Finite Element Modeling of Lattice Strains in Polycrystalline Materials with Comparisons to Diffraction Experiments

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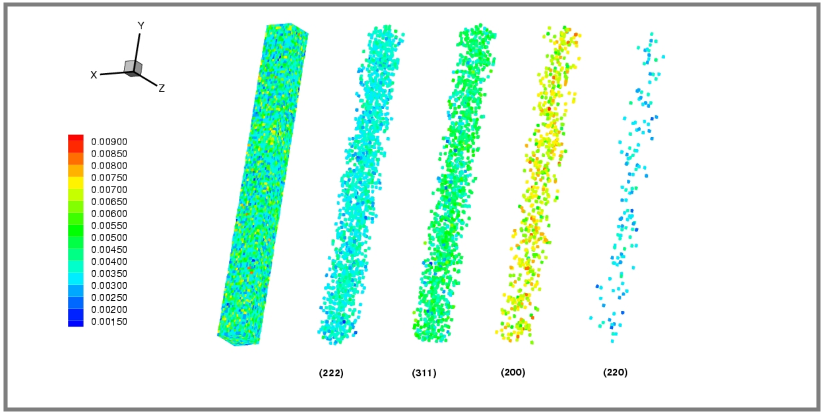
Cornell University



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Motivation from Applications

Structural Alloys:

- Severe service environments
  - high stress and low fault tolerance
- Tradeoff between reliability and performance
  - conservative practices prevail

Net effects:

- Fewer and fewer new materials used in designs
- Maintenance costs dominate

Progress limited by our understanding of:

- Basic properties: stiffness and strength
- Fatigue life: initiation of life-limiting flaws
- Deformation-induced microstructure evolution
- Phase transformations

Improving Materials

The rub:

- Microstructures are complex and dynamic
  - important features exist at several length scales
- Stress distribution depends on the microstructure
  - spatial variations across dimensions of grains
- Behavior depends on the stress
  - stress varies "substantially"
  - defects initiate in material under stress

Scientific Challenges:

- Address the competing demands:
  - neighborhood details are important
  - good statistics are needed to characterize rare behaviors
- Make the most of available data
  - peak profiles aren't well understood

Utilize a Simulation + Experiment Approach:

- Simulations that:
  - define realistic domains (adequate detail)
  - resolve enough volume (adequate numbers of grains)
  - capture correlation between stress and deformation
- Experiments that:
  - are coordinated with model development
  - provide complete records of strain and state

Finite Element Equilibrium Residual

Weighted residual:

$$R_u = \int_{\mathcal{B}} \boldsymbol{\psi} \cdot \left(\text{div} \boldsymbol{\sigma}^T + \boldsymbol{b} \right) d\mathcal{B}$$

Weak form:

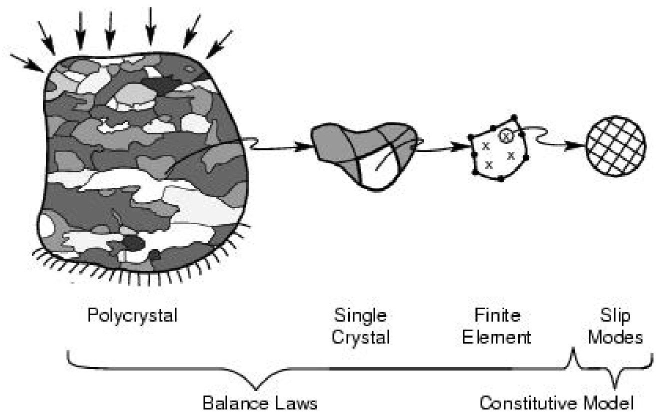
$$R_u = -\int_{\mathcal{B}} \text{tr} \left(\boldsymbol{\sigma}^T \cdot \ \text{grad} \boldsymbol{\psi} \right) d\mathcal{B} + \int_{\partial\mathcal{B}} \boldsymbol{t} \cdot \boldsymbol{\psi} d\Gamma + \int_{\mathcal{B}} \boldsymbol{b} \cdot \boldsymbol{\psi} d\mathcal{B}$$

Variables

Cauchy stress: σ
Crystal velocity gradient: $\mathbf{L} = \mathbf{D} + \mathbf{W}$

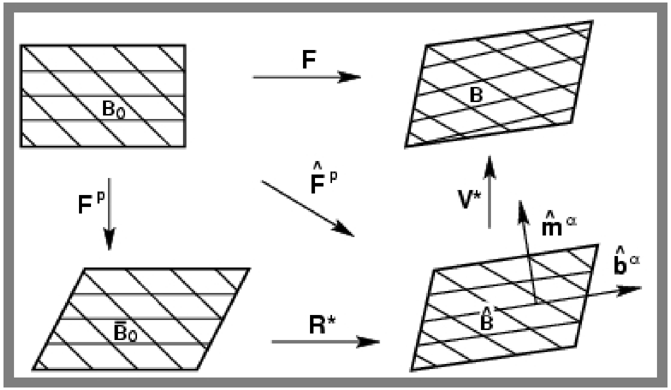
Implementation:

- Lagrangian formulation
- Velocity is the primary unknown
- Equations written in the current configuration
- Backward Euler time discretization
- Parallel architecture using F90/MPI



Elastoplastic Deformation Kinematics

Decomposition:



$$\boldsymbol{F} = \boldsymbol{V}^* \widehat{\boldsymbol{F}}^{\mathsf{p}}$$

where

$$\widehat{\boldsymbol{F}}^{\mathsf{p}} = \boldsymbol{R}^* \boldsymbol{F}^{\mathsf{p}}$$

Small elastic strains:

Elastic stretch:

$$\boldsymbol{V}^* = \boldsymbol{I} + \boldsymbol{\epsilon}^*$$

with

$$\mathrm{tr}(\boldsymbol{D}) = \mathrm{tr}(\dot{\boldsymbol{\epsilon}^*})$$

and

$$||\boldsymbol{\epsilon}^*|| << 1$$

Deformation rate:

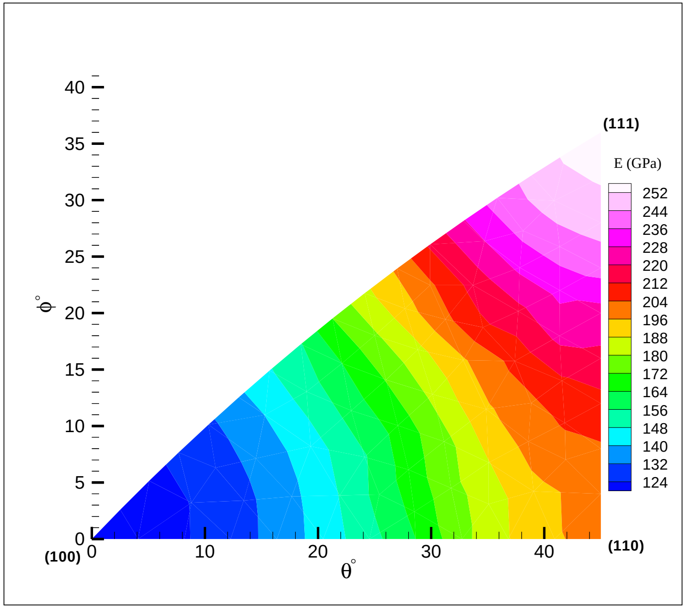
$$\boldsymbol{D}' = \dot{\boldsymbol{\epsilon}^{*\prime}} + \widehat{\boldsymbol{D}}^{\mathsf{p}} + \boldsymbol{\epsilon}^{*\prime}\widehat{\boldsymbol{W}}^{\mathsf{p}} - \widehat{\boldsymbol{W}}^{\mathsf{p}}\boldsymbol{\epsilon}^{*\prime}$$

Spin:

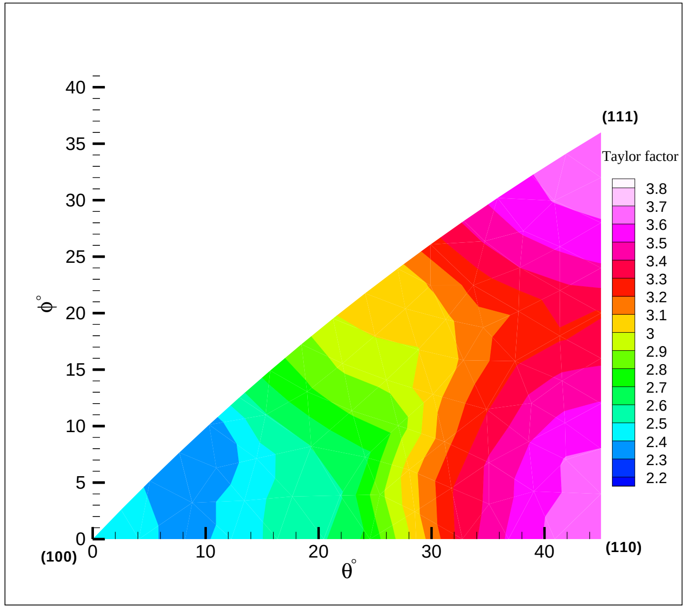
$$\boldsymbol{W} = \widehat{\boldsymbol{W}}^{\mathsf{p}} + \boldsymbol{\epsilon}^{*\prime}\widehat{\boldsymbol{D}}^{\mathsf{p}} - \widehat{\boldsymbol{D}}^{\mathsf{p}}\boldsymbol{\epsilon}^{*\prime}$$

Single Crystal Anisotropy

Directional Elastic Modulus



Uniaxial Flow Strength



Grain interactions depend on alloy

- Range in $\frac{E_{111}}{E_{100}}$ from ≈ 1 to > 3 (above plot for stainless steel)
- Strength-to-stiffness distribution depends on alloy:

Aluminum: $(\frac{\tau}{E})_{100} < (\frac{\tau}{E})_{111}$ Stainless steel: $(\frac{\tau}{E})_{100} > (\frac{\tau}{E})_{111}$

Microdiffraction Experiments of a Cu Alloy

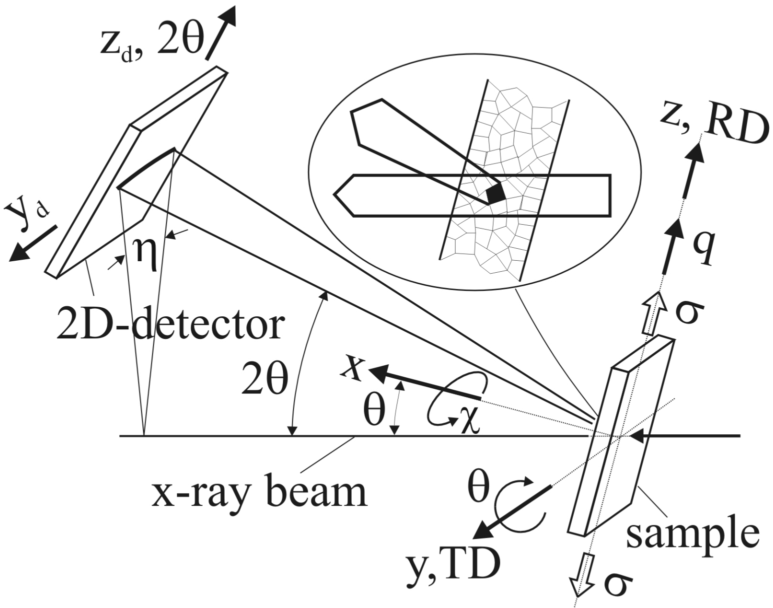
Microdiffractometer

- X-ray synchrotron source
- Single grain diffraction volume
- In-situ loading
- Nominally same *hkl*

Experiments

- Polycrystalline copper
- Axial scattering vector
- Measurements taken on ≈ 20 grains
- Loaded in tension to ≈ 2% strain

Schematic of experiment



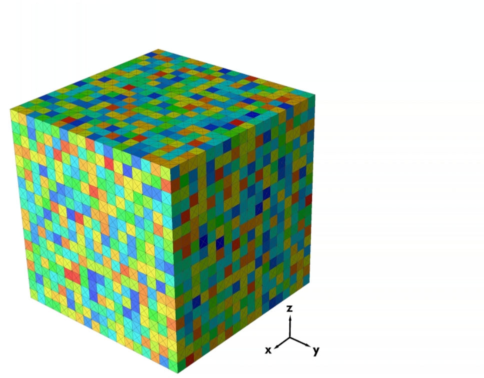
Reference: Lienert, U. *et al.*, **Acta Materialia**, in press.

Microdiffraction Experiments of a Cu Alloy

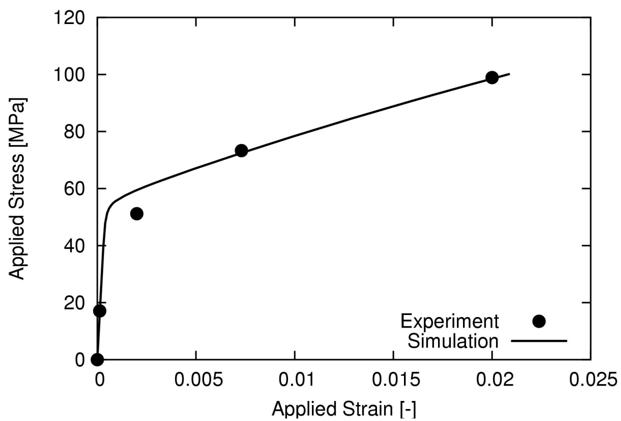
Simulations

- Elastoplastic formulation
- Dodecahedral grains
- Tetrahedral elements

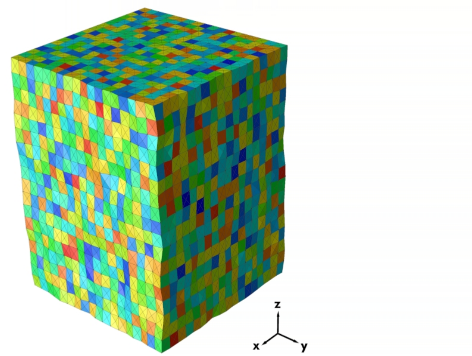
Undeformed polycrystal



Aggregate response:

