **If β phase grows from pre-existing β grains expect bcc rolling texture, i.e. (111) parallel to rolling normal.**

Dramatic Pause …

β- 1120 C



- **β phase above transformation temperature.**
- **(111) parallel to rolling normal direction.**
- **Texture of β phase is a strong indication for growth from pre-existing grains.**

HIPPO

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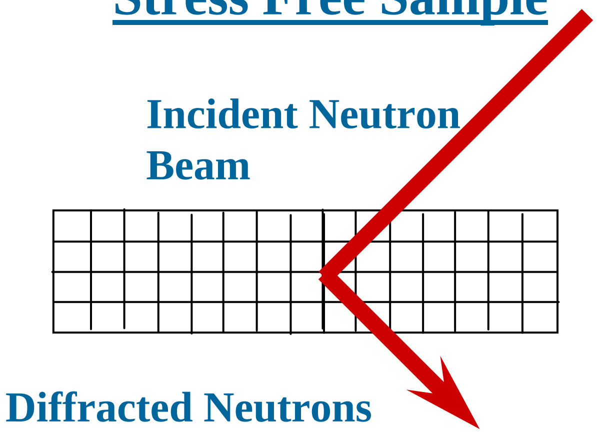
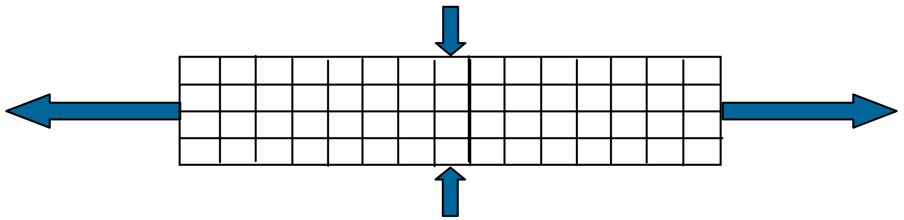
How do we measure strain?

Stress Free Sample



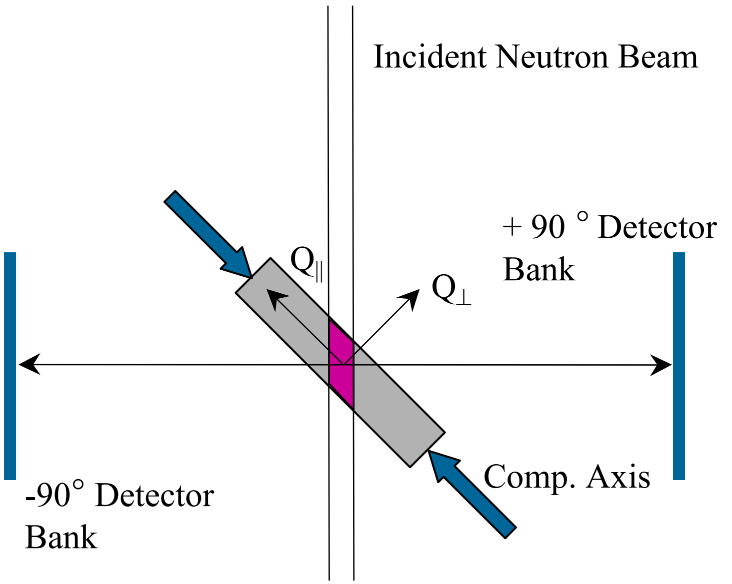
Applied Tension

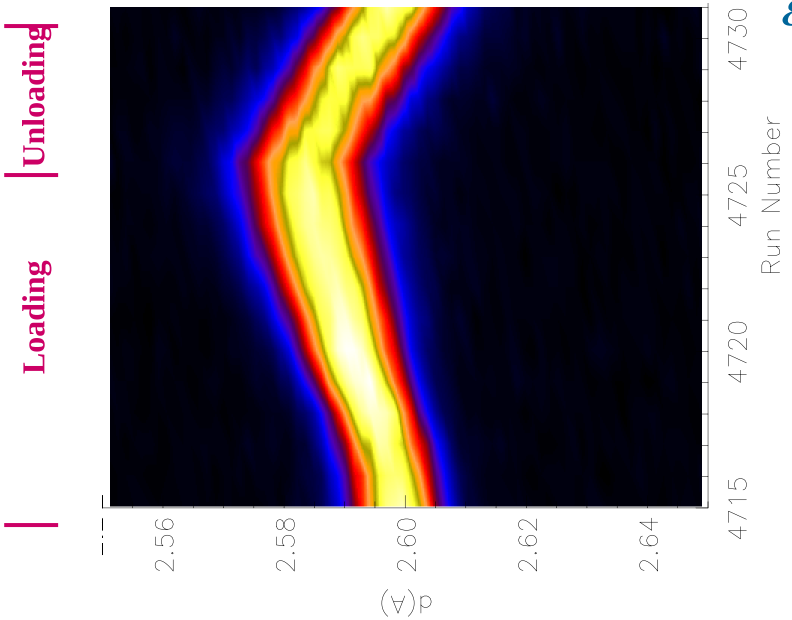


Poisson's Ratio Contraction

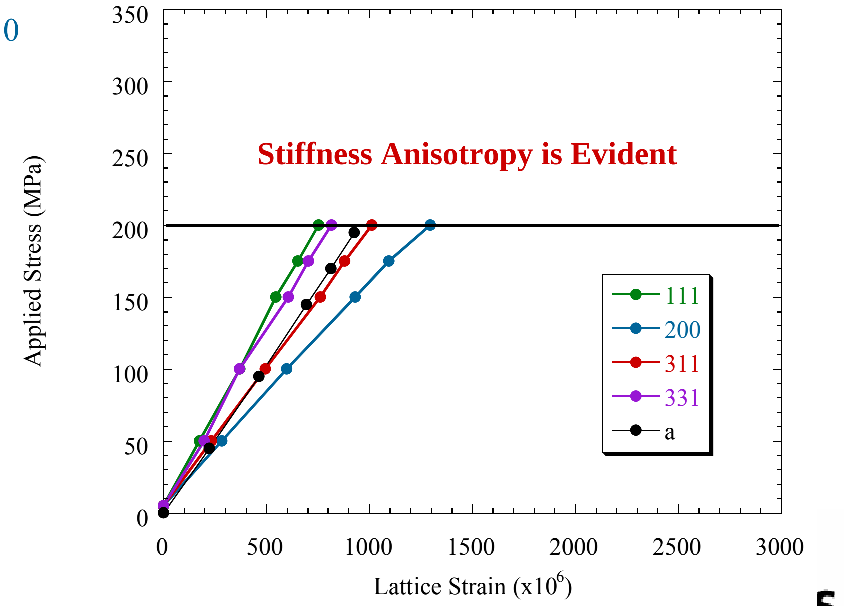
- $\lambda = 2d\sin\theta$
  - Measure d very accurately, 1 part in 10^5.
- Lattice Plane Specific Strains Determined From Deviations From Unstrained Lattice.
  - $\varepsilon_{hkl} = \dfrac{d_{hkl} - d_0}{d_0}$
  - Directly Sensitive to Elastic Strains Only.
- Indirectly Get Information About Plastic Deformation.
- Applied Stress is one example, others include residual stress,temperature, chemistry…

Lattice Response to Applied Stress



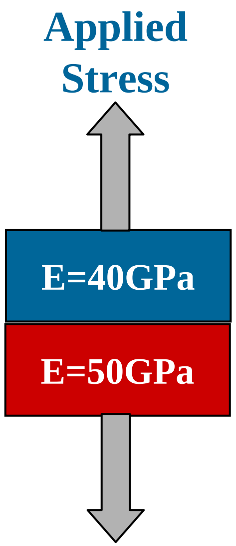


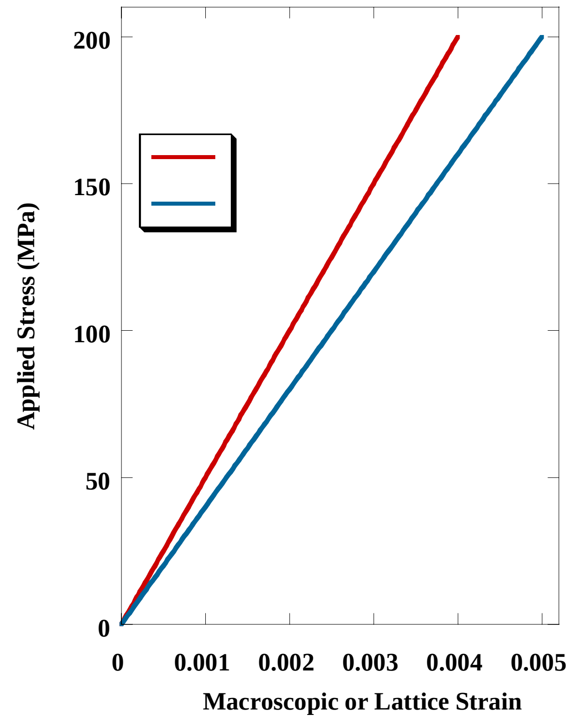
$$\varepsilon = \frac{d - d_0}{d_0}$$



Consider the case of a bi-metallic sample : Elastic loading in series

*(rubber band demo)



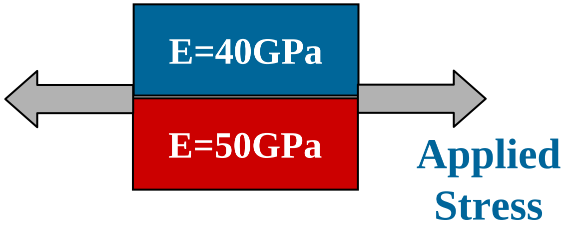


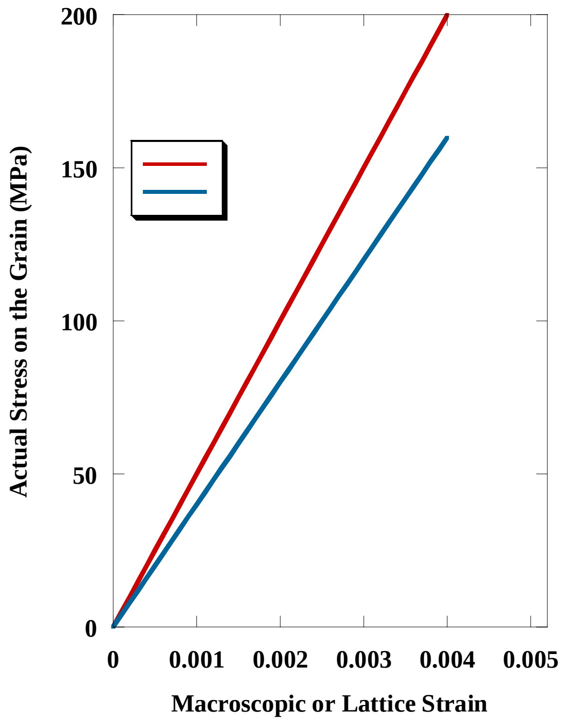
Lattice strain $=(d-d_0)/d_0$

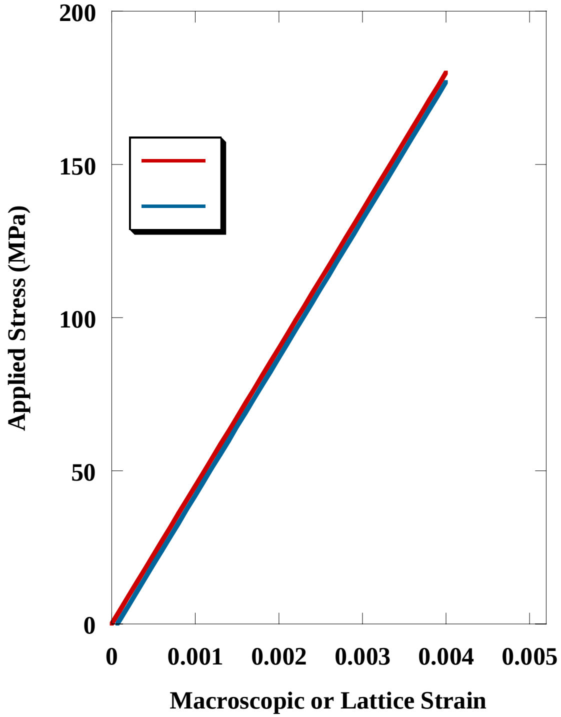
Macroscopic strain $= (l-l_0)/l_0$

- Stress on each is constant, but strain varies.
- Lattice and macroscopic strain are equivalent.

Consider the case of a bi-metallic sample : Elastic loading in parallel

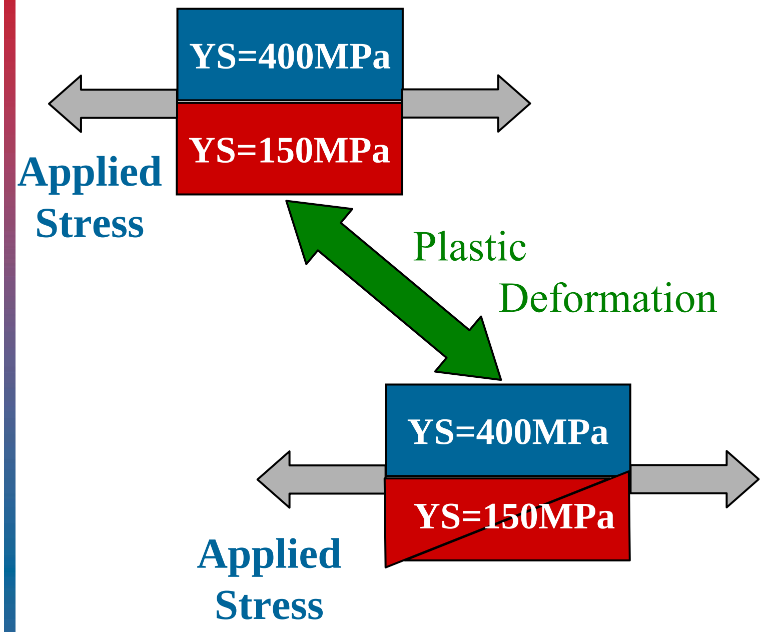


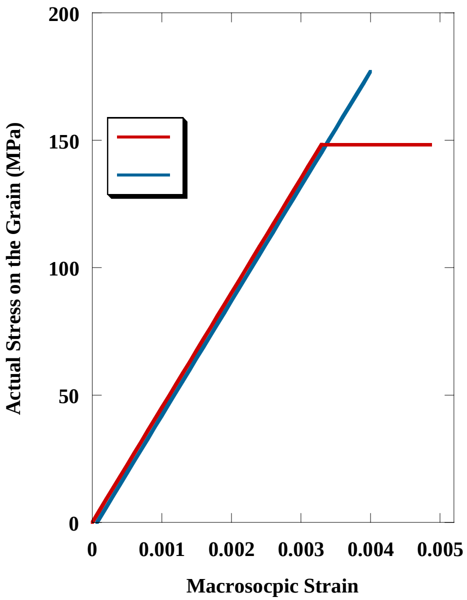


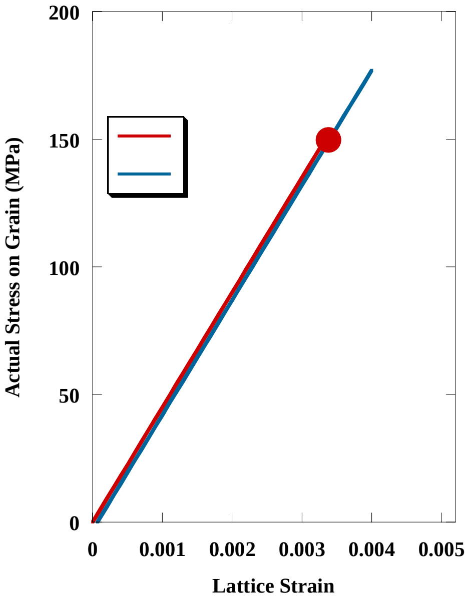


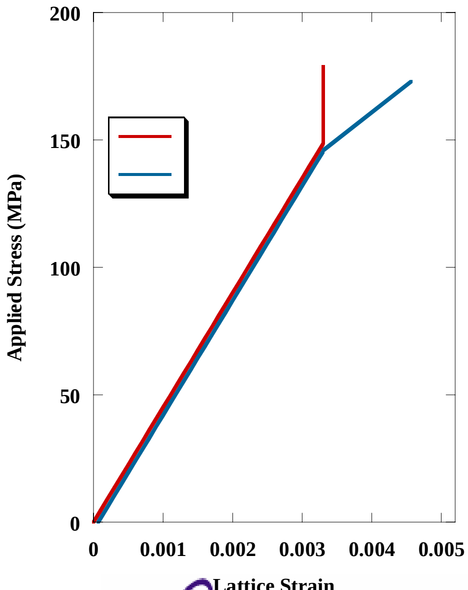
- Stain on each is constant.
- But Stress=Modulus*Strain
- ∴ Actual Stress on each "grain" varies.
- We can only measure Applied Stress macroscopically.

Consider the case of a bi-metallic sample : plastic loading in parallel.









- Plasticity : Macrocopic strain and lattice strain are no longer equivalent.
- Once one component yields, the stress on that component is fixed while macroscopic strain increases (perfect plasticity).
- Similarly, lattice strain is also fixed.
- Again, we can only measure Applied Stress vs Lattice Strain.
  - Characteristic Y shape associated with plastic deformation.
  - Deviatiation of lattice strain from linear is the “Intergranular Strain”.

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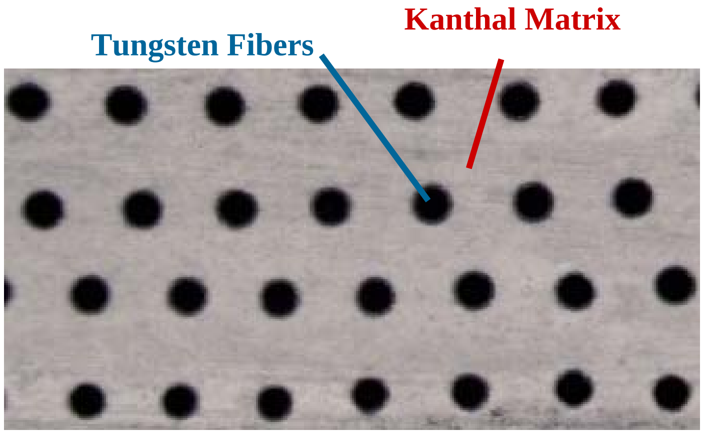
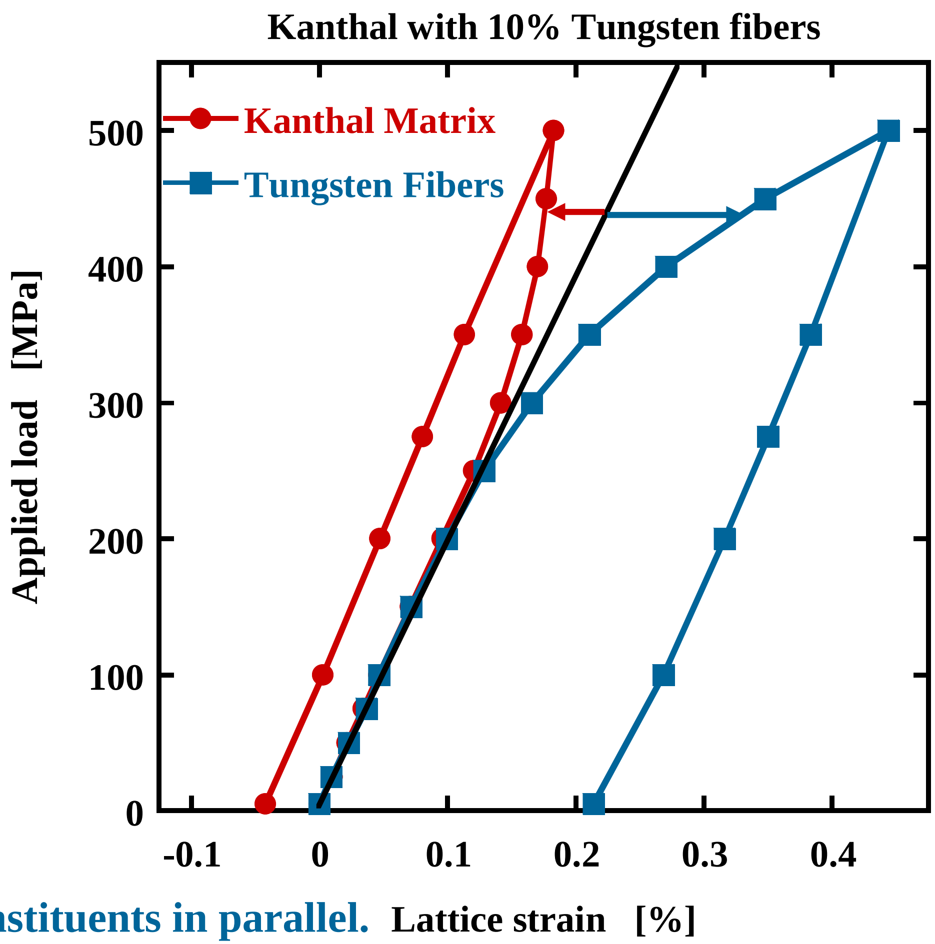
Next step in complexity : a two phase composite





- Microstructure represents loading 2 constituents in parallel.
- In elastic regime, lattice strains are equivalent.
- Saturation of lattice strain in plastic regime in Kanthal indicates that it has yielded.
  - Call Kanthal the “soft” phase.
  - Intergranular strain = deviation from linearity.