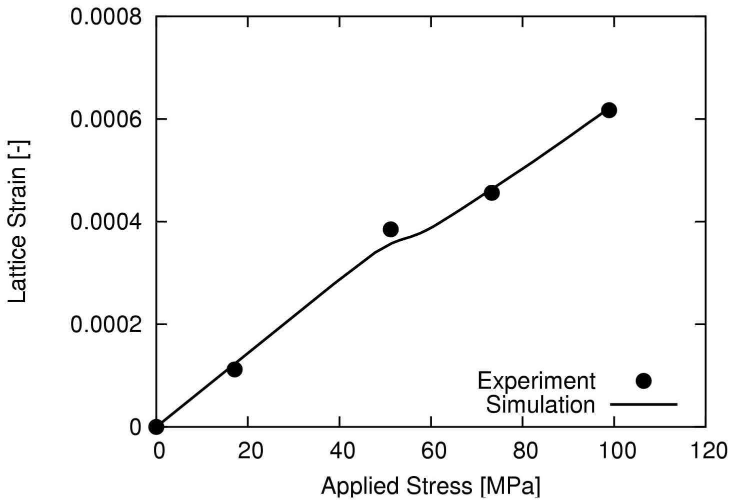


Deformed polycrystal

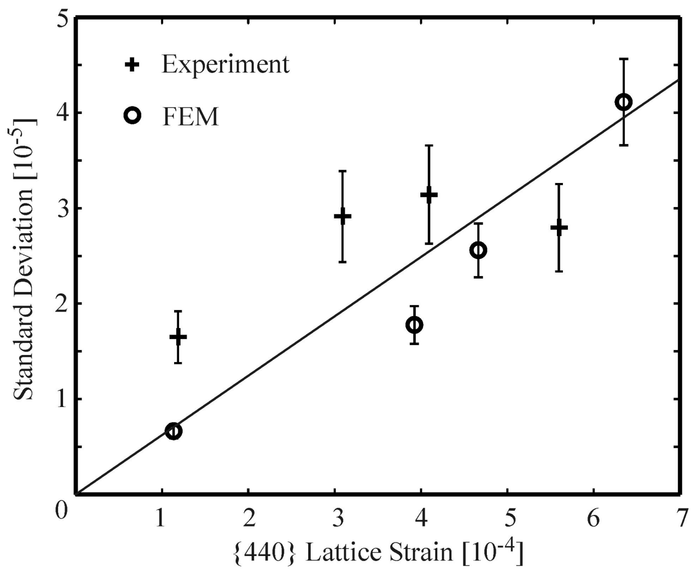


Microdiffraction Experiments of a Cu Alloy

Lattice strains average



Lattice strain variability



Comparisons of variations

- Similar levels
- $\approx 8\%$ of mean
- Significant for low rate sensitivity

Stress Partitioning in Polyphase Systems

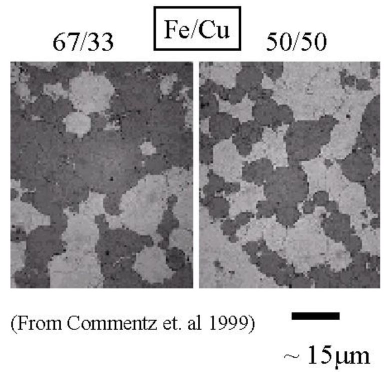
Material system:

- Iron-Copper
- Mechanically alloyed
- Initially untextured

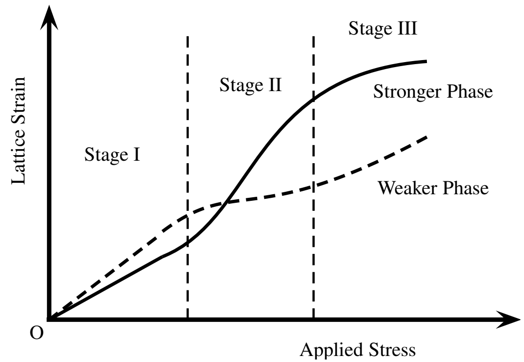
Mechanical tests

- Conventional macroscale tests
- In-situ loading diffraction tests
  Neutrons (SMARTS)
  Synchrotron x-rays (CHESS)