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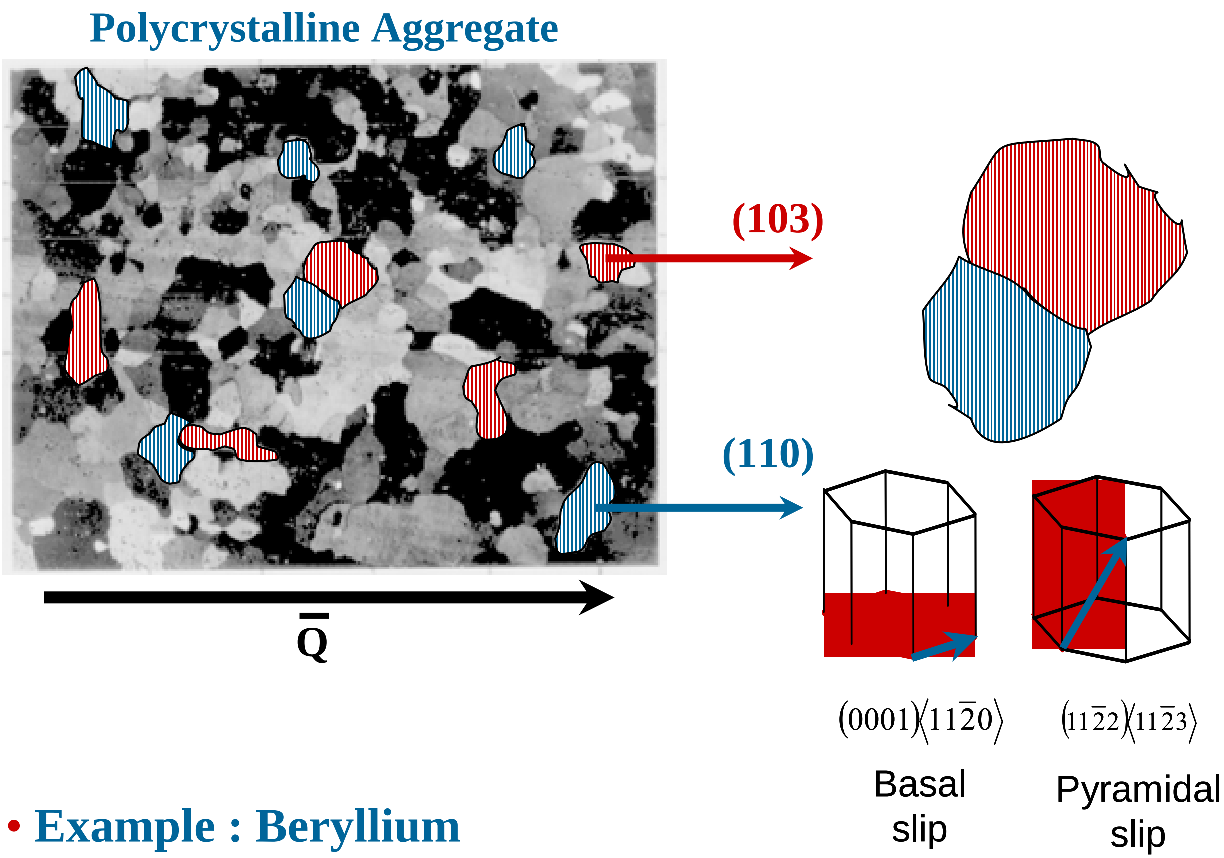
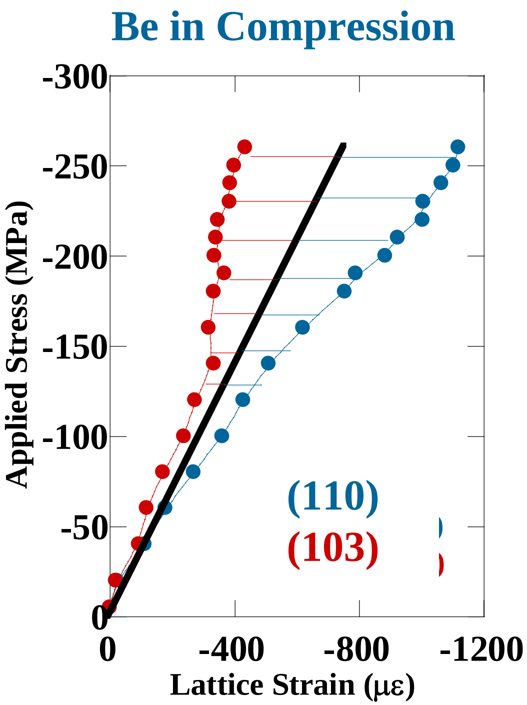
Next Consider Anisotropic Polycrystalline Samples : “The Mother of All Composites”.





- **Example : Beryllium**
  - **Microstructure is somewhere between loading in parallel and series.**
  - **Yield strength when loaded along different plane normals is disparate.**
  - **Saturation of elastic strain indicates plastic deformation in a unique set of grain orientations.**
  - **(103) is “soft orientation”; (110) is “hard orientation”.**

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  - If we have time : Residual Stresses in Welds

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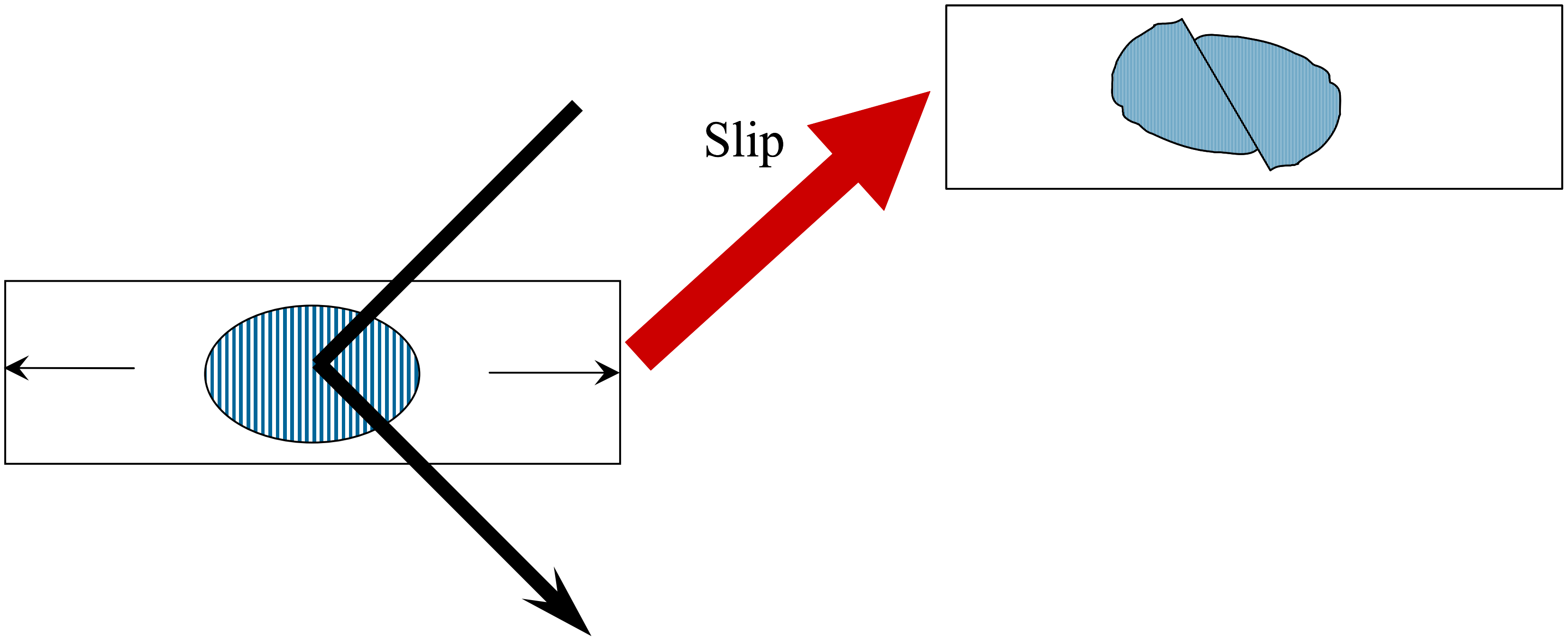
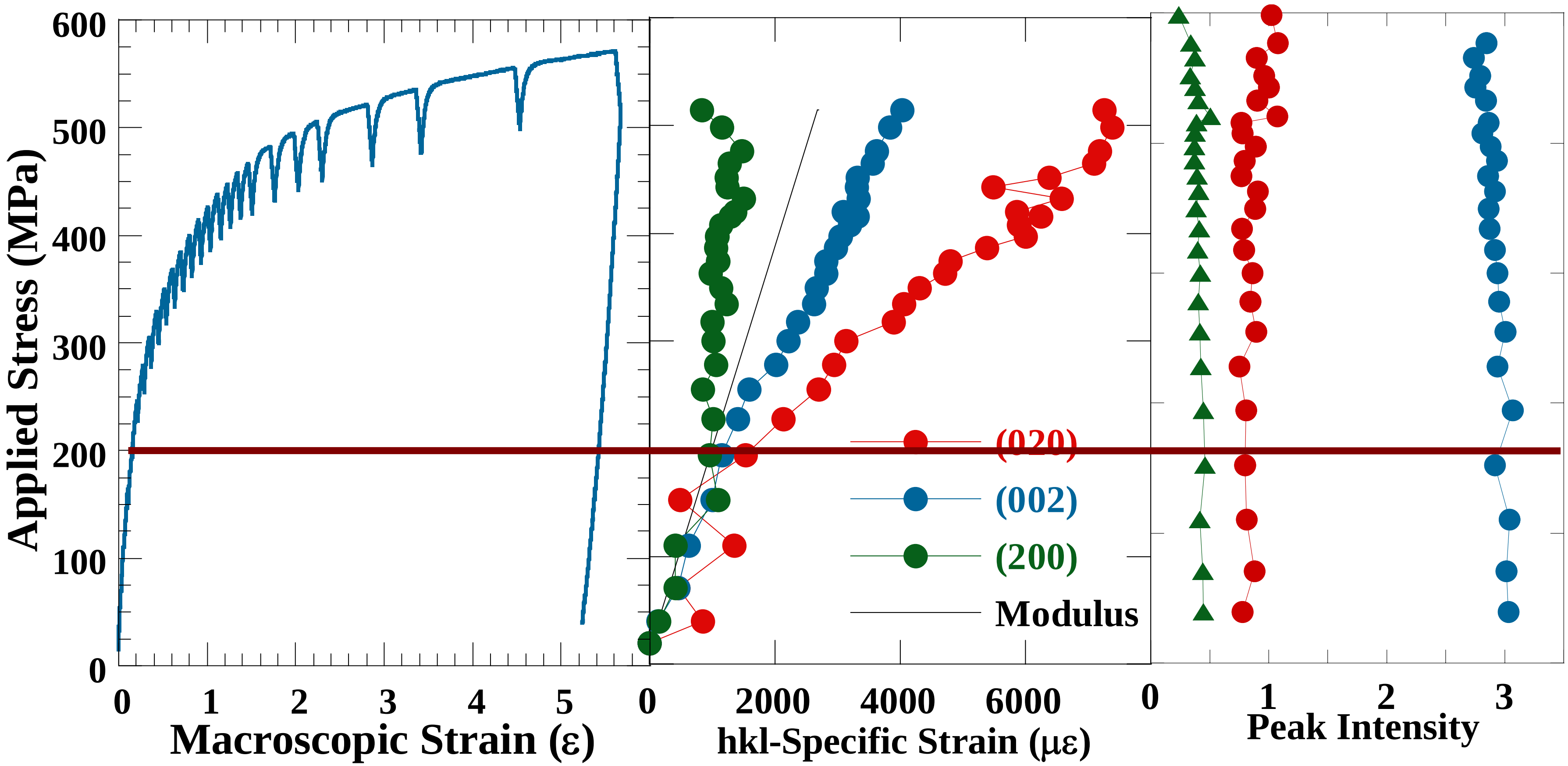
Plastic Deformation Mechanisms Have Distinct Diffraction Signatures



• **Slip : little if any change in peak intensity, broadening proportional to dislocation density.**

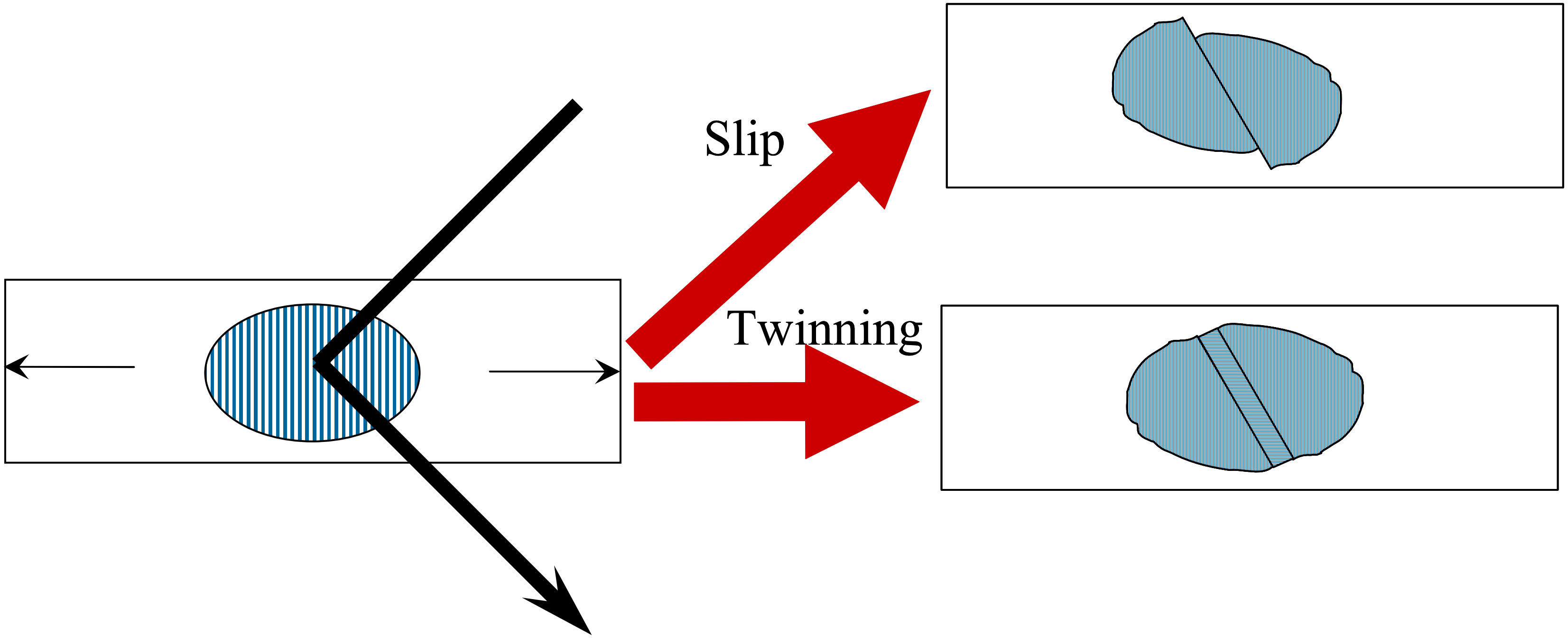
Plastic Deformation of Uranium



• Deviation of lattice strains from linearity indicates that plastic deformation has initiated.

• Lack of change of peak intensity suggests it is slip dominated.

Plastic Deformation Mechanisms Have Distinct Diffraction Signatures



- Slip : little if any change in peak intensity, broadening proportional to dislocation density.
- Deformation twinning : large changes in single peak diffraction intensity.

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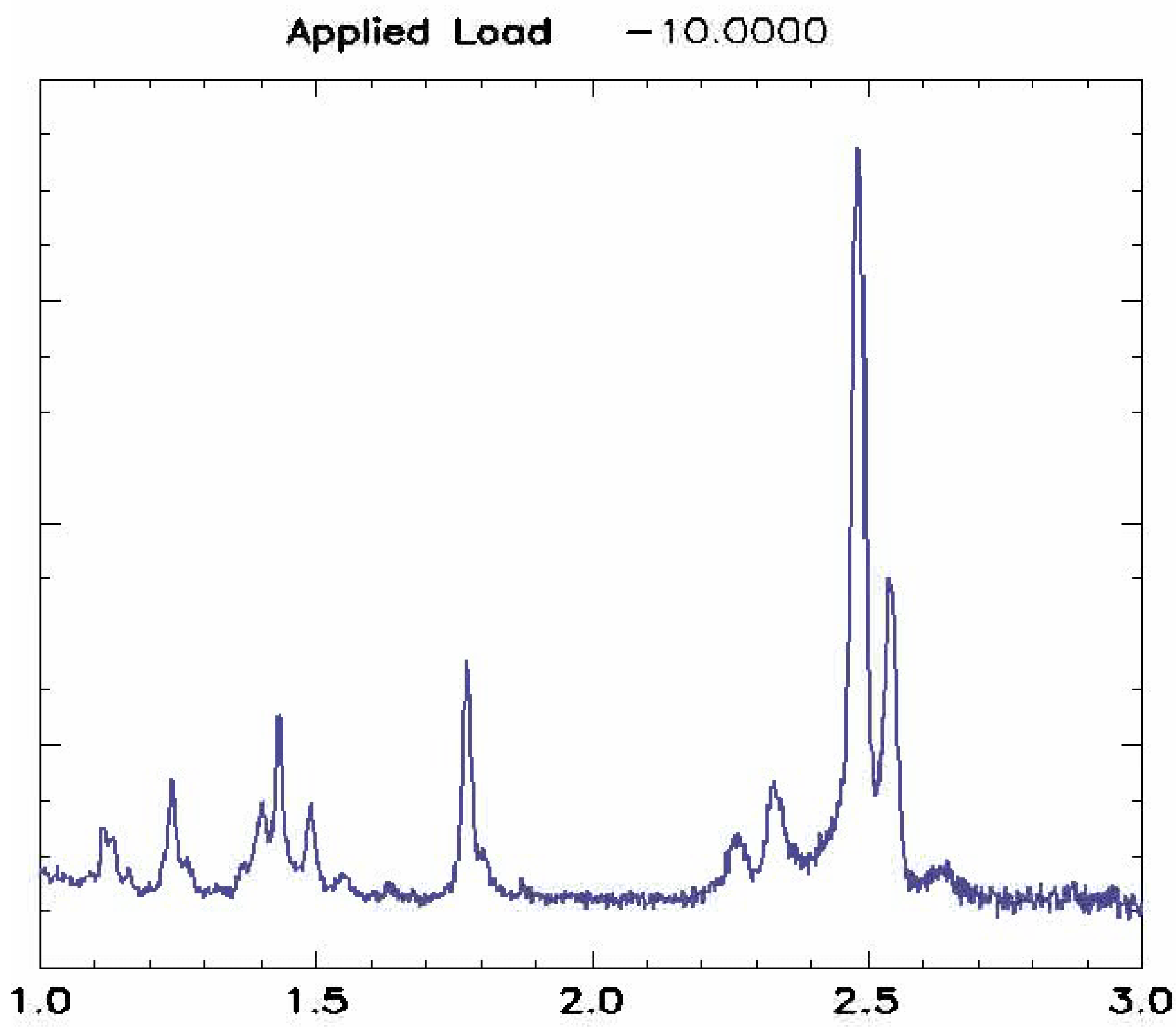
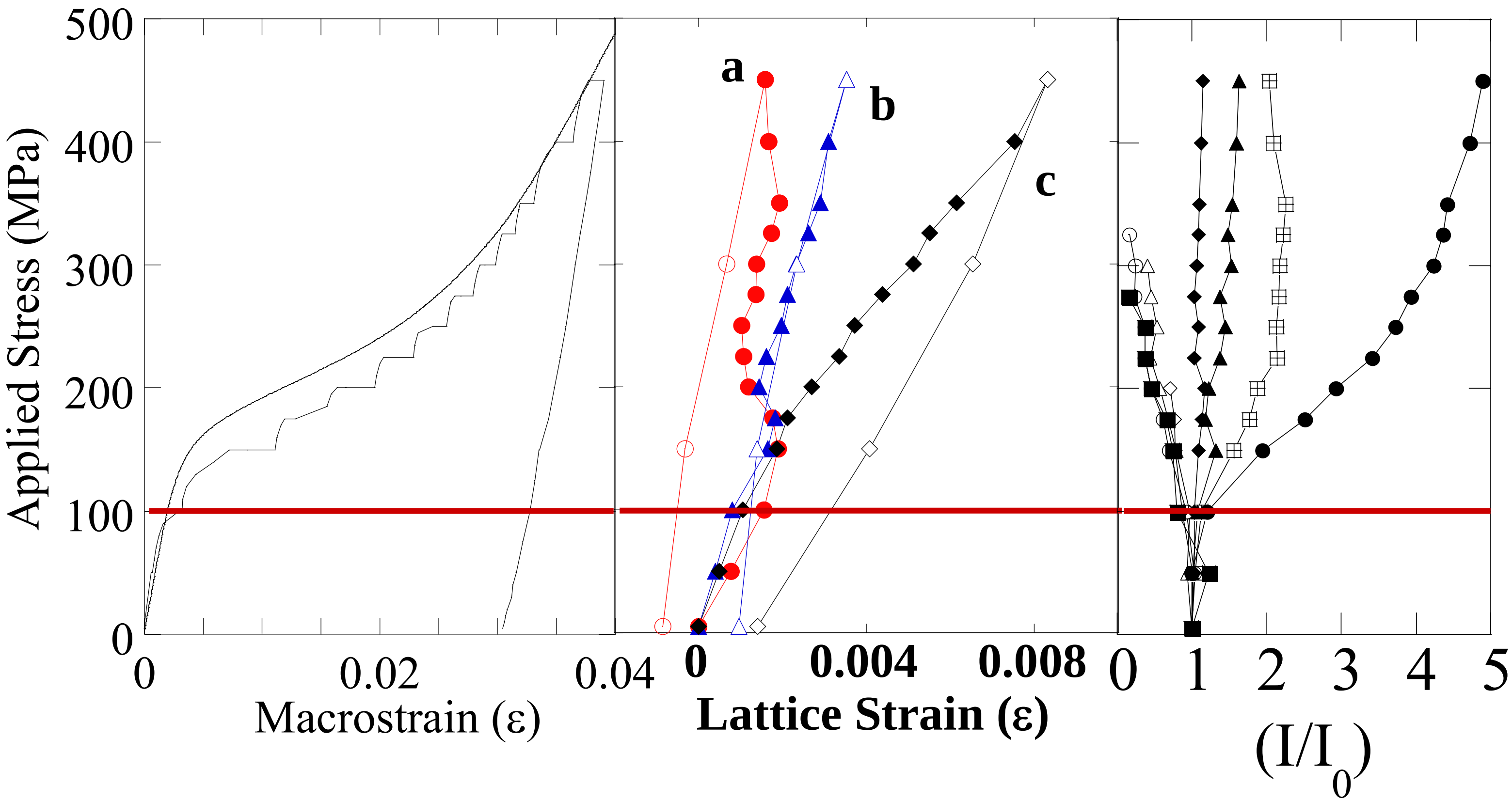
Neutron Diffraction Indicates Twinning Reorientation During Deformation of U6Nb



Deformation Twinning is a Relaxation Mechanism for Twinning Grains



- Deviation of lattice strains from linearity indicates that plastic deformation has initiated.
- Significant change of peak intensity suggests it is twinning dominated.

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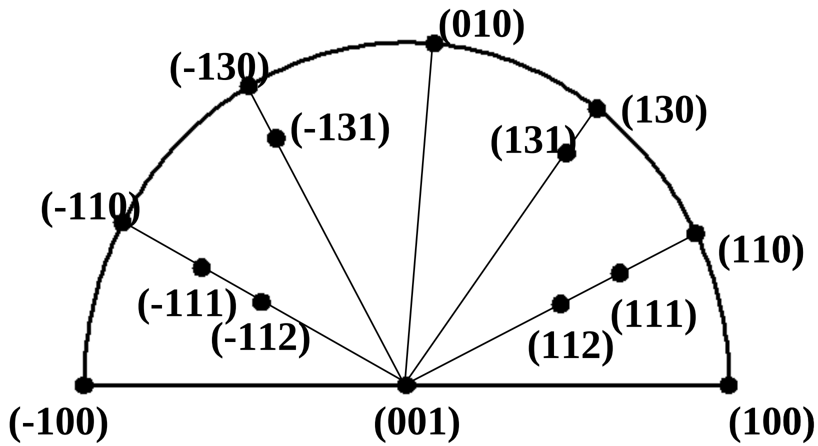
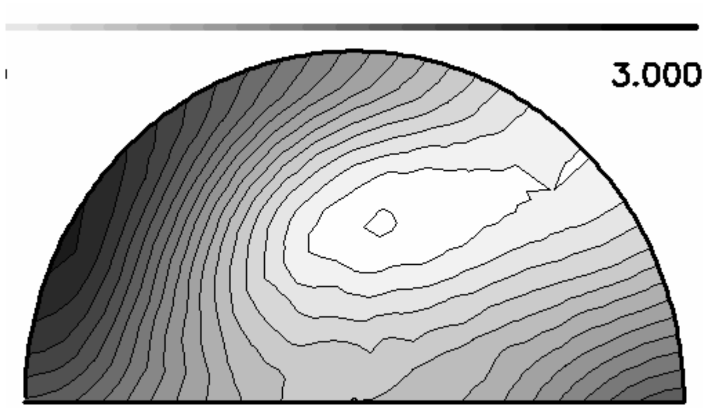
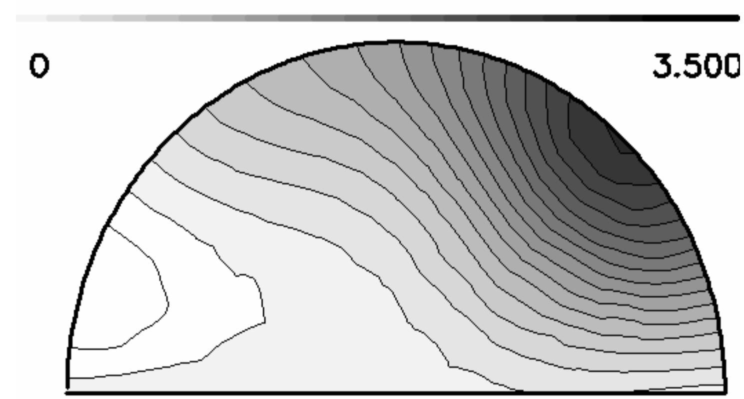
Texture Development During Deformation of U6Nb Indicates Deformation Twinning



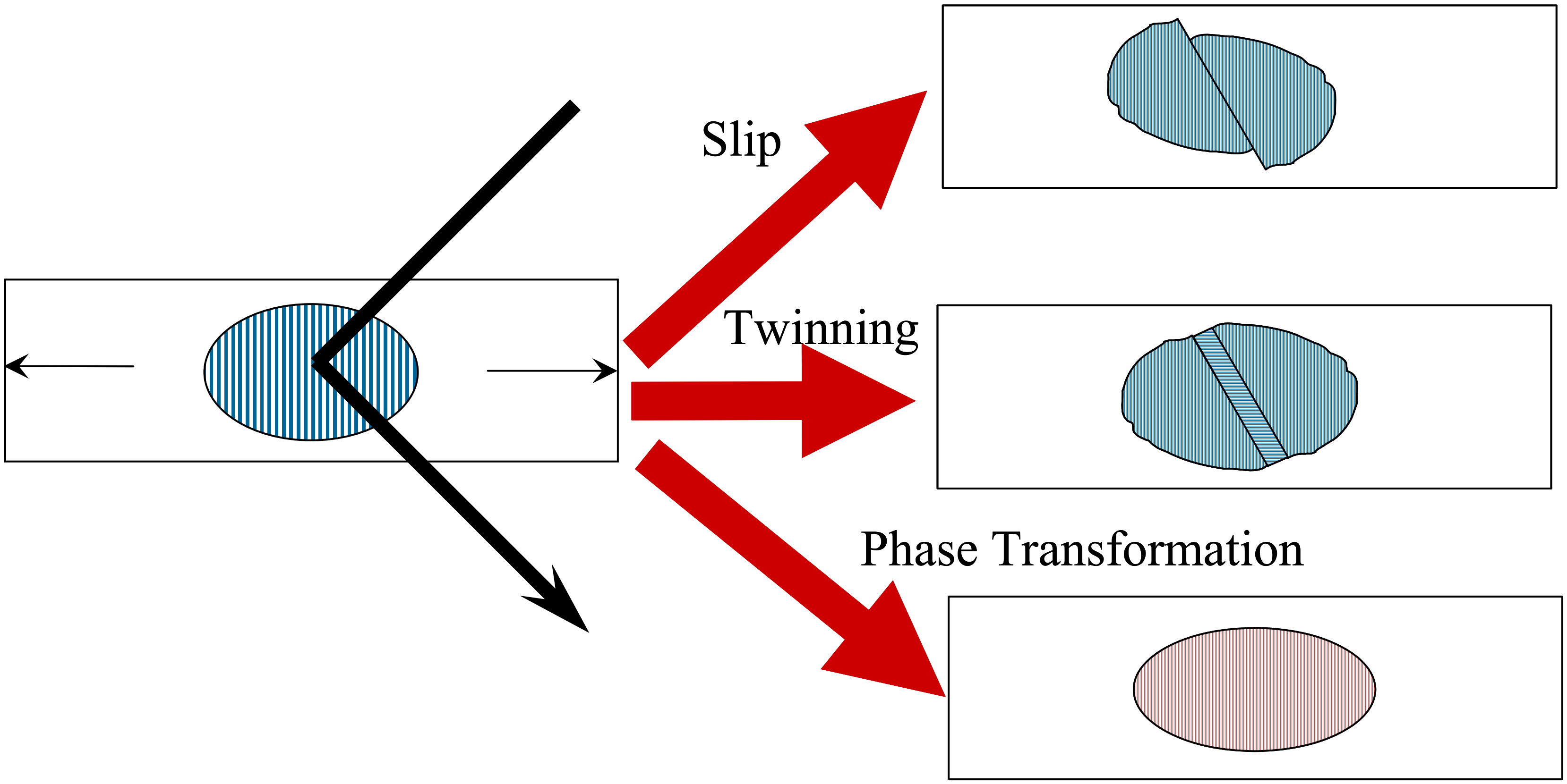


Compression



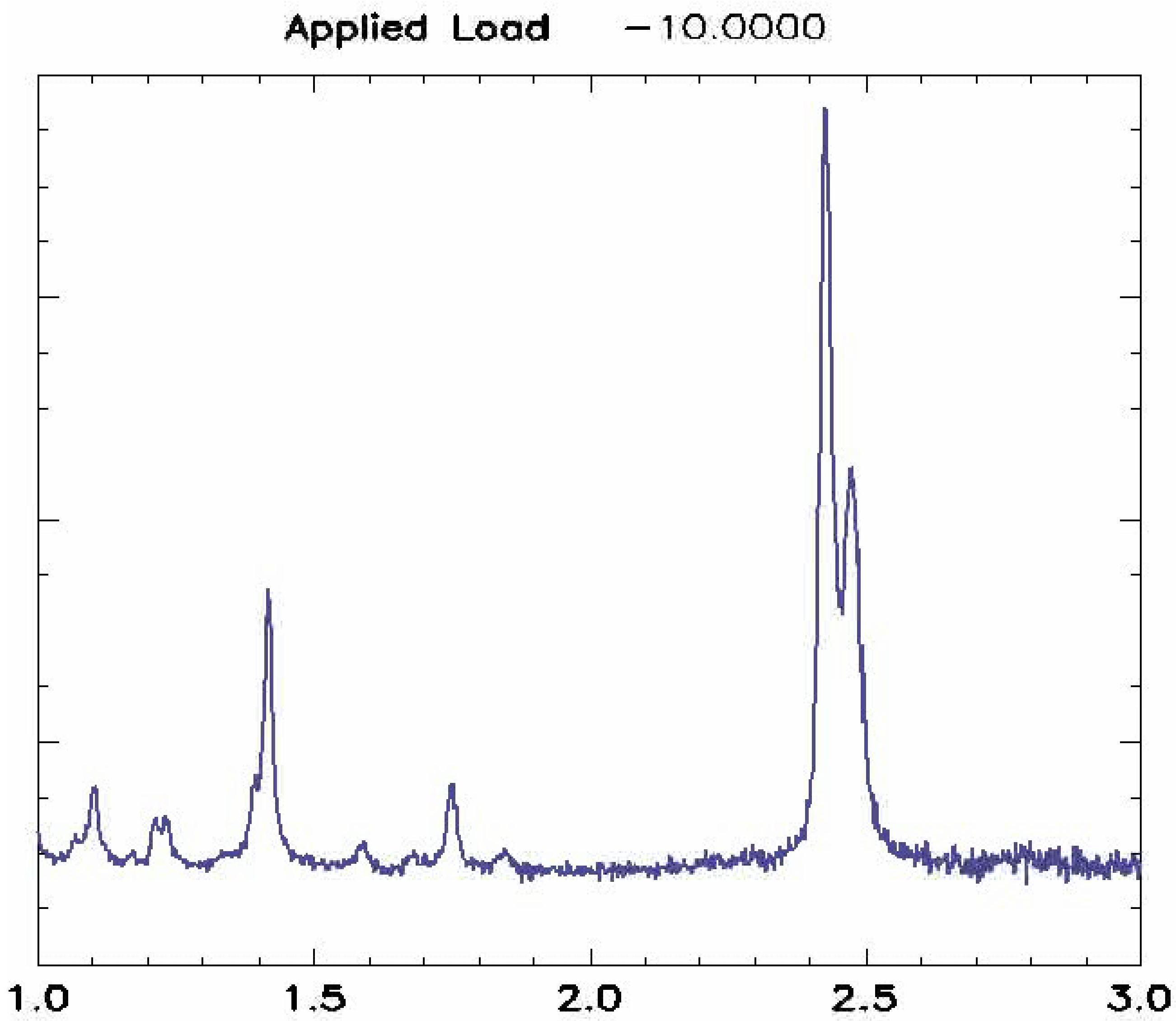
Tension

Plastic Deformation Mechanisms Have Distinct Diffraction Signatures

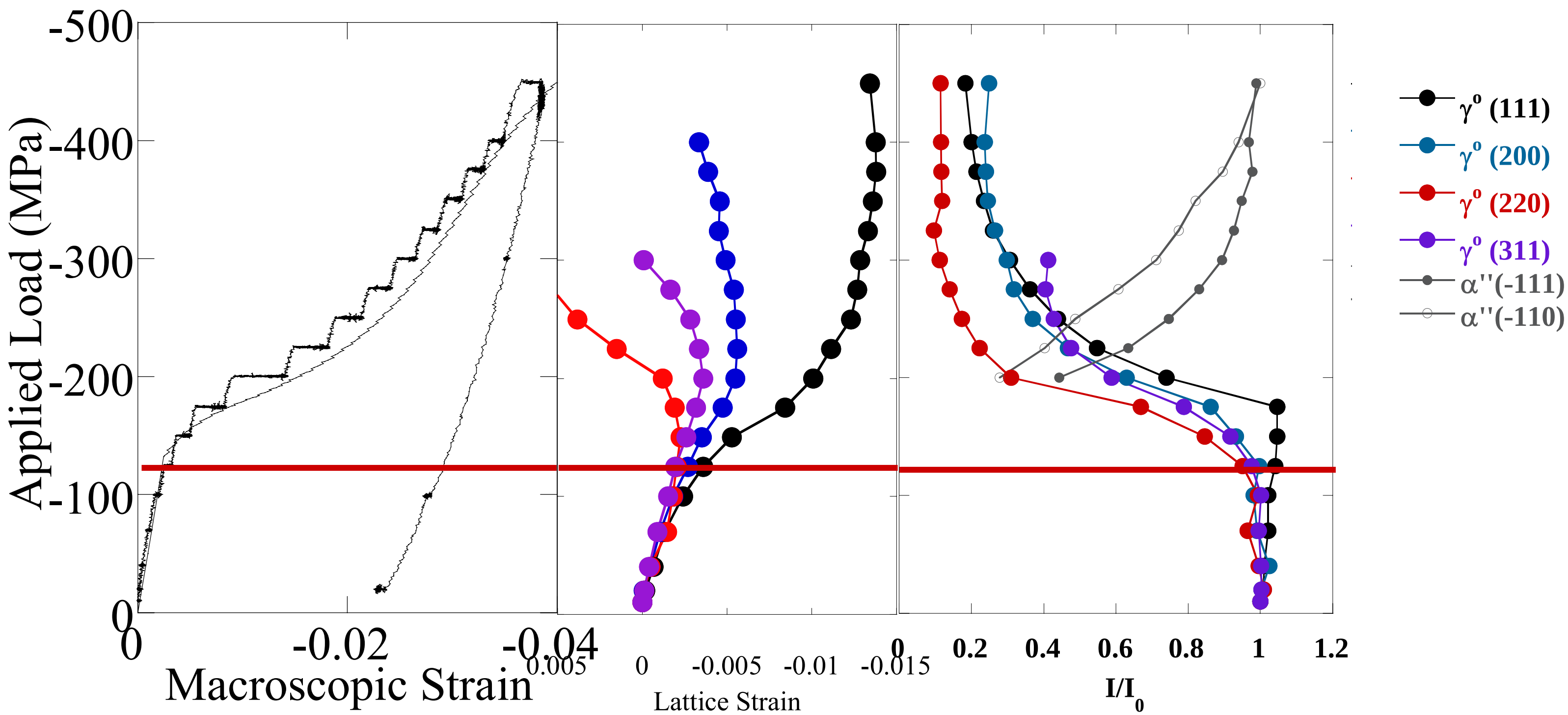


- Slip : little if any change in peak intensity, broadening proportional to dislocation density.
- Deformation twinning : large changes in single peak diffraction intensity.
- Phase transformation : appearance of new crystal symmetry.

New Peaks In U7Nb Indicate Stress Induced Phase Transformation.



Deformation Twinning is a Relaxation Mechanism for Parent Grains



• Deviation of lattice strains from linearity indicates that plastic deformation has initiated.

• Addition of new peaks suggests stress induced phase transformation.

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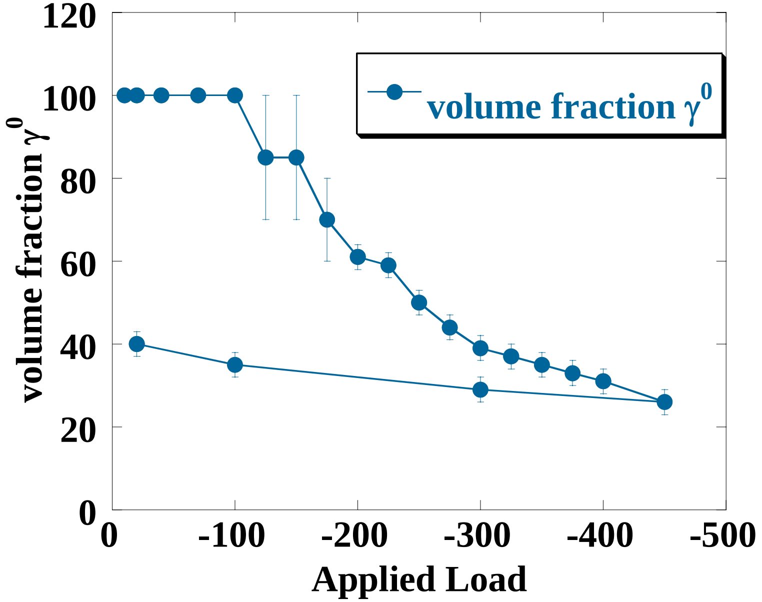
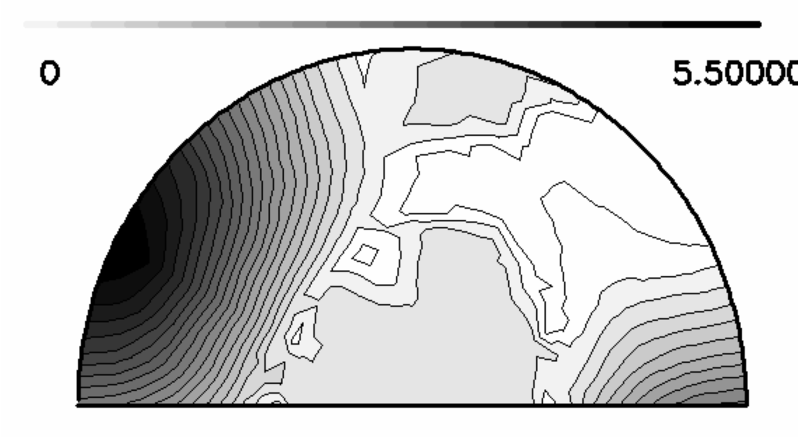
In-Situ Neutron Diffraction Monitors Volume Fraction and Texture During Deformation





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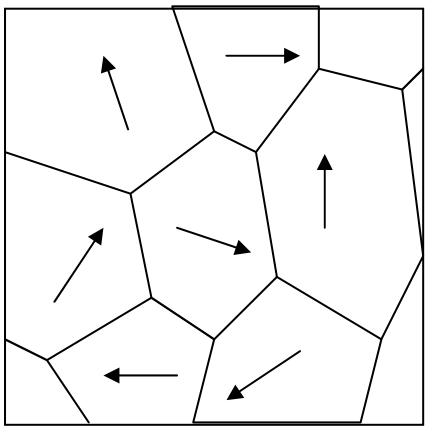
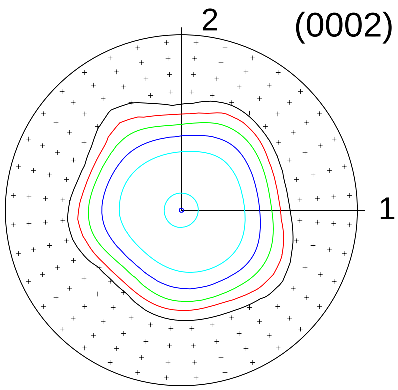
Polycrystalline Plasticity Models

The aggregate is modeled as a collection of crystal orientations with associated volume fractions chosen to reproduce the texture.



Aggregate properties are given by averages performed over the grains.