Micrographs

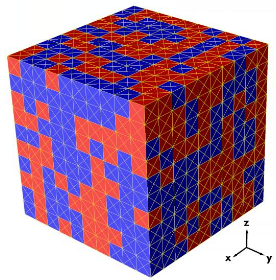


Qualitative behavior

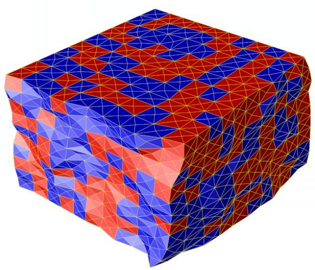


Stress Partitioning in Polyphase Systems

Undeformed Polycrystal



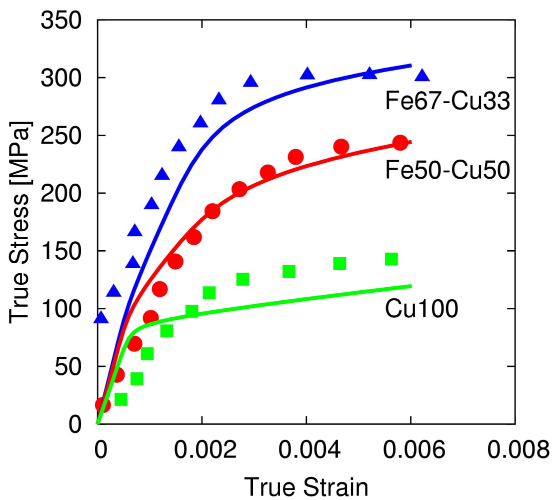
Polycrystal Deformed 30%



Calibration and Prediction

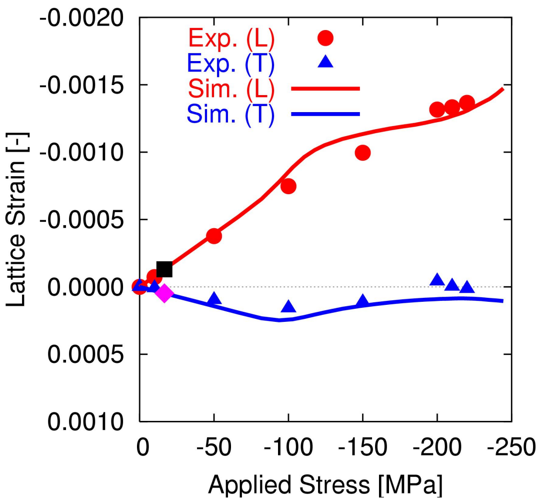
- Determine single crystal parameters
  Fit Cu using Cu100 test
  Fit Fe using Fe67-Cu33 test
- Predict the Fe50-Cu50 test