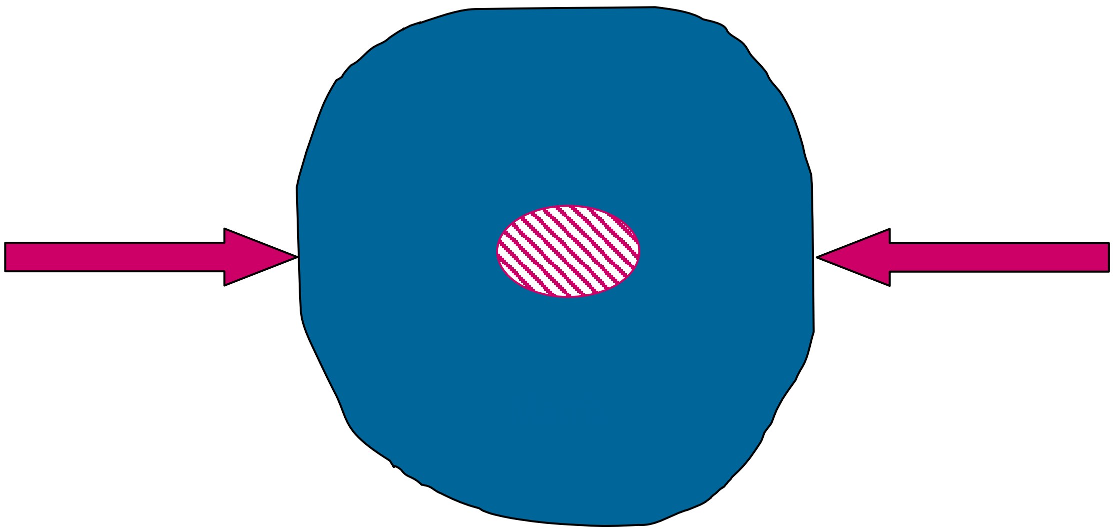
Anisotropy follows from texture and averaging procedure.



rolled Mg
(1944 orientations)

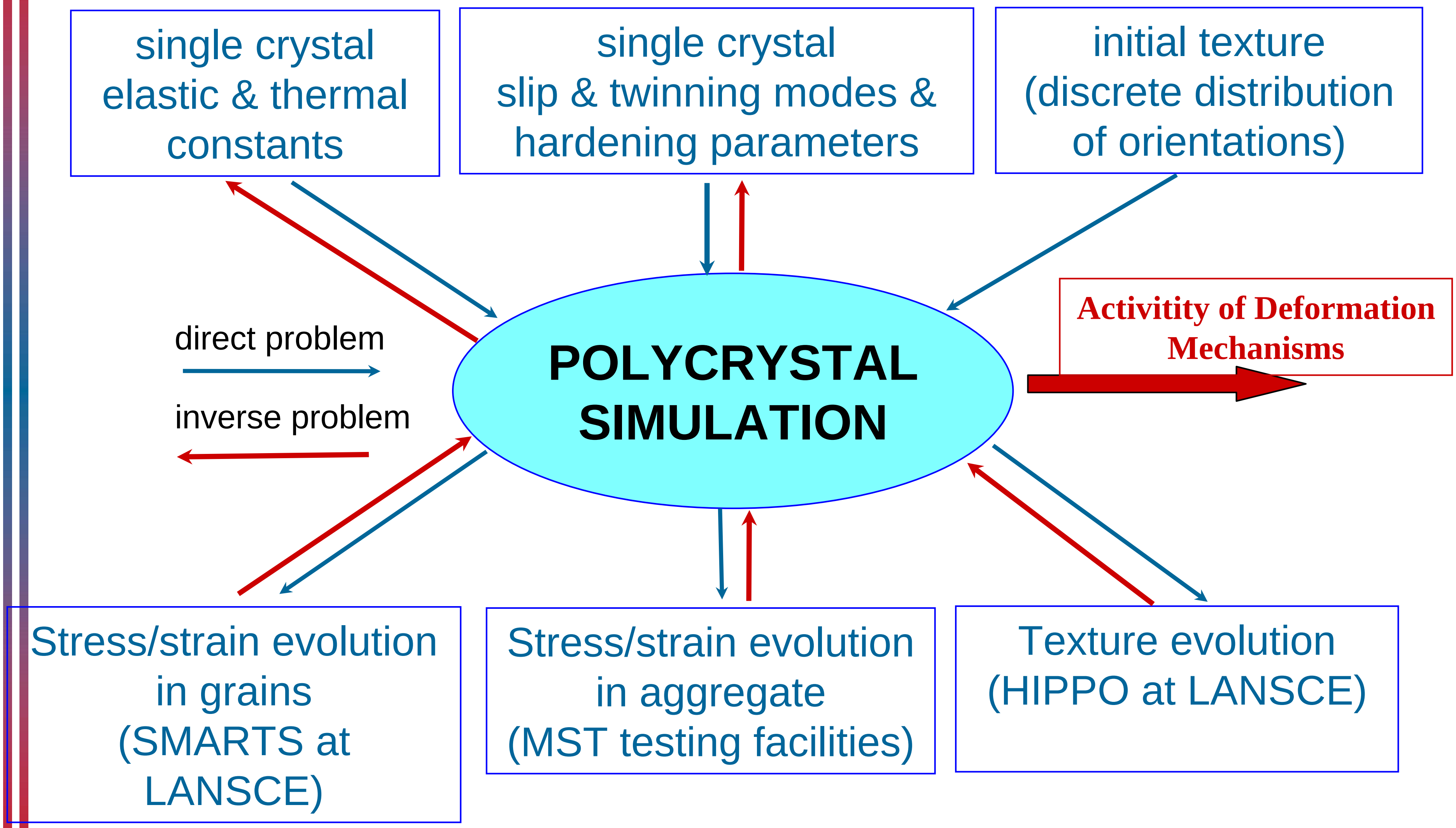
Polycrystal models provide a link between macroscopic response and microstructure

Use Visco-Plastic Self-Consistent Model to Help Interpret Diffraction Data



- Input : Material properties : CRSS's, hardening, texture…
- Calculates deformation in an elliptical included grain in homogeneous matrix (HEM).
  - Eshelby inclusion theory.
- Repeat for distribution of grain orientations : match known texture.
  - HEM properties equal to a weighted average of all grains.
- Keeps track of deformation activities and texture development.

Input/output To Polycrystal Model



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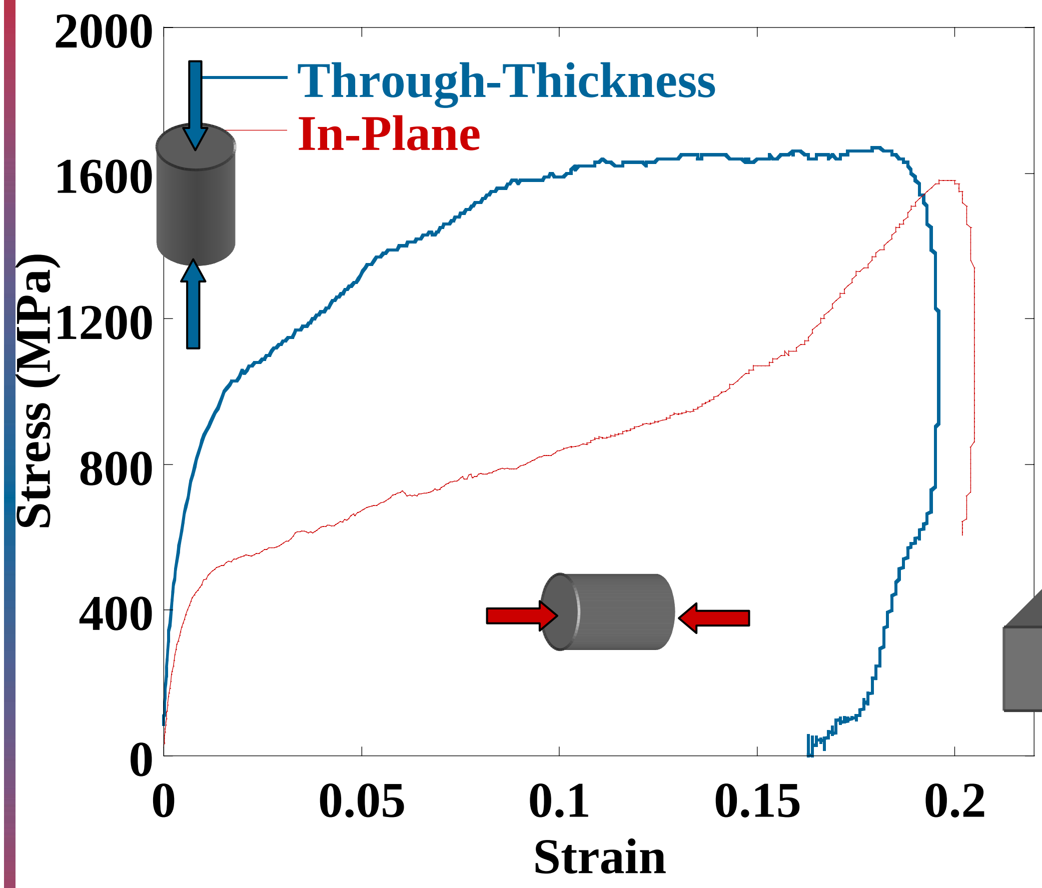
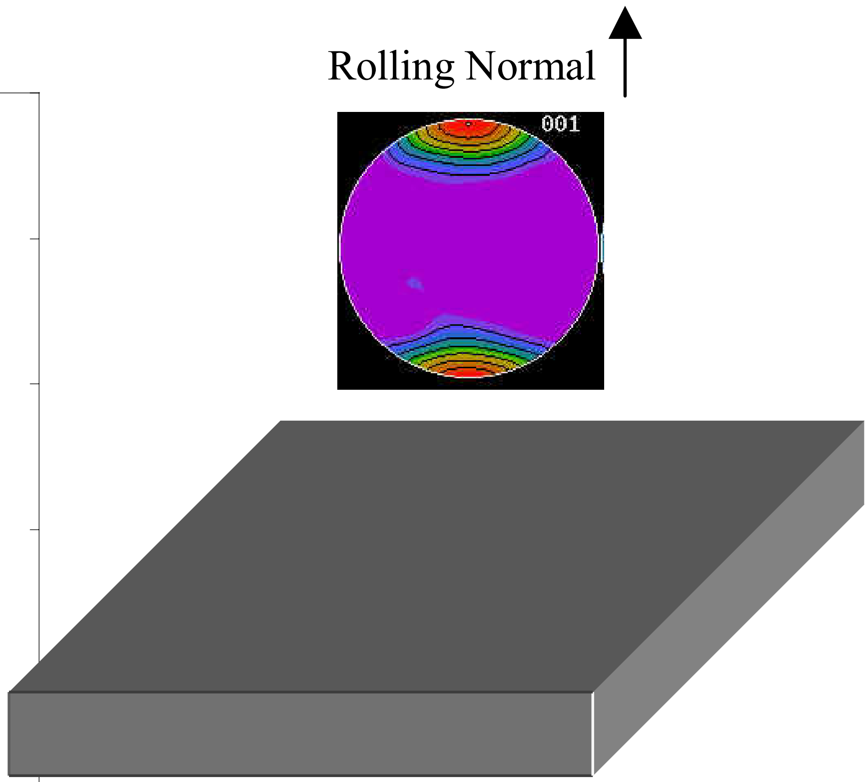
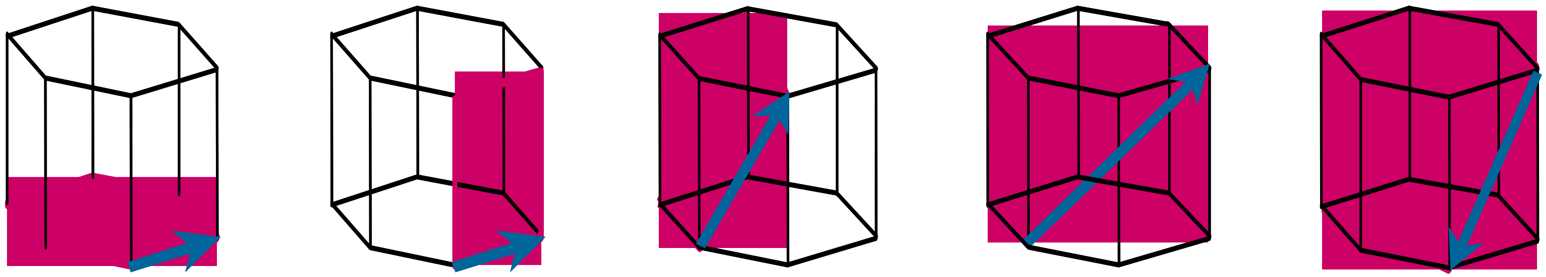
Example 4 : Anisotropy of Rolled Beryllium Plate



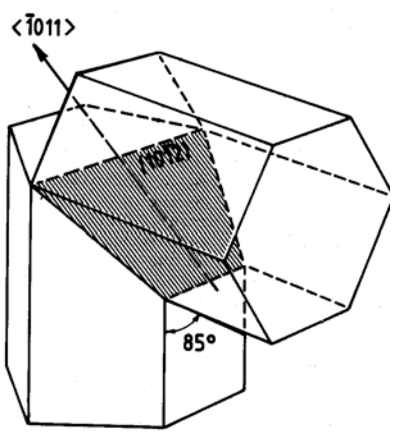


• Macroscopic response to applied load is dramatically orientation dependent.

Background : Viable Deformation Mechanisms in Hexagonal Metals

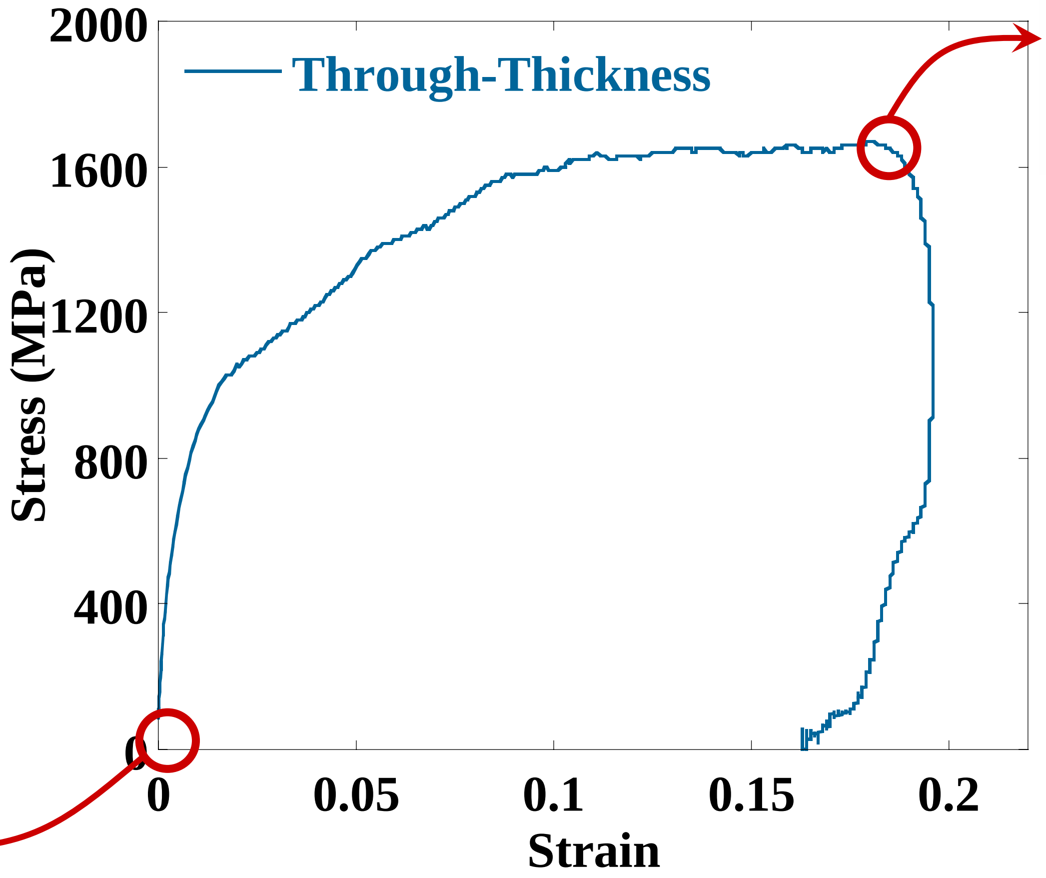


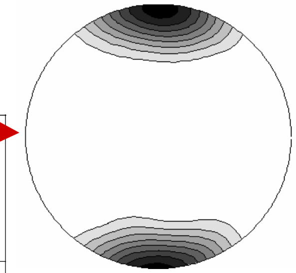
$(0001)\langle 11\bar{2}0\rangle$	$(10\bar{1}0)\langle 11\bar{2}0\rangle$	$(11\bar{2}2)\langle 11\bar{2}3\rangle$	$(10\bar{1}2)\langle 10\bar{1}1\rangle$	$(10\bar{1}1)\langle 10\bar{1}2\rangle$
Basal slip	Prismatic slip	Pyramidal slip	Tensile twin	Compressive twin

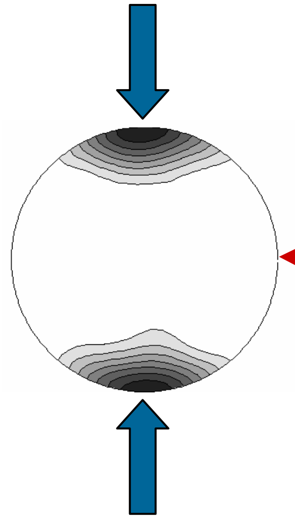


- Operation of twin mechanism alloys grain to extend or contract depending on c/a ratio.
- Causes discrete reorientation of crystal axis.
- In beryllium, convenient switching of a and c axis directions.

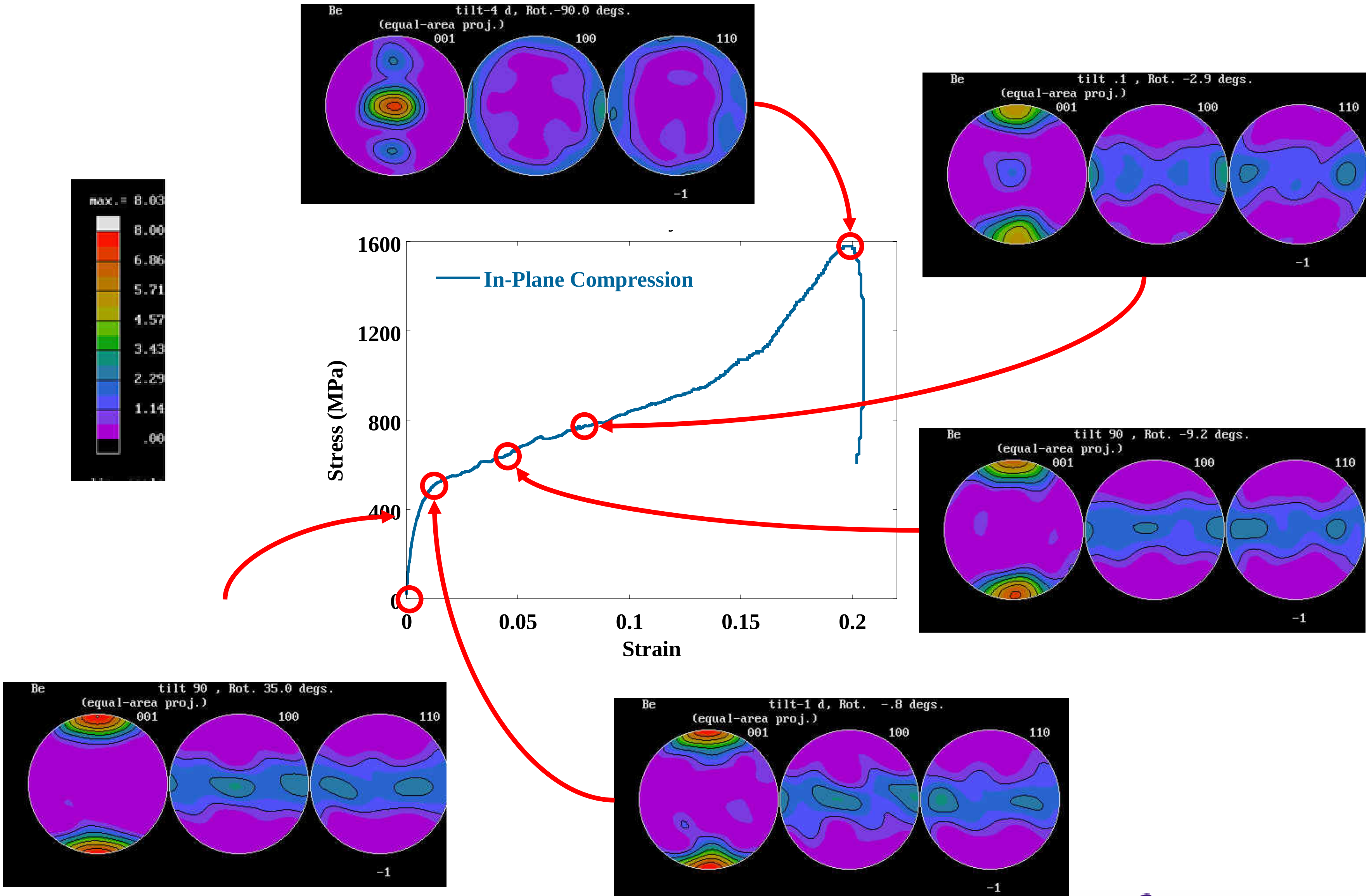
Experiment : Ex-Situ Post-Portem Texture Measurements After Interrupted Deformation







Texture Development of Rolled Beryllium During In-Plane Compression



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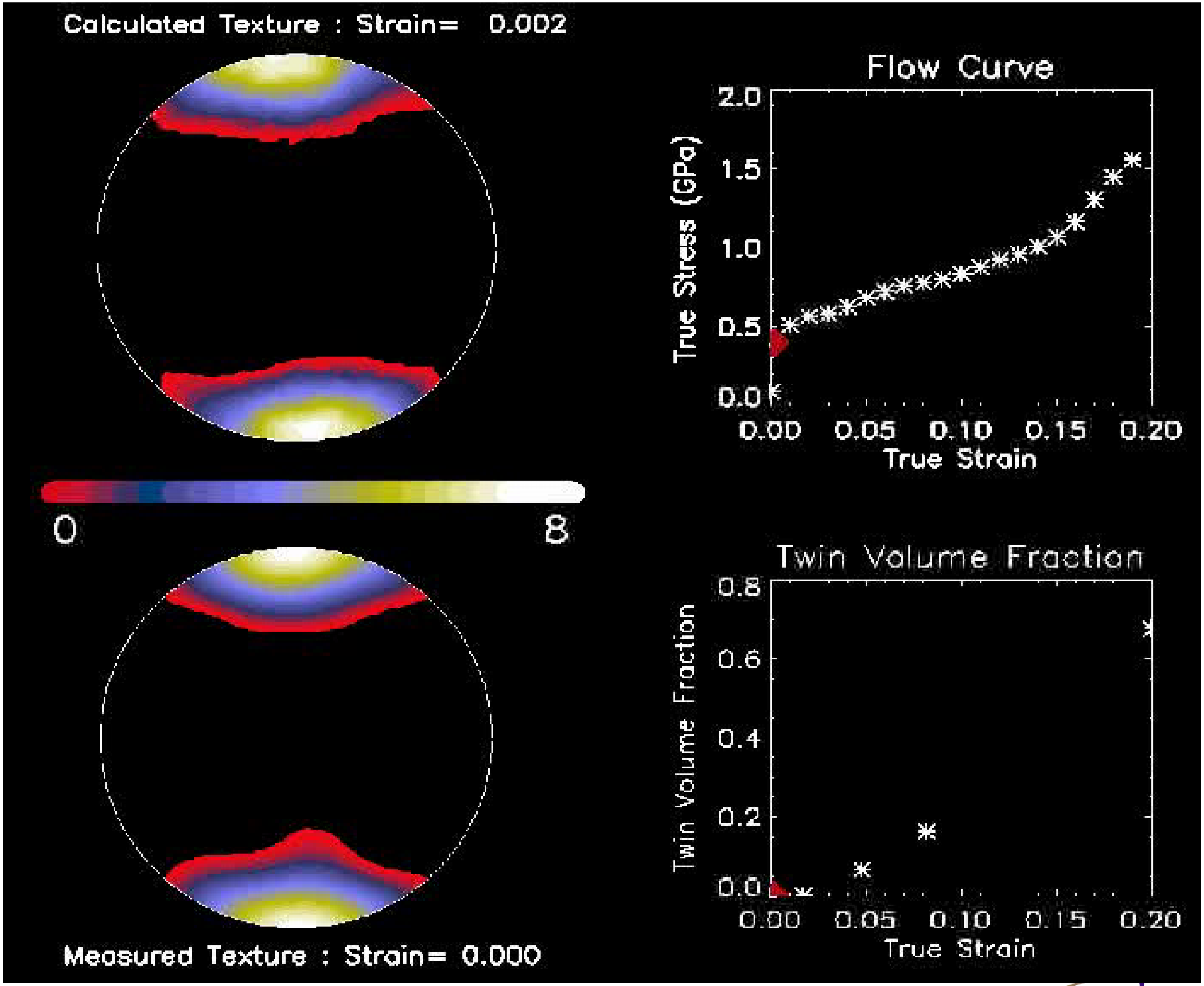
After Iteration of Input Parameters, Model Compares Well With Data



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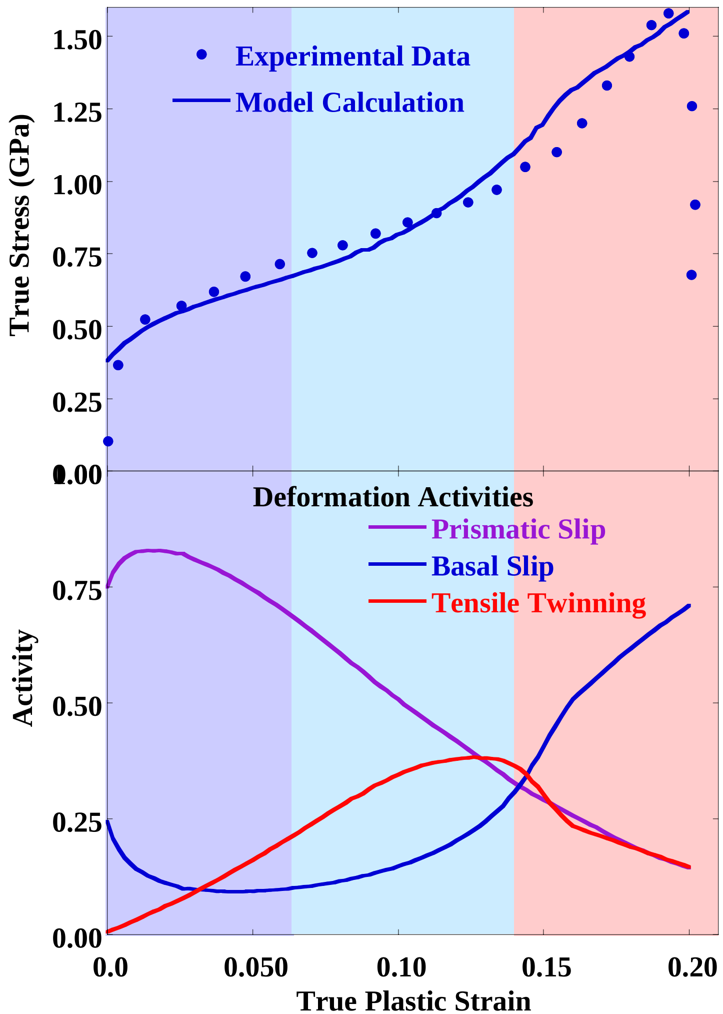
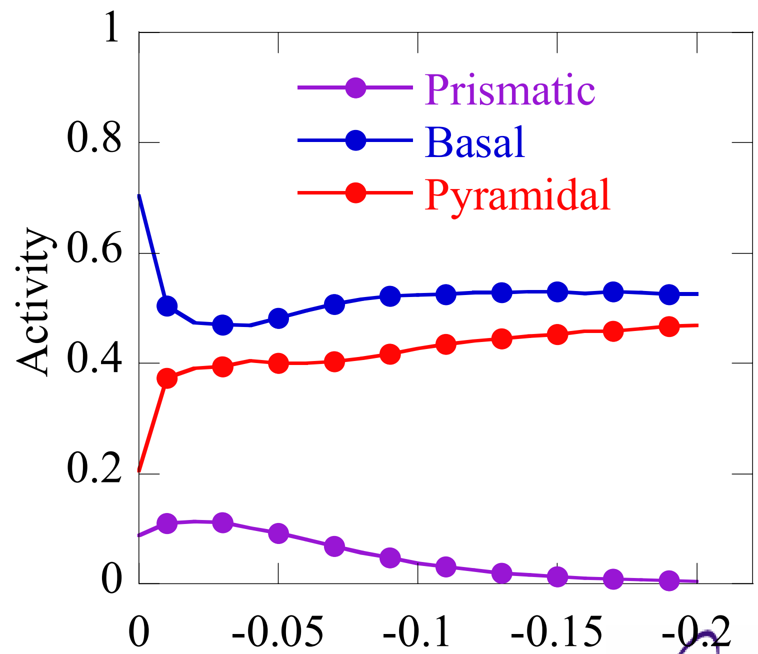
Model Provides Detailed Understanding of Microscopic Deformation Mechanisms.



- Low Strain : few grains aligned for basal slip.
  - Prismatic slip dominates deformation at ε < 6%.
- Intermediate Strain : Prism grains hardening
  - Twinning important at 6% < ε < 14%.
- Large texture : Twinning exhausted.
  - New texture allows for basal slip.
  - Basal slip dominates at ε > 14%.



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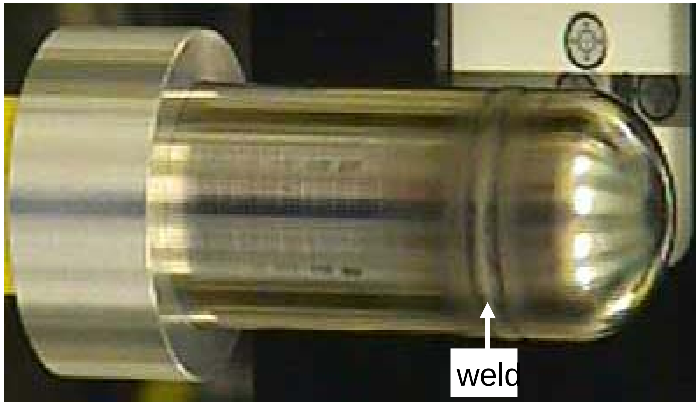
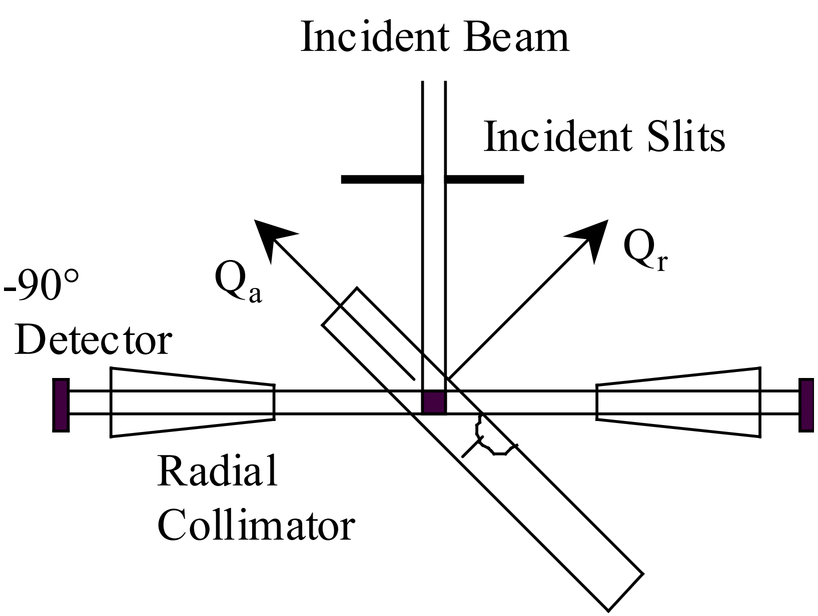
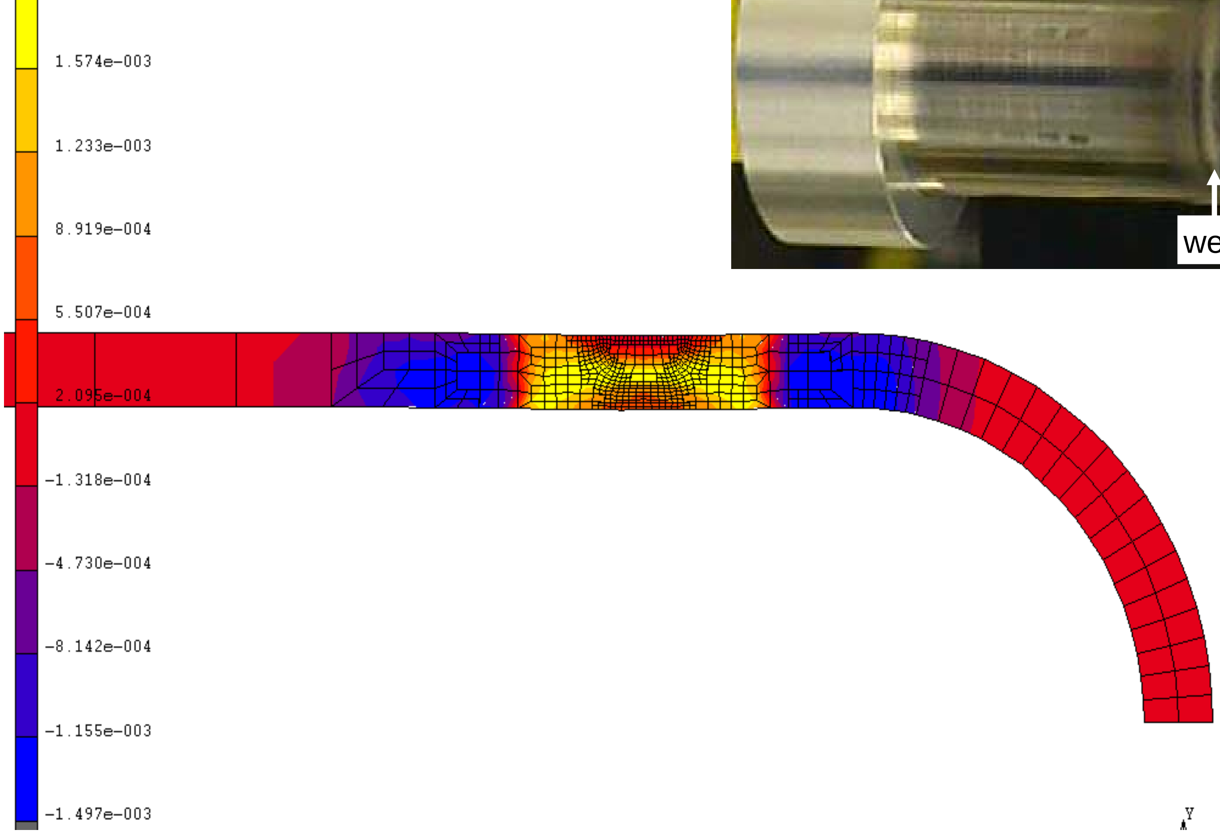
Example 5 : Residual Stresses in Welded Haynes 25 (Cobalt) Container.

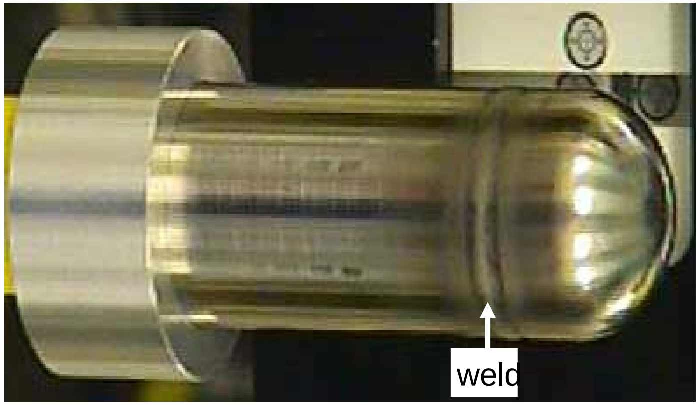




a.

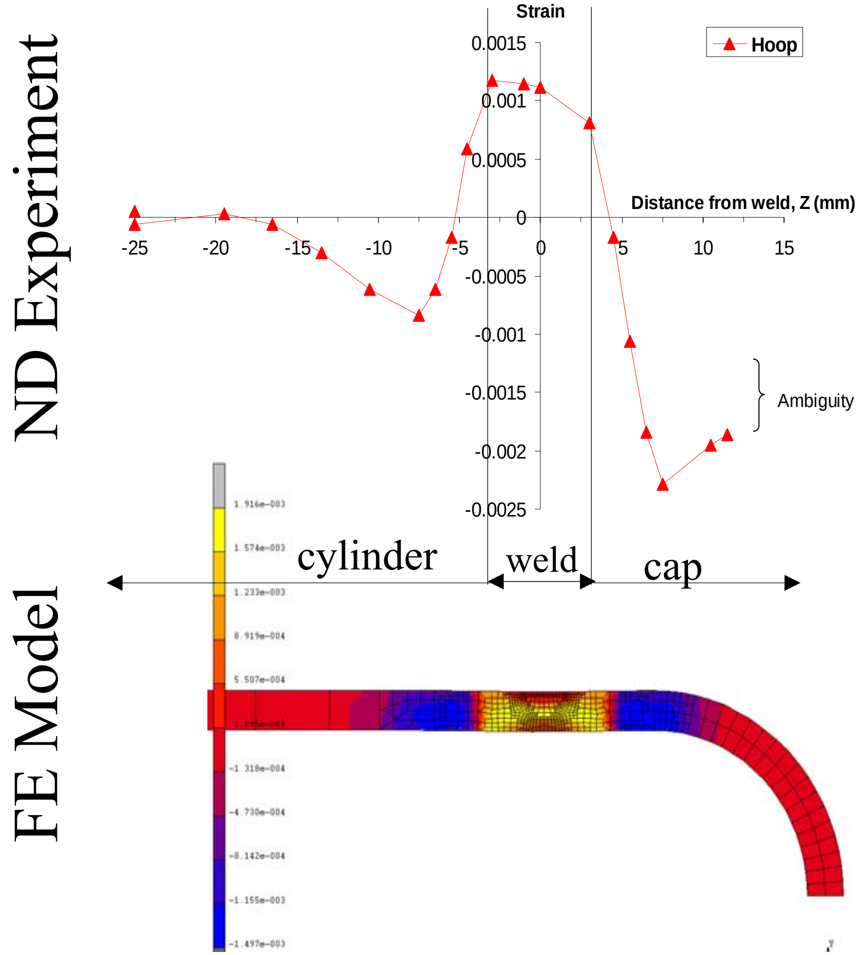
Finite Element Model Calculates Residual Stresses/Strains.





- If you believe model, do not need measurements.
- Moreover, if you validate model with one measurement, you do not need more.

Neutron Diffraction Strain Map Used to Validate Finite Element Model



Now the model can be used to optimize weld procedure or predict lifetime …

Larsson et al., accepted by Mat. Sci. Eng. A (2004)

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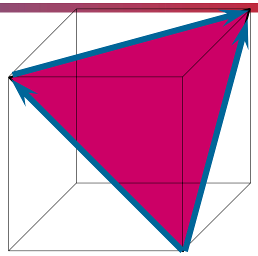
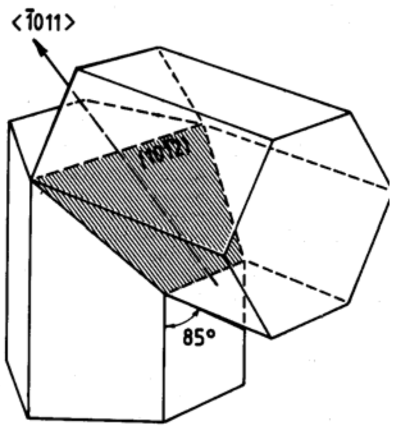
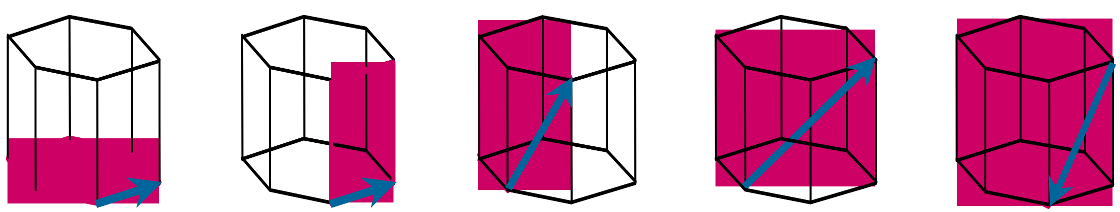
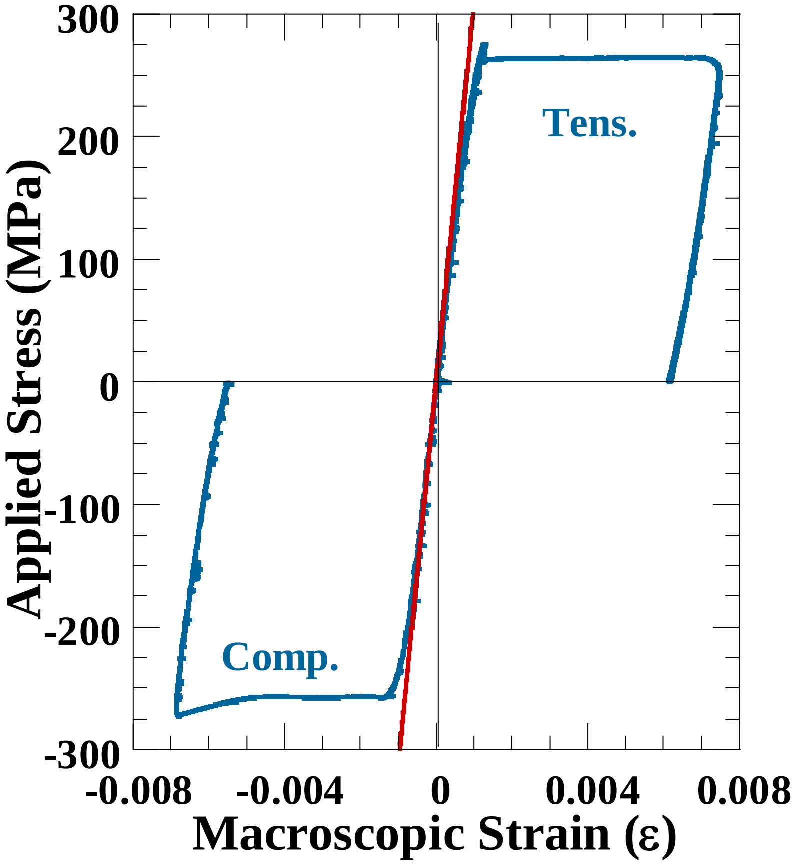


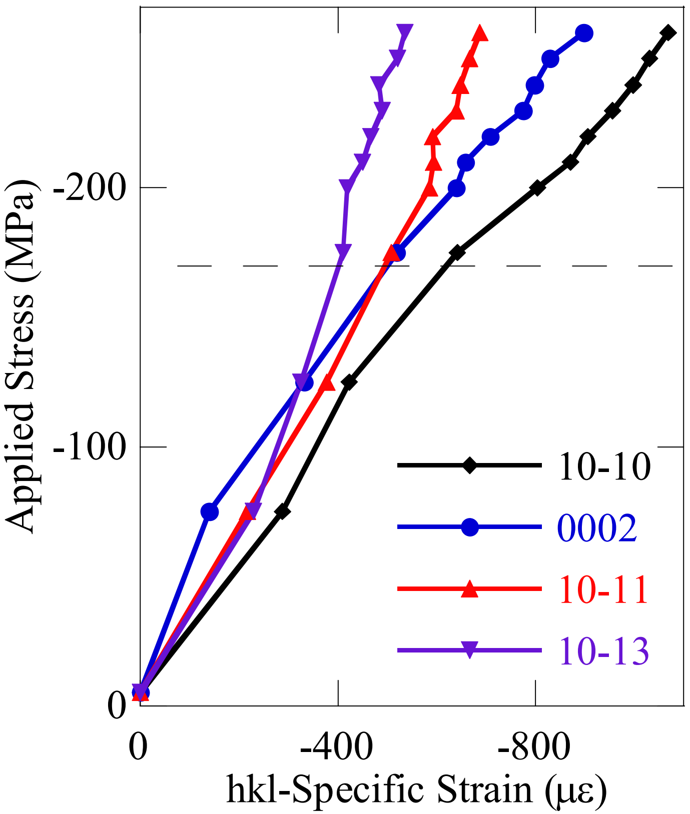
- Face Center Cubic materials : Deform on {111}<110> slip system
  - 12 equivalent modes.
  - Can manipulate mechanical properties with texture.
    - e.g. strength, ductility, hardening…
- Hexagonal and lower symmetry materials often lack the necessary slip systems for arbitrary deformation by slip.
  - Can manipulate deformation mechanisms by choice of crystallographic texture.
    - e.g. slip, twinning, fracture…
- Example Materials :
  – BES Program interest in Magnesium, Zirconium, Nickel-Titanium Alloys.
  – DP Program interest in Uranium-Niobium, Beryllium





$(0001)\langle 11\bar{2}0\rangle$	$(10\bar{1}0)\langle 11\bar{2}0\rangle$	$(11\bar{2}2)\langle 11\bar{2}3\rangle$	$(10\bar{1}2)\langle 10\bar{1}1\rangle$	$(10\bar{1}1)\langle 10\bar{1}2\rangle$
Basal slip	Prismatic slip	Pyramidal slip	Tensile twin	Compressive twin


300
200
100
0
-100
-200
-300
-0.008
-0.004
0
0.004
0.008
Applied Stress (MPa)
Macroscopic Strain (ε)
Tens.
Comp.