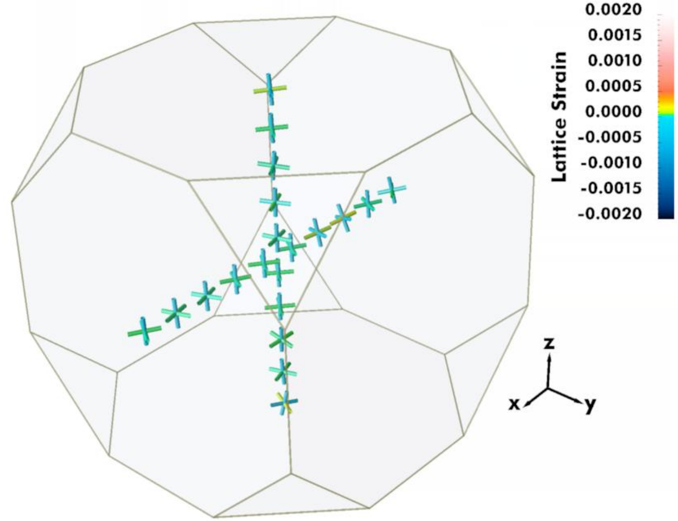
Aggregate response



Stress Direction Evolution

Macro Stress = 17MPa



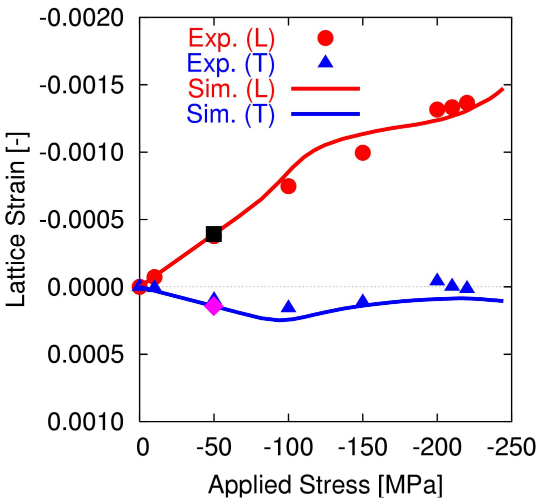


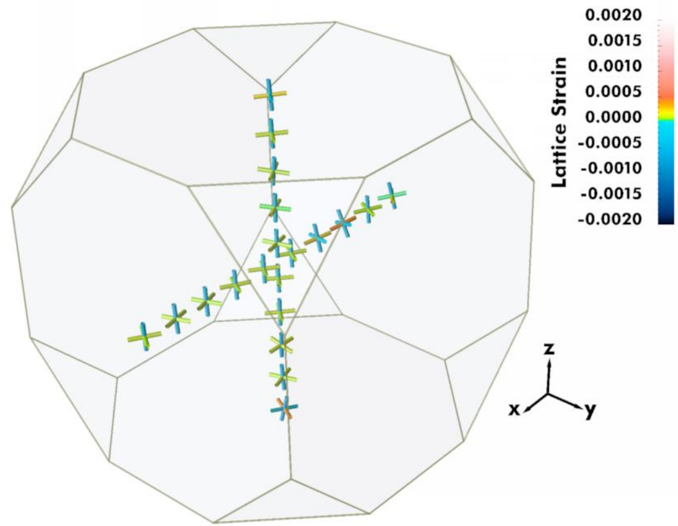
Average Fiber Lattice Strain

Principal Strains along Fibers

Stress Direction Evolution

Macro Stress = 50MPa



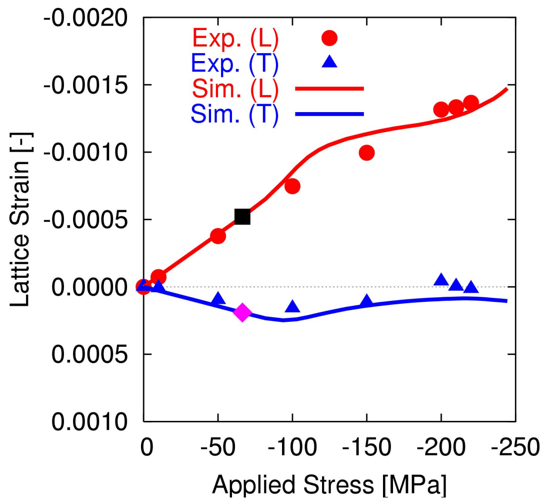


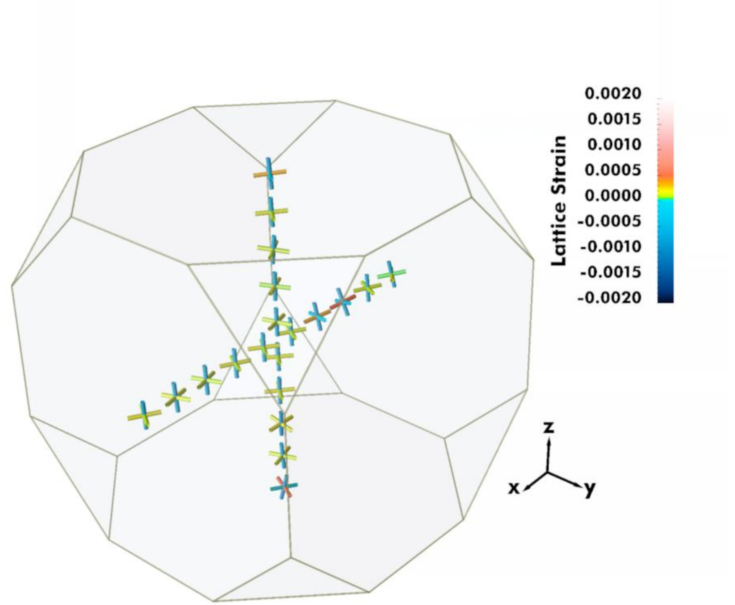
Average Fiber Lattice Strain

Principal Strains along Fibers

Stress Direction Evolution

Macro Stress = 66MPa