-200
-100
0
0
-400
-800
Applied Stress (MPa)
hkl-Specific Strain (με)
10-10
0002
10-11
10-13

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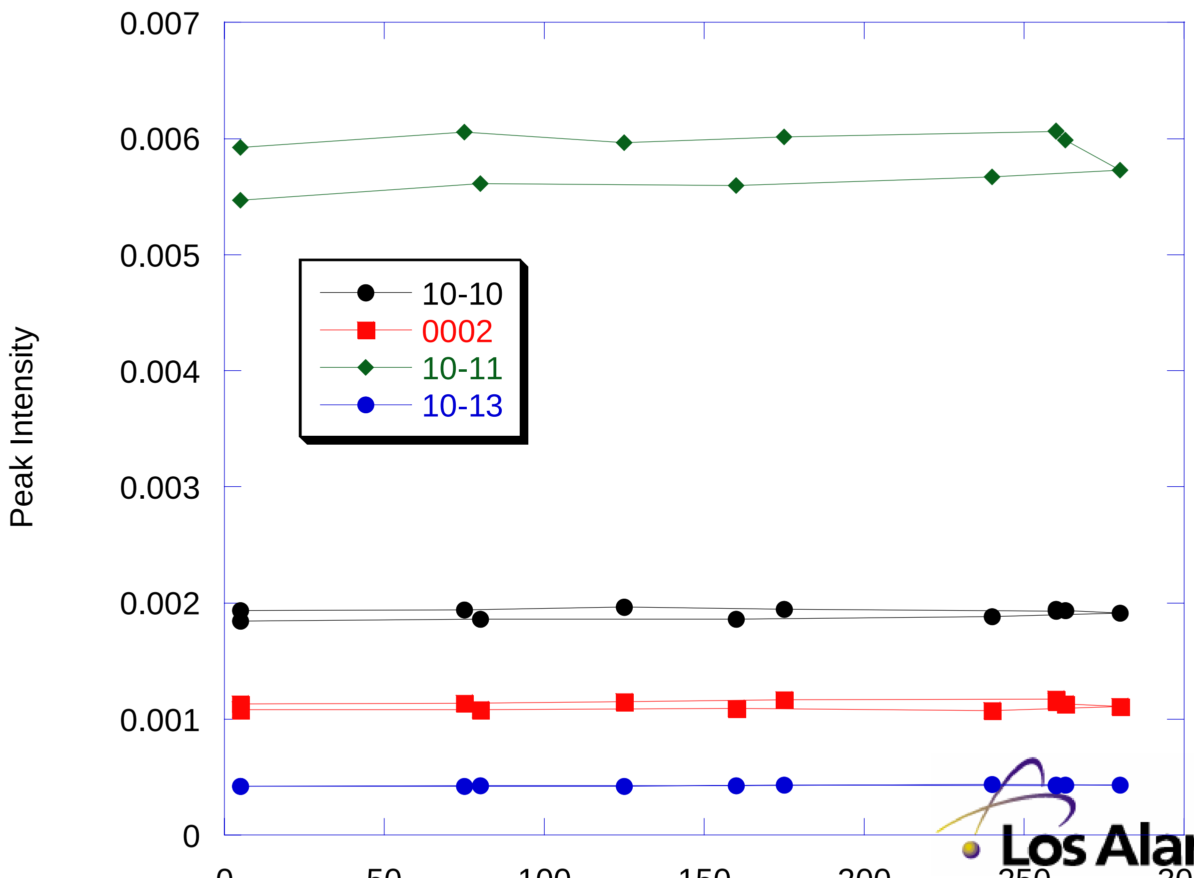
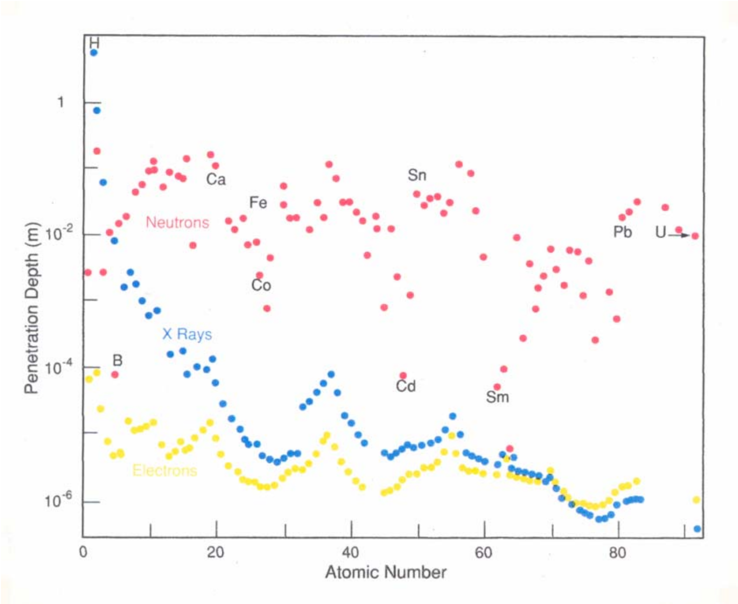
Peak Intensities Nearly Constant : No Twinning



How Do We Measure Texture and Strain?



- Any diffraction technique is possible.
  - Peak position (Bragg's law) lets us measure interatomic spacing.
  - Individual peak intensity lets us determine texture.
- Question is which technique is optimal for the problem.
- Electron diffraction :
  - Penetration depth is very small, ~1μm.
    - Surface technique.
  - Does not determine interatomic spacing accurately enough to use for strain.
  - Very effective for measuring texture over small length scales, 10μm-1mm.
  - Most materials science labs have TEM/SEM available.
- Conventional (bench-top) X-ray diffraction :
  - Penetration small, ~10μm.
  - Traditional technique for surface texture and strain measurements.
  - Sources are very common.

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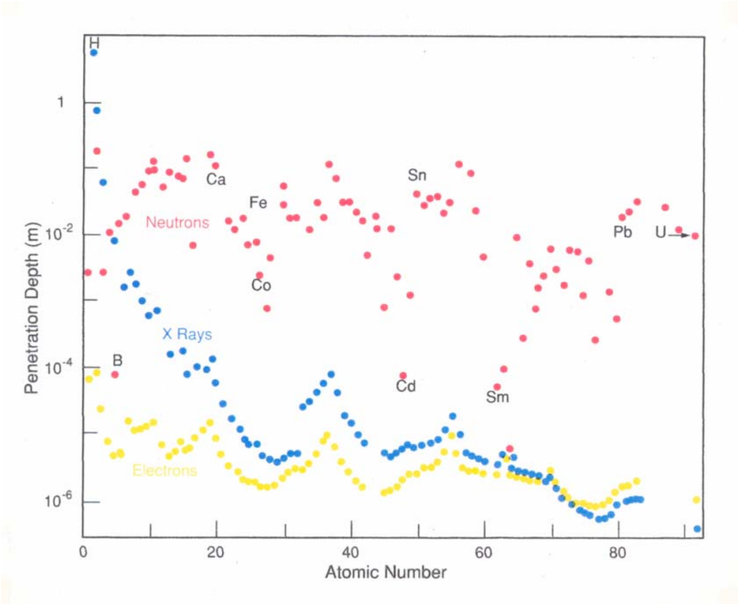
How Do We Measure Texture and Strain? (cont.)



- Thermal neutron diffraction :
  - Large Penetration, ~1cm.
  - Effective measurement of bulk texture and strain.
    - Neutrons sources are few and far between, not an everyday technique.
- High energy synchrotron X-ray diffraction :
  - Large Penetration, ~1cm.
  - Effective measurement of bulk texture and strain.
  - Again, not an everyday technique

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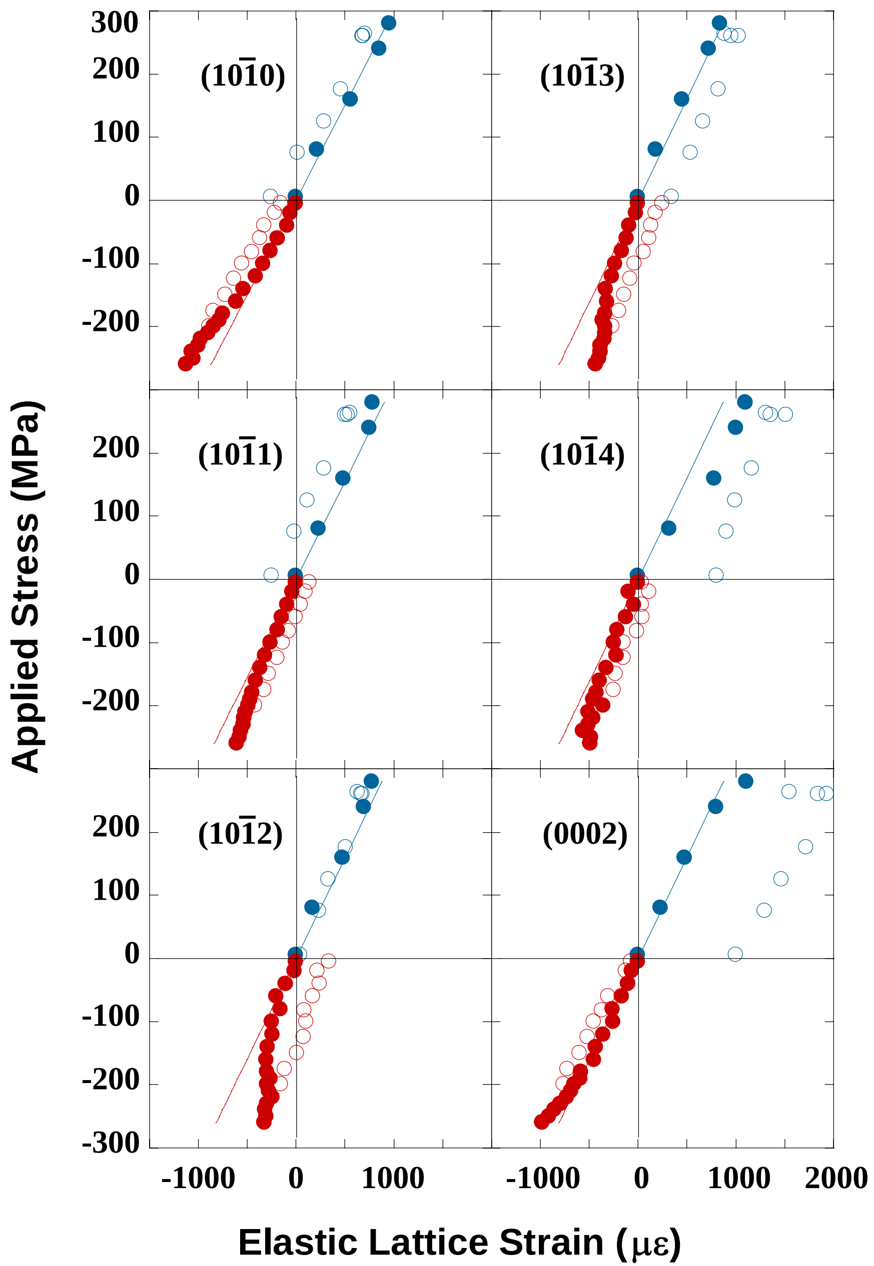
Microscopic (hkl-Specific) Flow Curves



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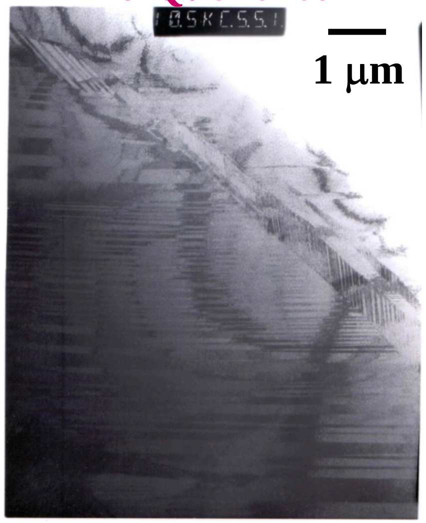
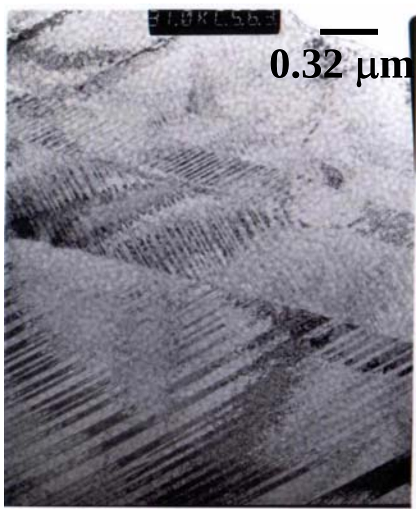
TEM Provides Details of Deformation of U6Nb.

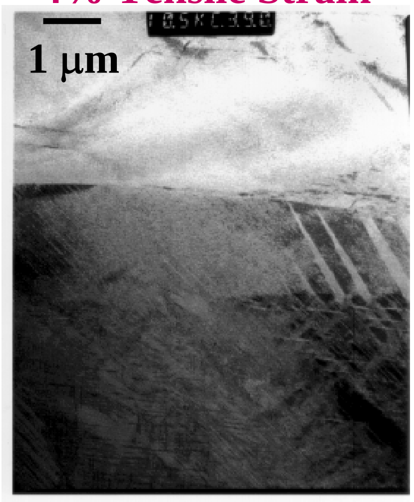
As-Quenched

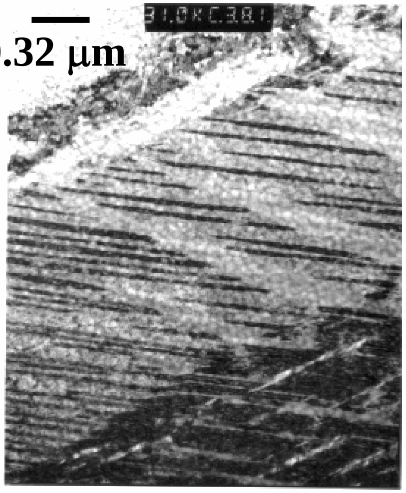




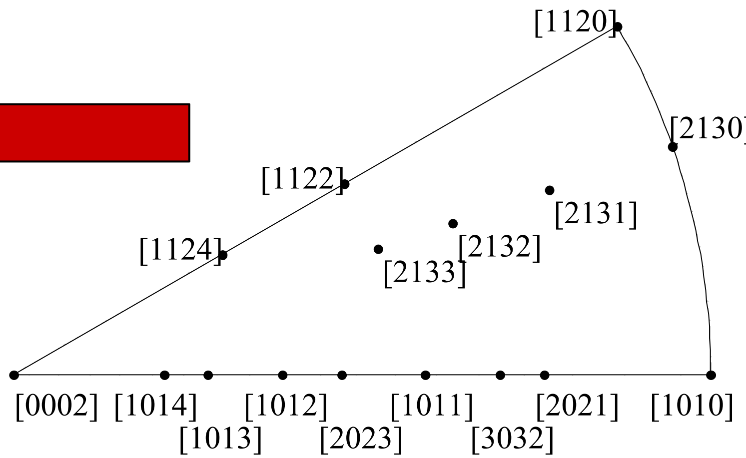
- As-Quenched
  - U6Nb Heavily Twinned.
  - (-130) Twin Boundaries
  - (021) Lath Boundaries.
- Post 4% Tensile Strain.
  - Large Single Orientation Areas.
  - (-172) Fat Lenticular Twins.
  - (-130) Fine Lamellar Twins.
- Growth and Assimilation of Preferred Variant.
- Nucleation of Deformation Twins.

4% Tensile Strain

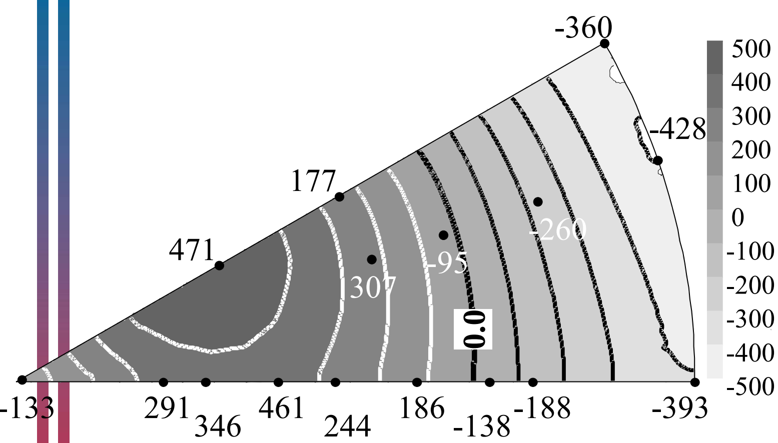




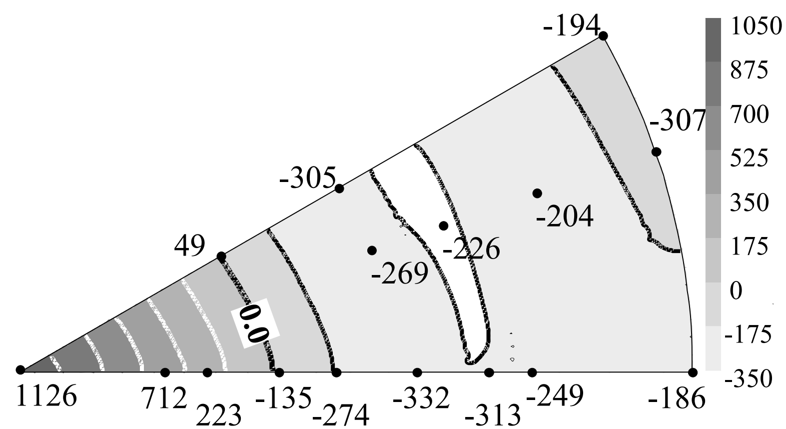
Compression



Tension



-0.70% Total strain



0.70% Total Strain

Compression : Contour Interval 60 με

Tension : Contour Interval 175 με

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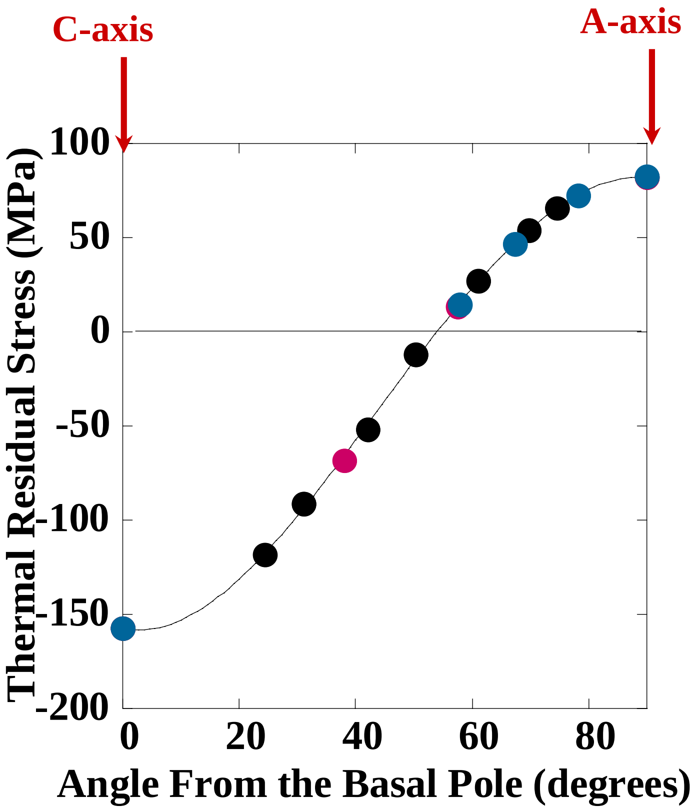
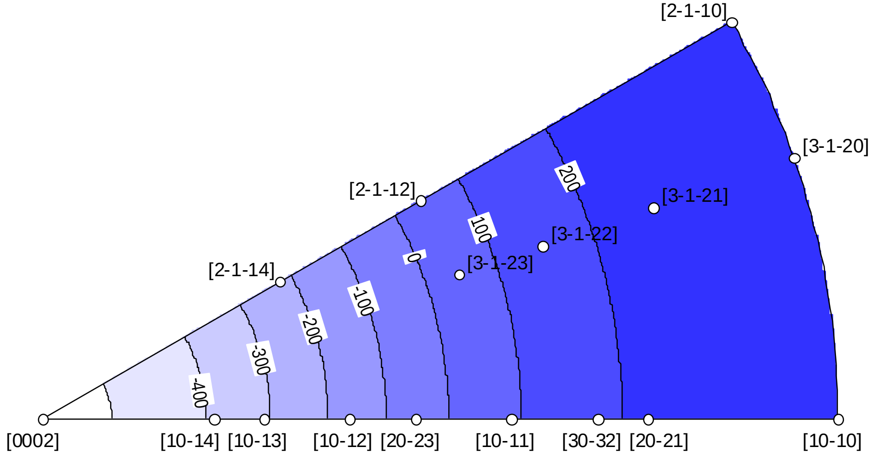
Calculated Thermal Residual Stresses





EPSC

- Beryllium Has an Anisotropic CTE : α_a=13.9, α_c=10.4 10^{-6} K^{-1}.
- Thermal Residual Stresses are Significant.
- C-axis in Residual Compression (A-axis in Tension).
  - Poles Near C-axis Predisposed to Yield in Compression.

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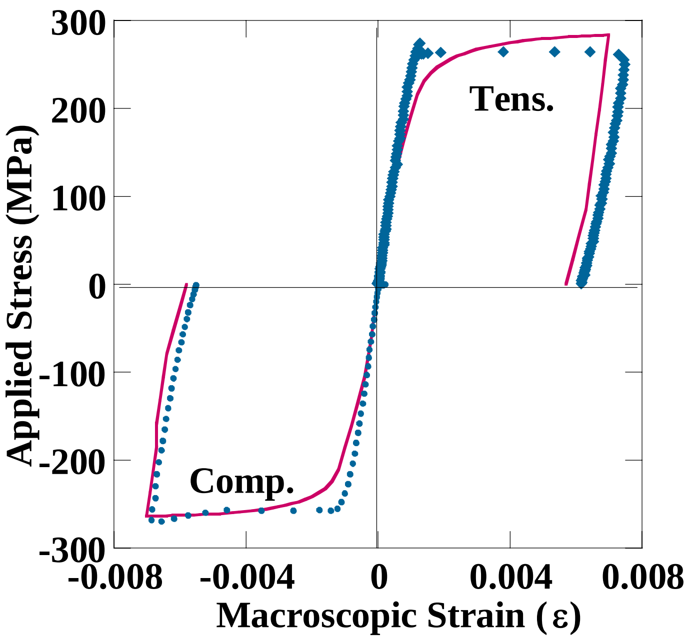
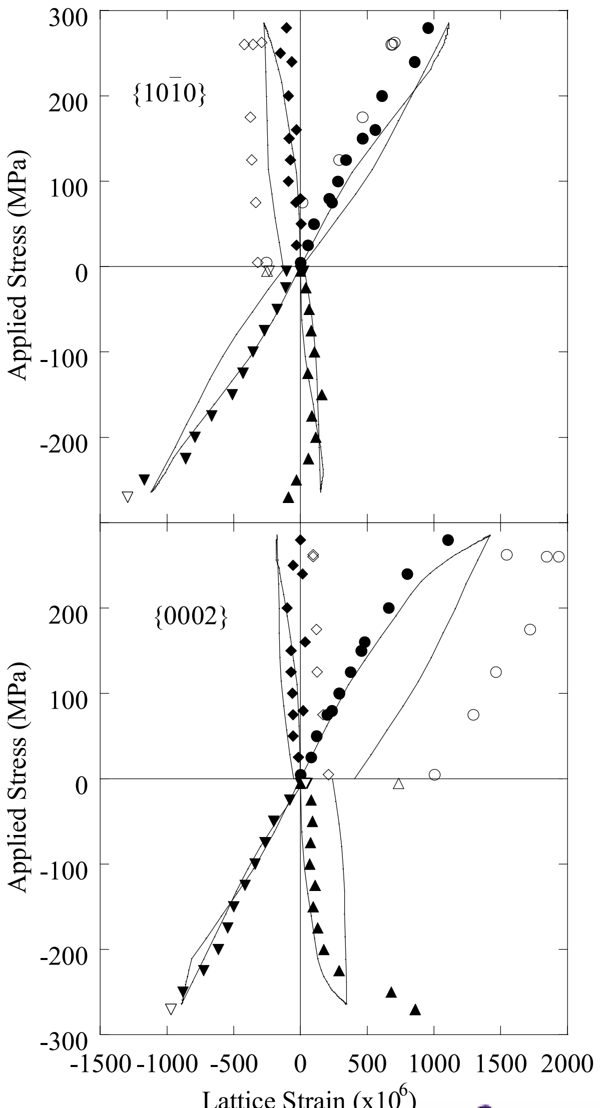
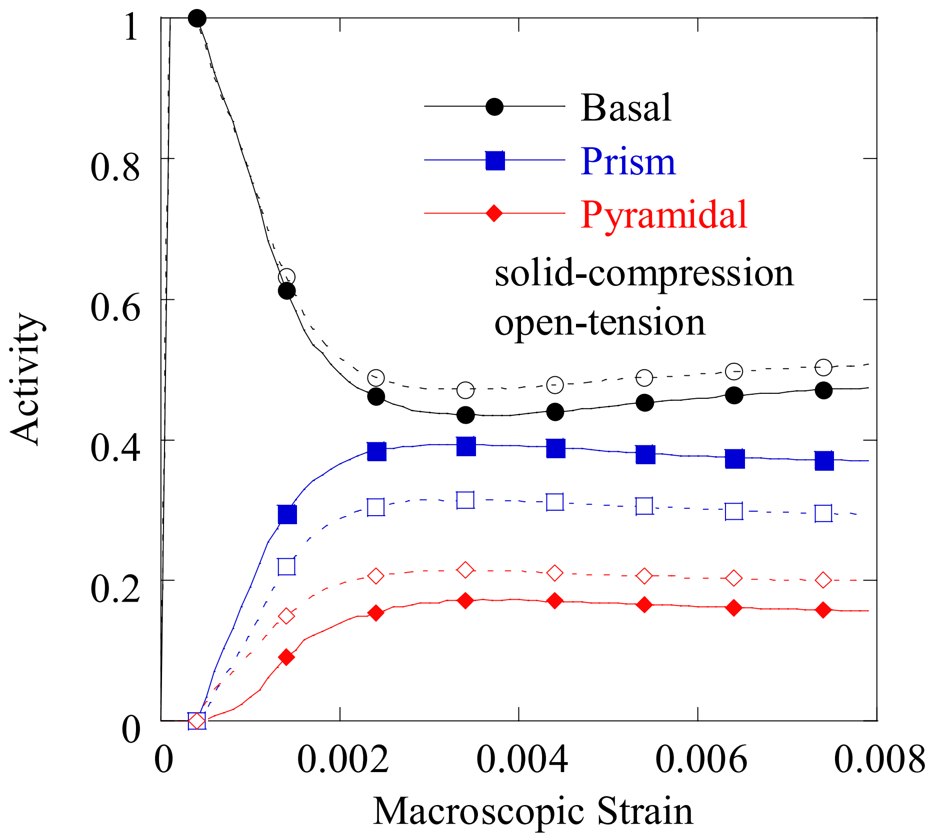
Elasto-Plastic Self Consistent Model Captures Lattice Strains

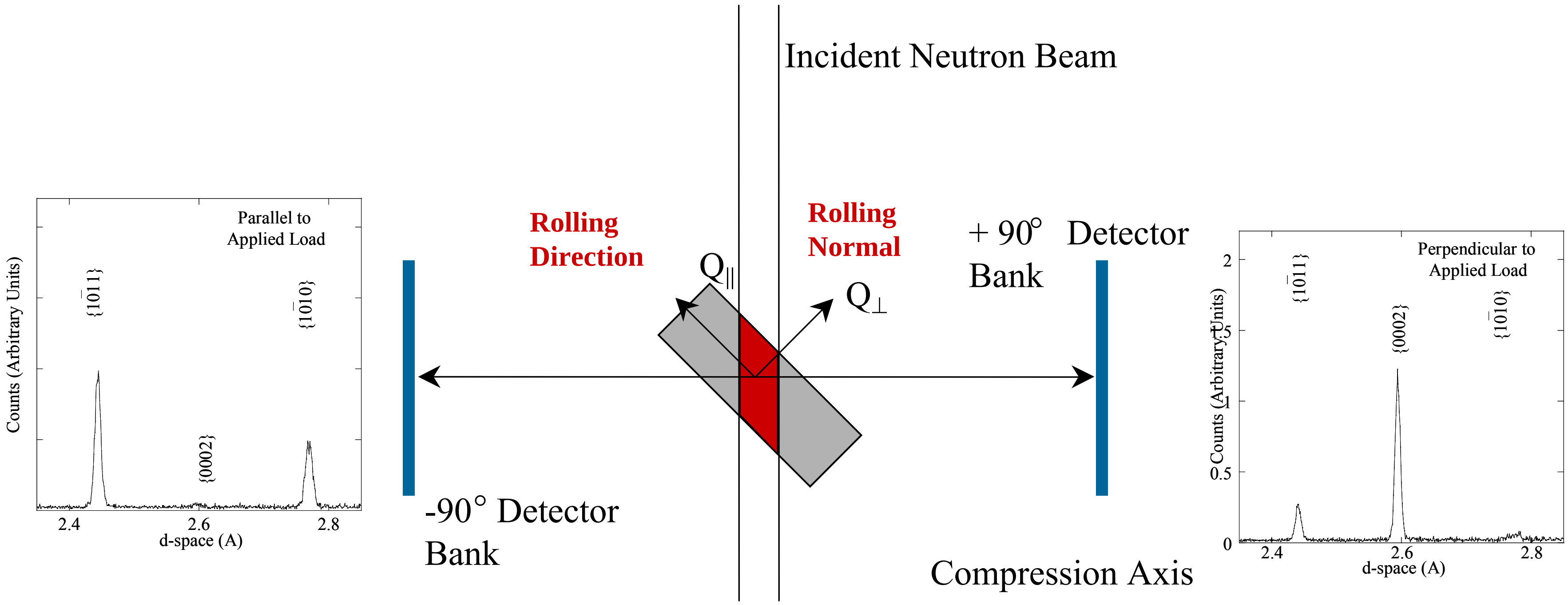




Combination of ND and Modeling Yields Deformation Mode Activity.

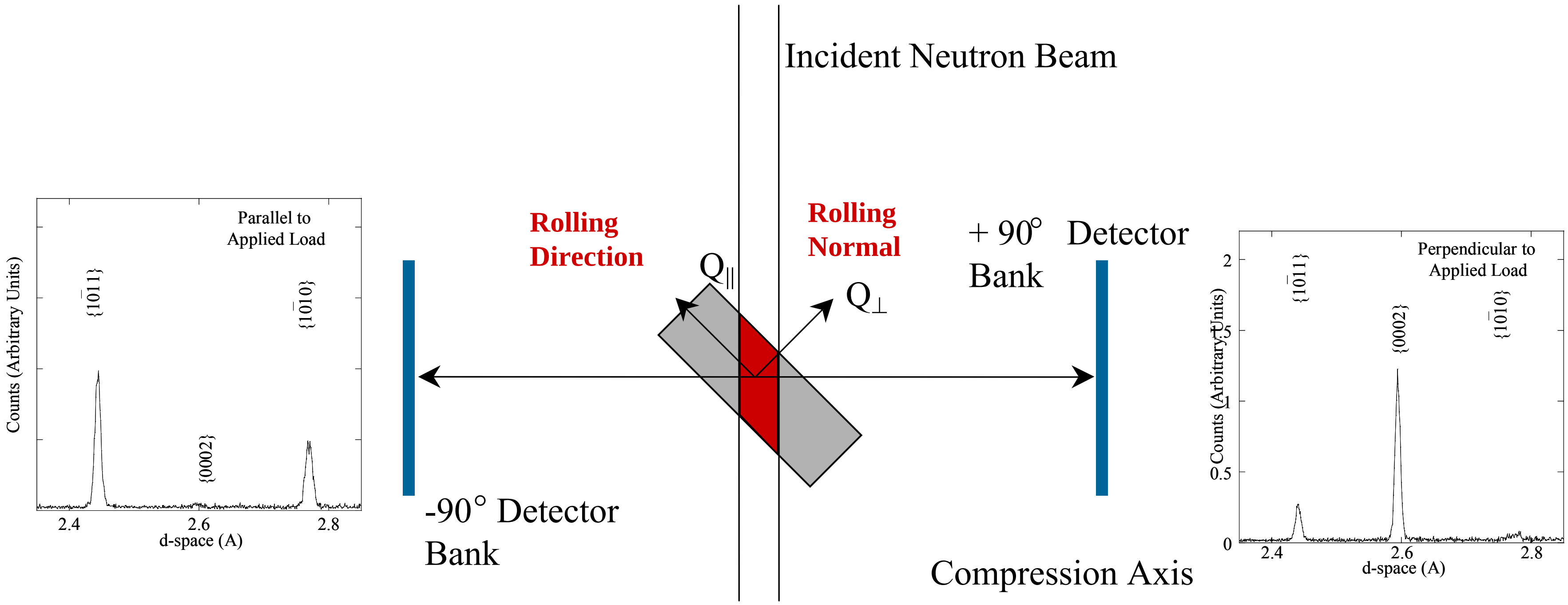


Time of Flight Neutron Diffraction Measures Texture and Strain



- **Intensity of diffraction peaks is proportional to the pole density parallel to the diffraction vector**
- **Position of diffraction peaks is related to the strain**

Time of Flight Neutron Diffraction Measures Texture and Strain



- Intensity of diffraction peaks is proportional to the pole density parallel to the diffraction vector
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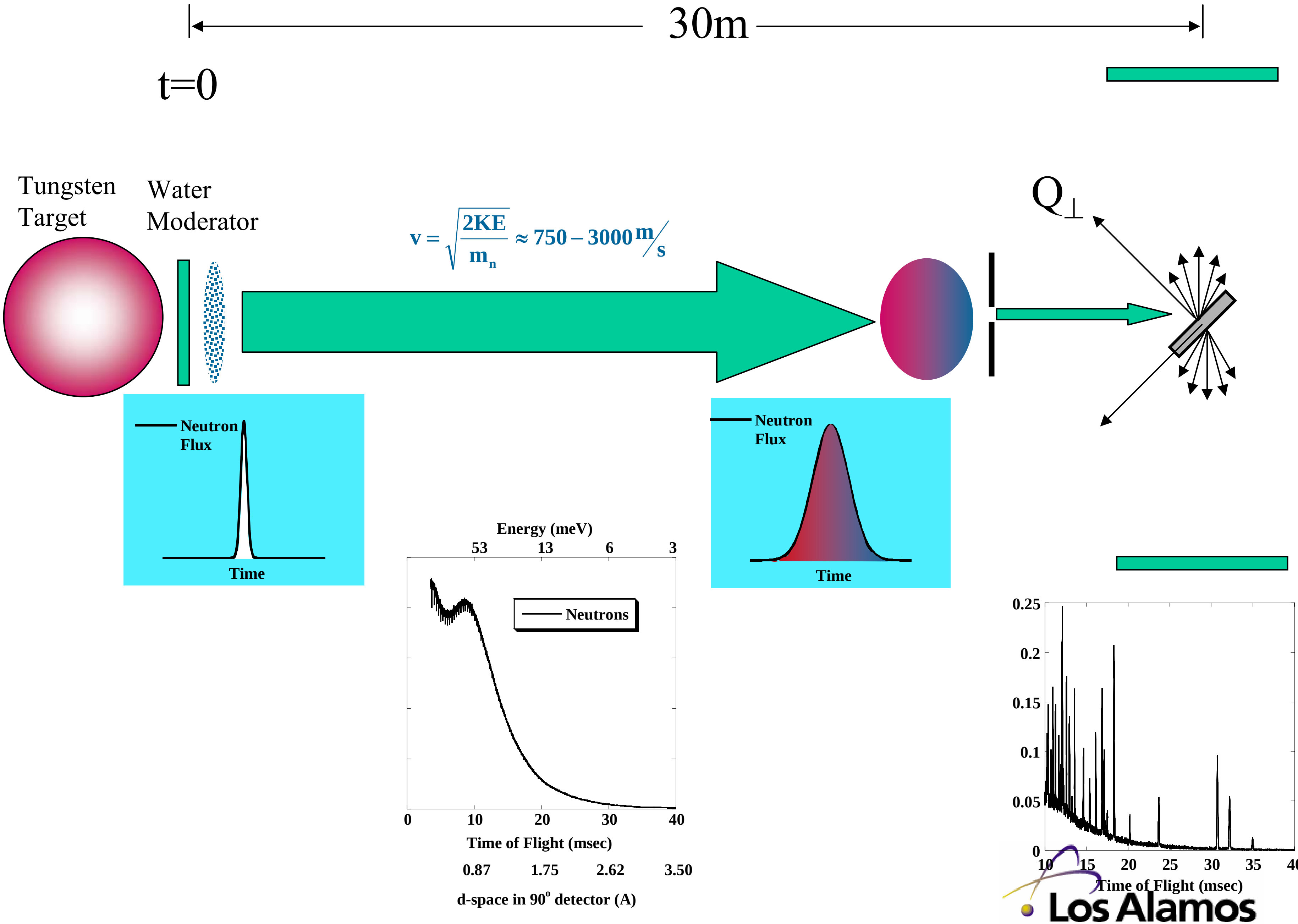
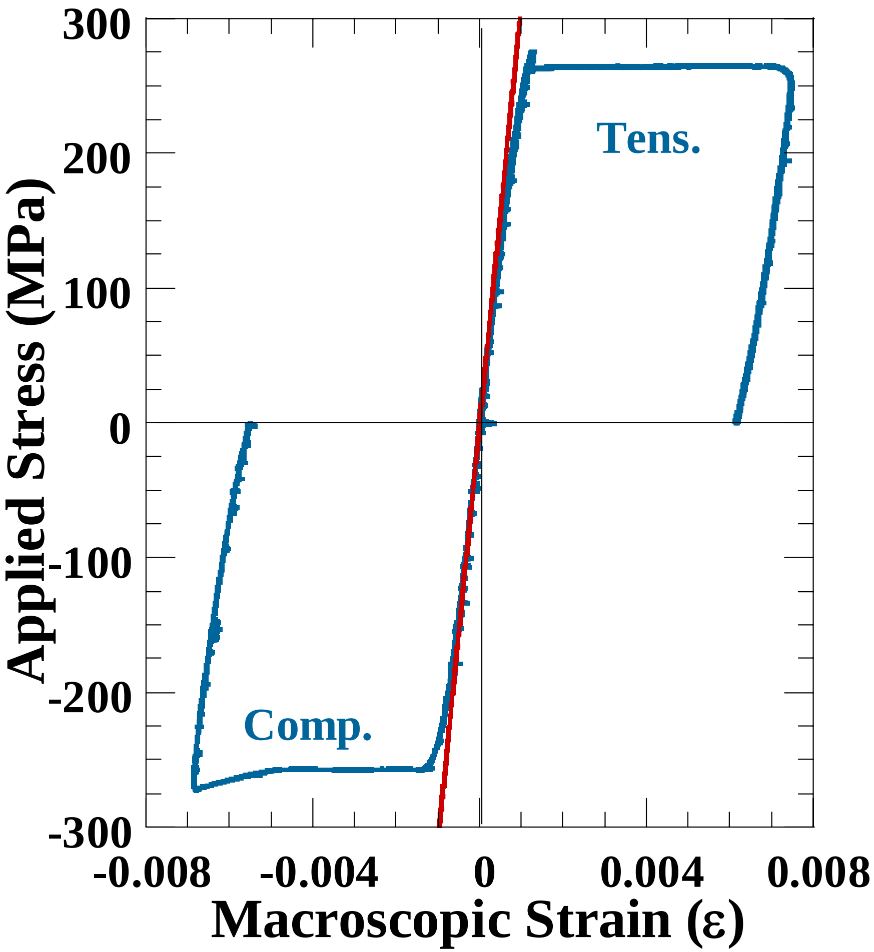
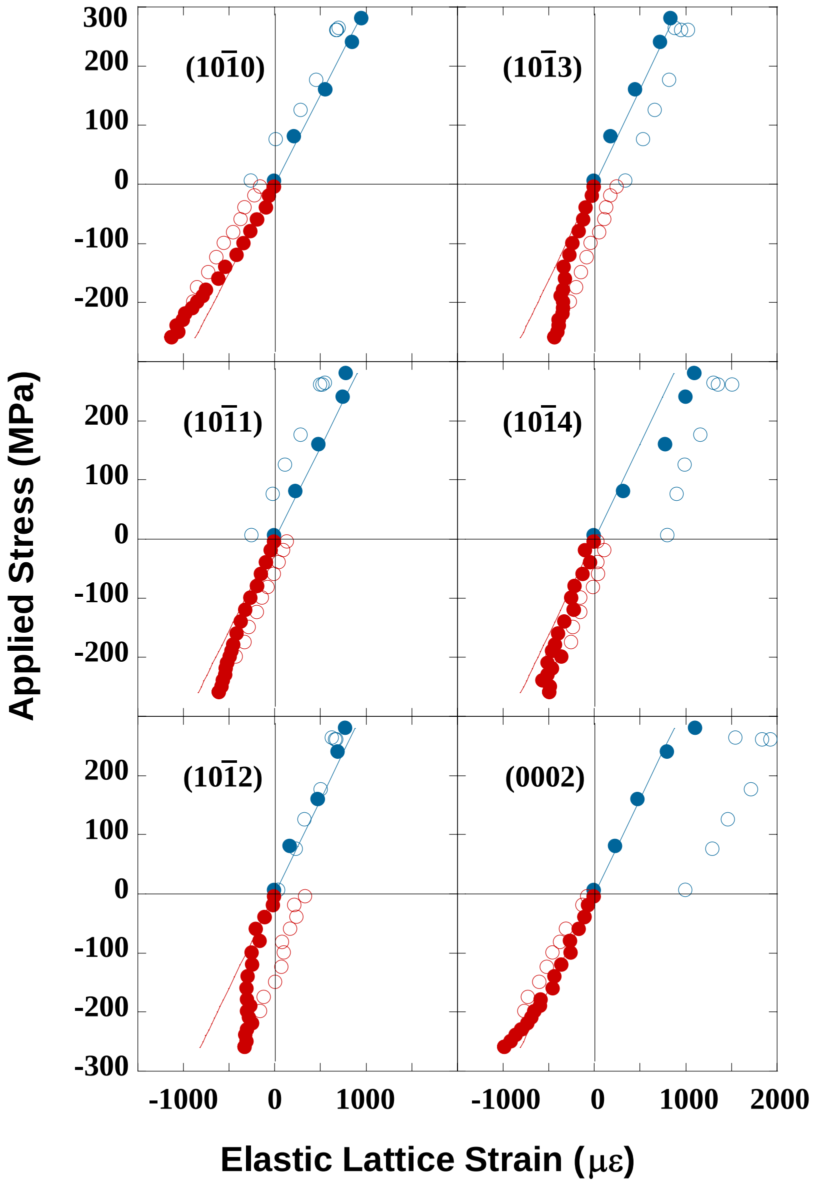
Time of Flight Technique at a Spallation Source