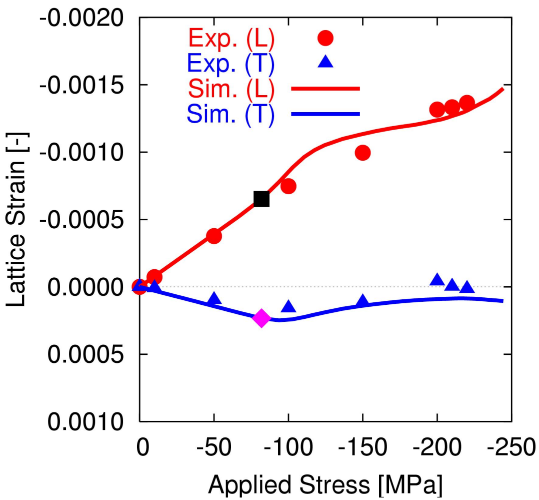


Average Fiber Lattice Strain

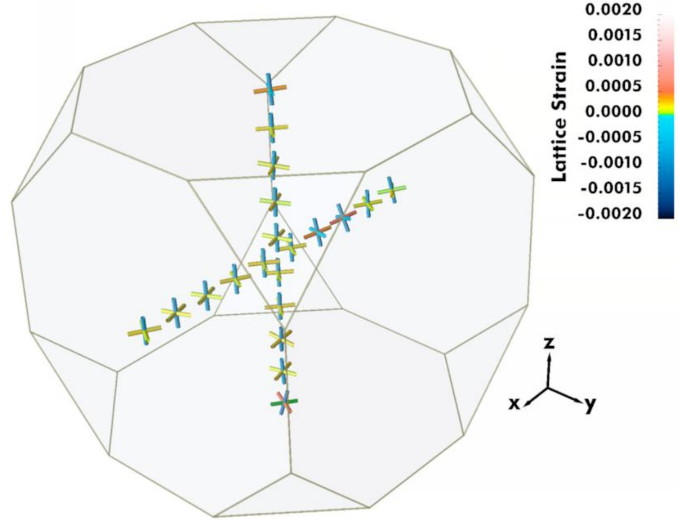
Principal Strains along Fibers

Stress Direction Evolution

Macro Stress = 82MPa



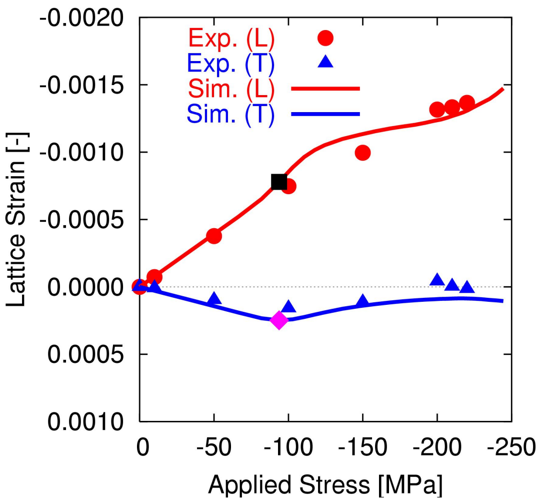
Average Fiber Lattice Strain

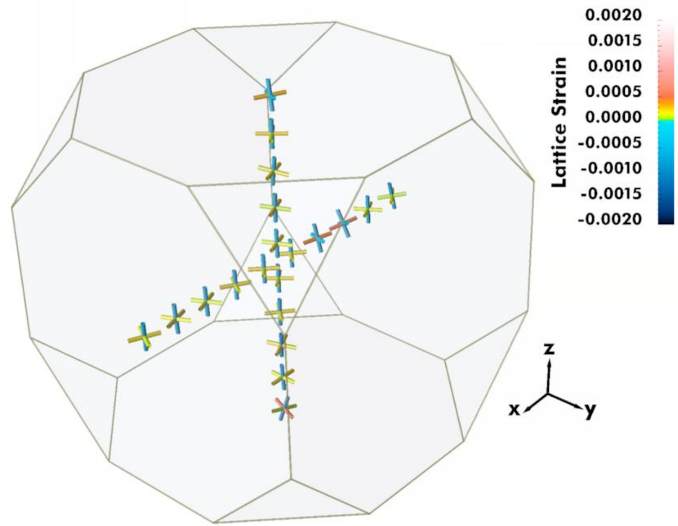


Principal Strains along Fibers

Stress Direction Evolution

Macro Stress = 94MPa



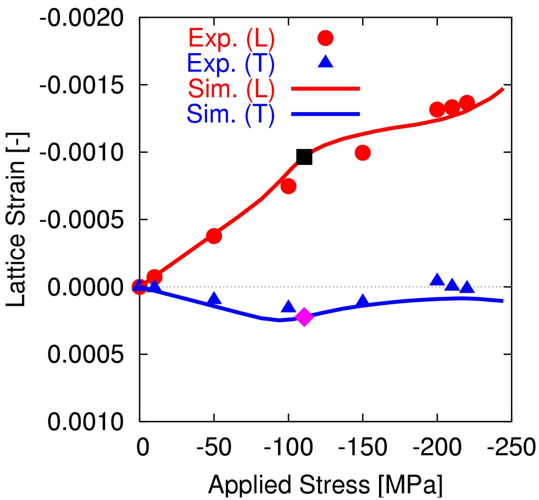


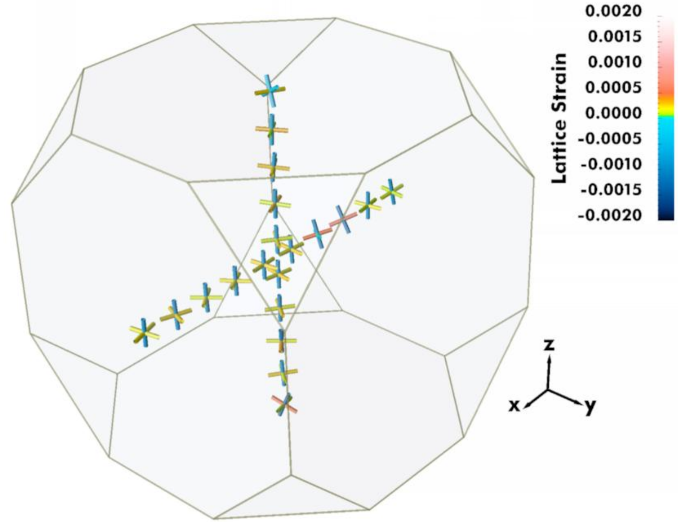
Average Fiber Lattice Strain

Principal Strains along Fibers