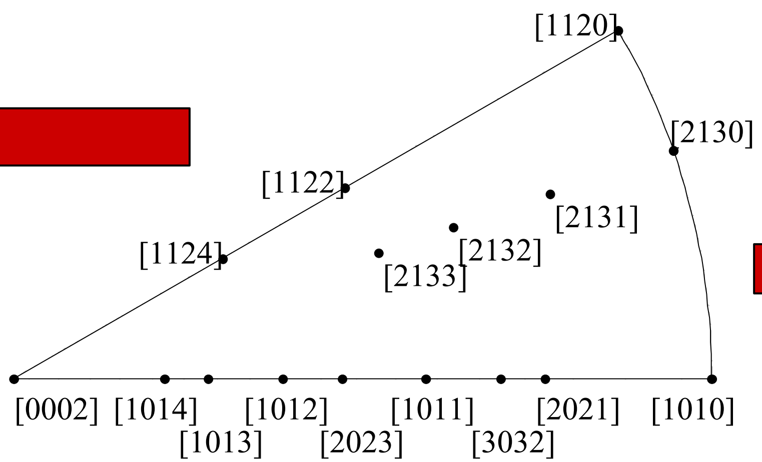
Plastic Deformation of Beryllium

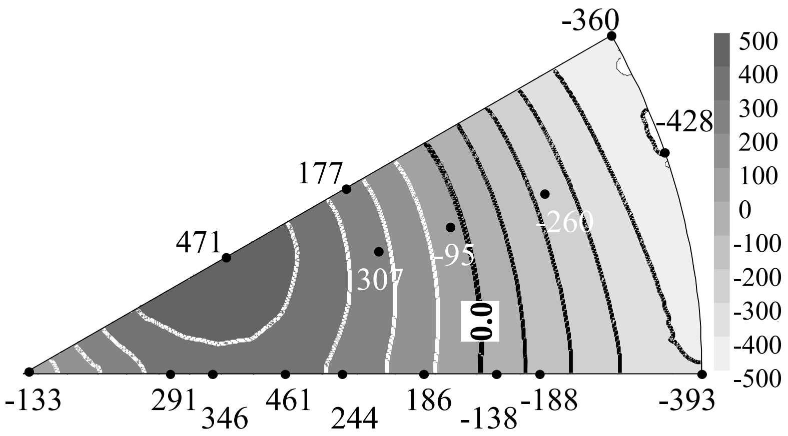




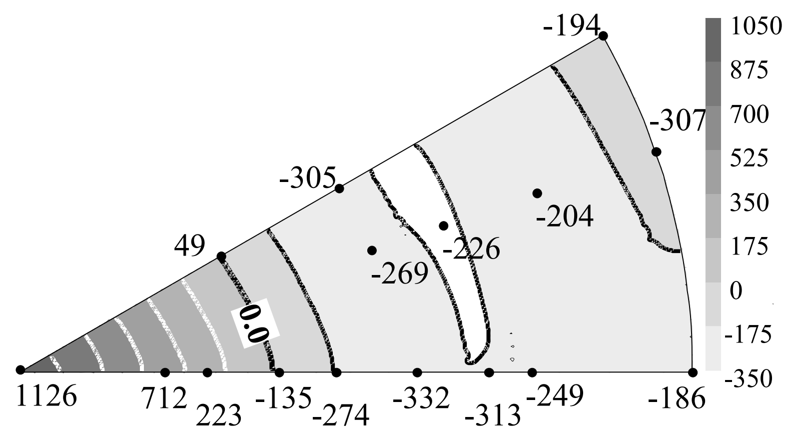
Compression

Tension





-0.70% Total strain



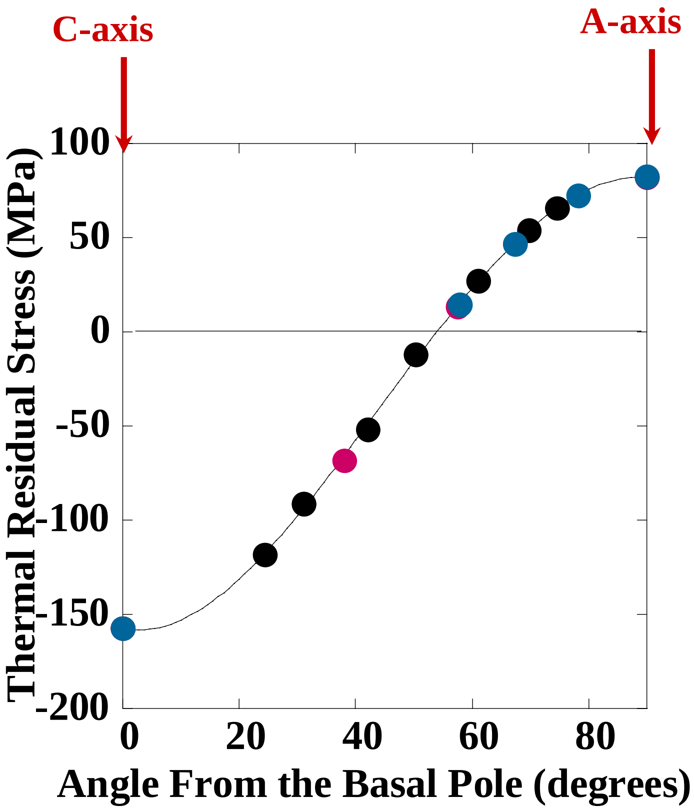
0.70% Total Strain

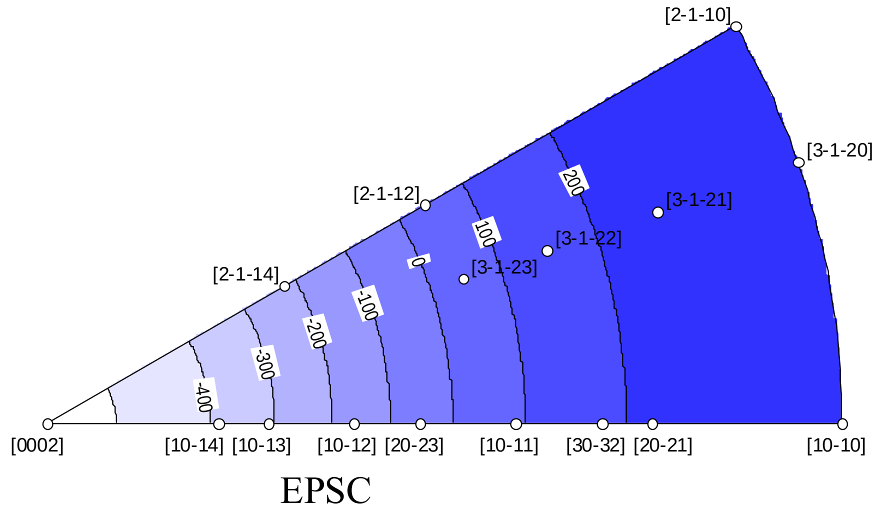
Compression : Contour Interval 60 με

Tension : Contour Interval 175 με

Los Alamos

Calculated Thermal Residual Stresses





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- Thermal Residual Stresses are Significant.
- C-axis in Residual Compression (A-axis in Tension).
  - Poles Near C-axis Predisposed to Yield in Compression.

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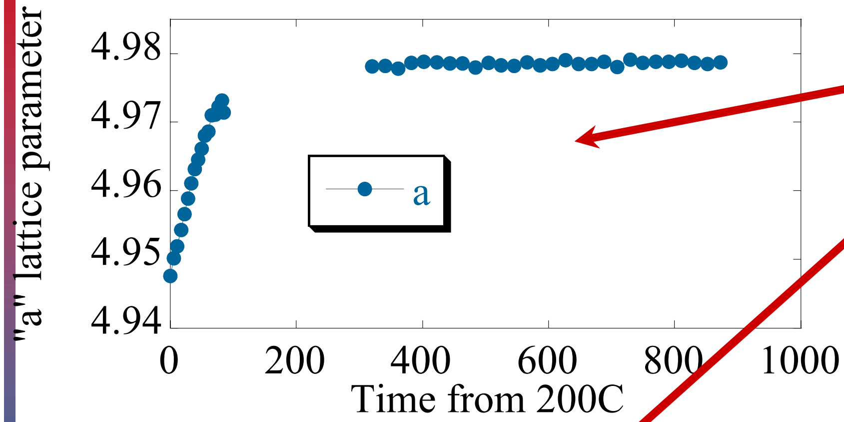
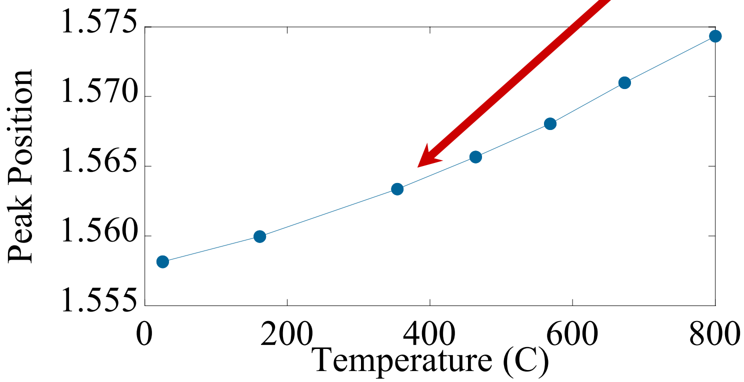
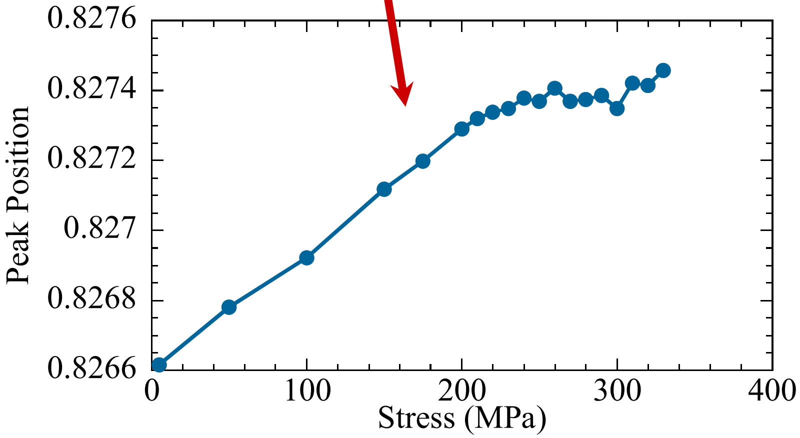
Peak Position is Sensitive To :



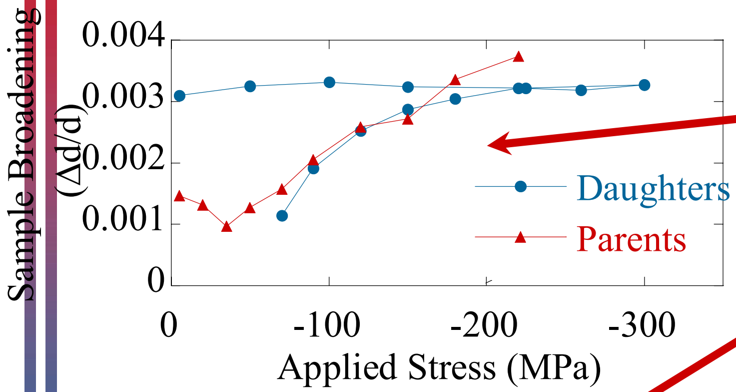


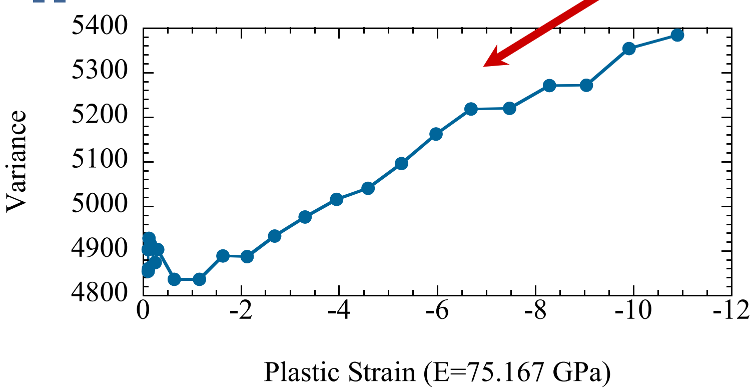
- Chemical composition
- Temperature
- Stress
  - Residual Stress Field
  - Macrostress – tractions (Type I)
  - Intergranular stress- (Type II)
  - Intragranular stress – (Type III)

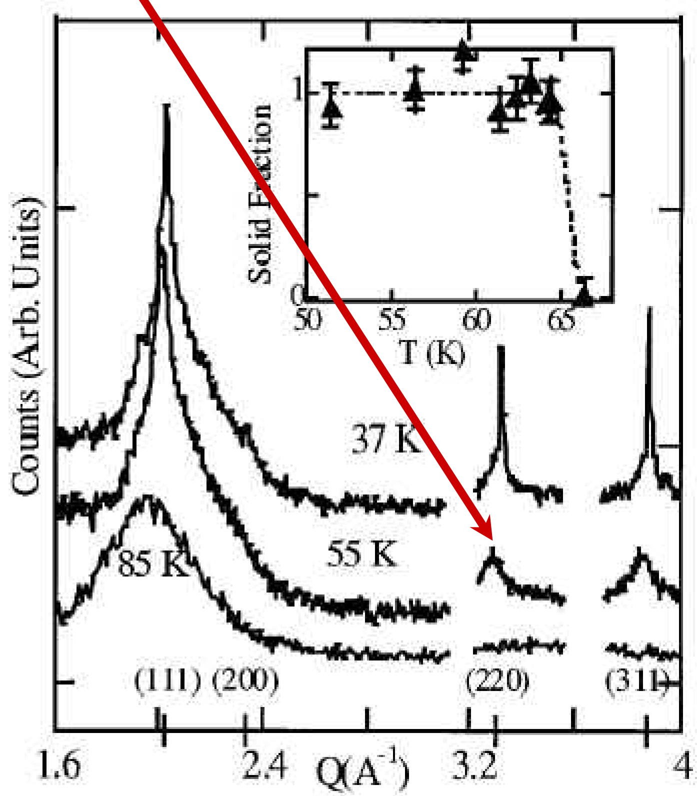


Peak Width is Sensitive To :

- **Heterogeneous Stress Distribution**
- **Dislocation Density**
- **Finite Size Effects**







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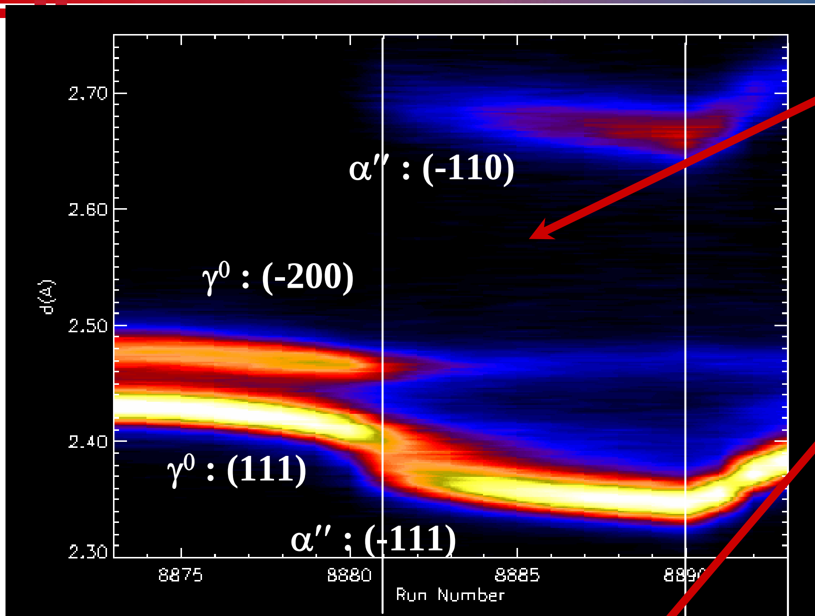
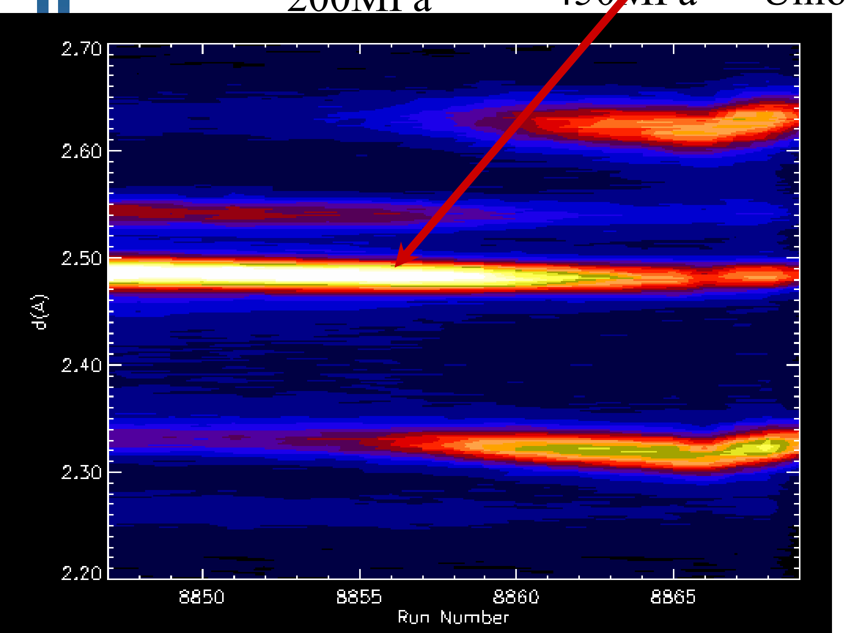
Peak Intensity is Sensitive To :

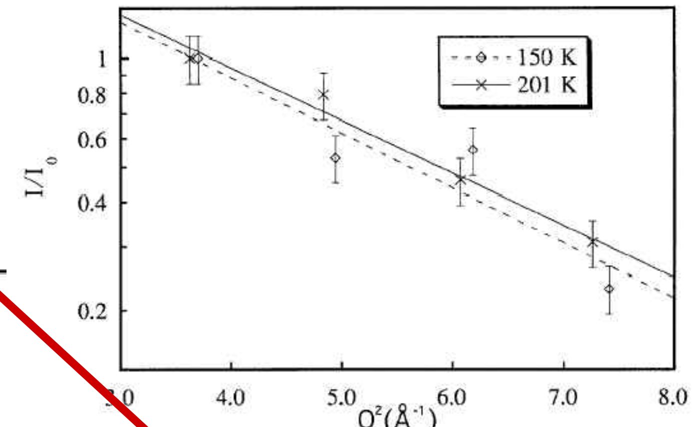
- **Volume Fraction**
  - Composite
  - Stress induced phase transformation
- **Texture**
- **Disorder**



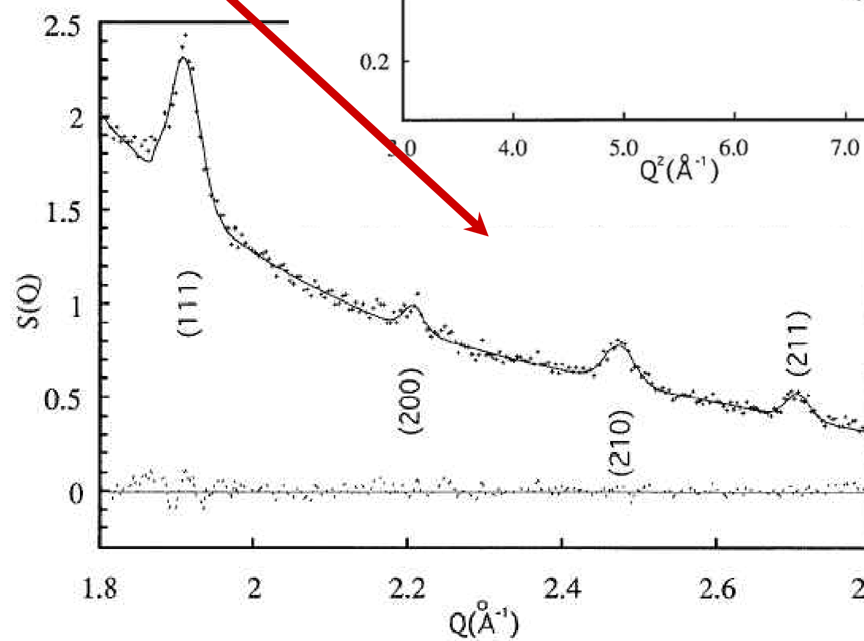
200MPa 450MPa Unloaded



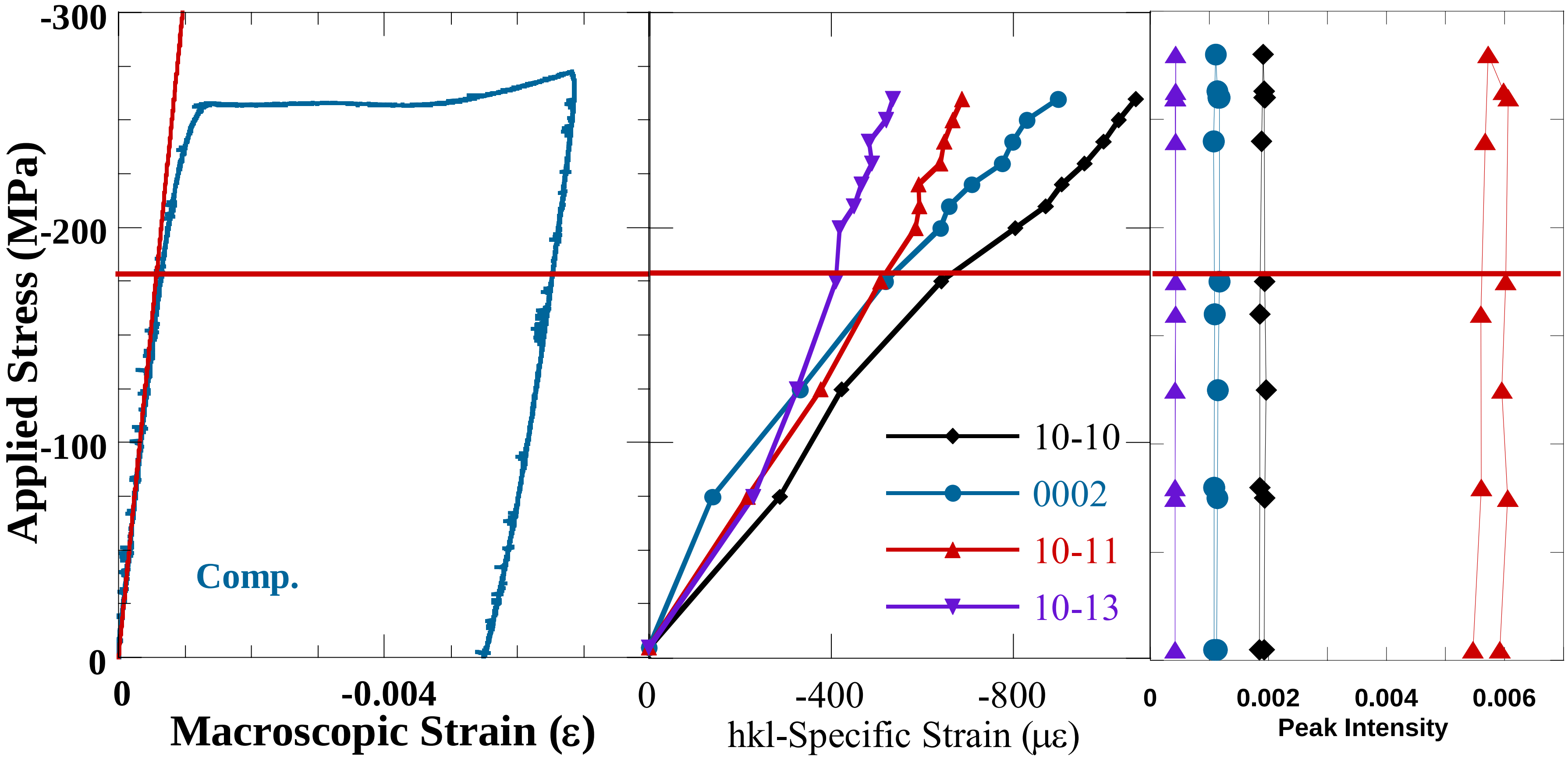
D W Brown et al



D W Brown et al



Plastic Deformation of Beryllium



• Deviation of lattice strains from linearity indicates that plastic deformation has initiated.

• Lack of change of peak intensity suggests it is slip dominated.

Los Alamos