Stress Direction Evolution

Macro Stress = 111MPa



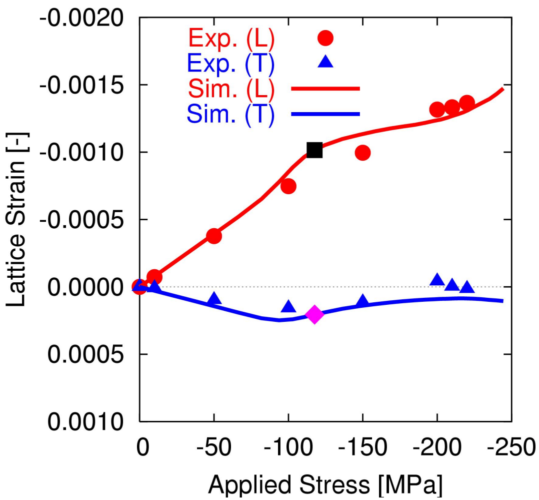


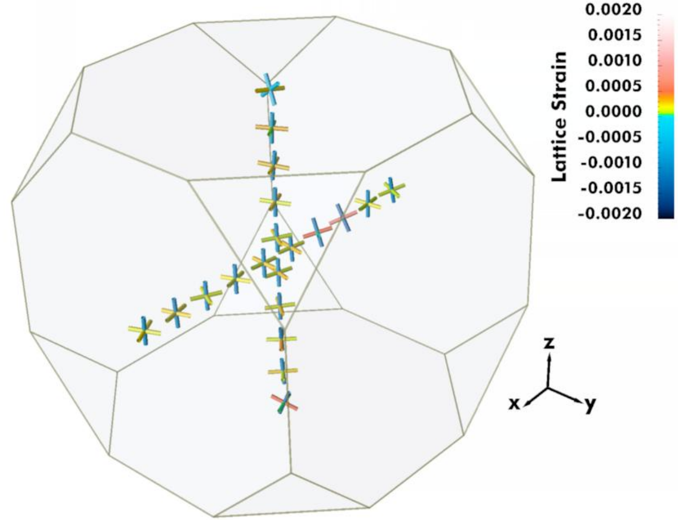
Average Fiber Lattice Strain

Principal Strains along Fibers

Stress Direction Evolution

Macro Stress = 118MPa



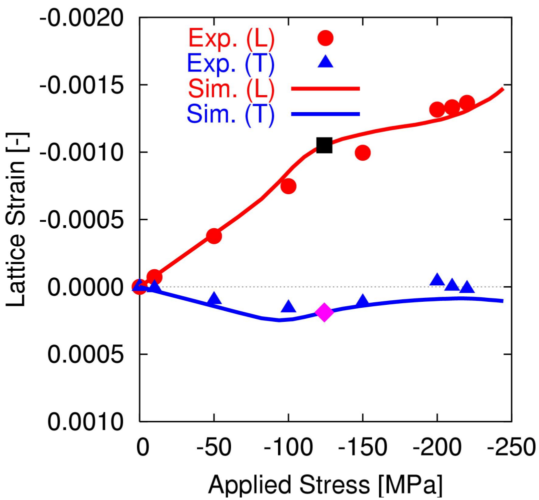


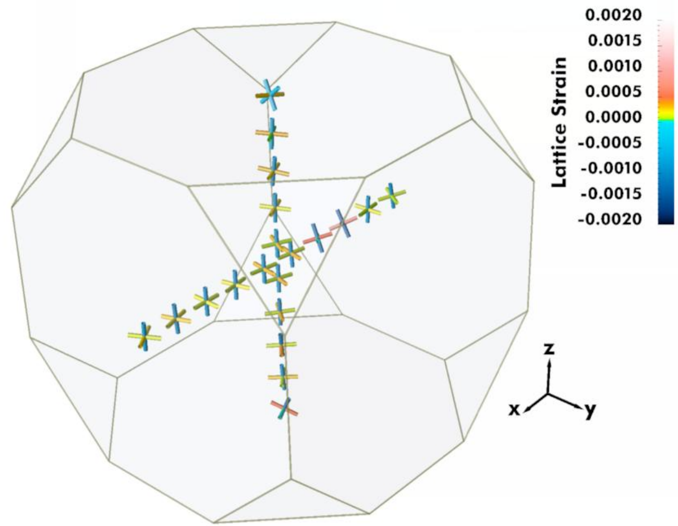
Average Fiber Lattice Strain

Principal Strains along Fibers

Stress Direction Evolution

Macro Stress = 124MPa



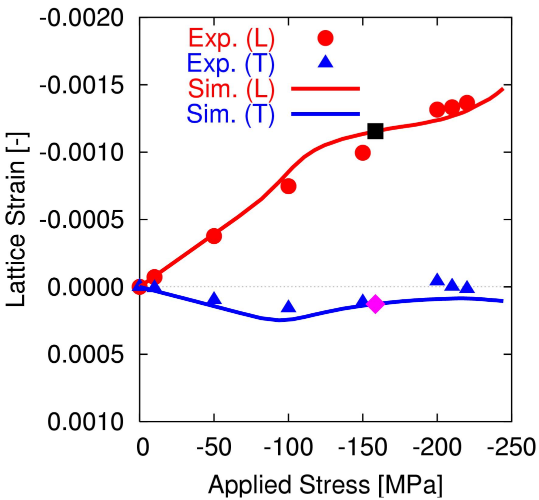


Average Fiber Lattice Strain

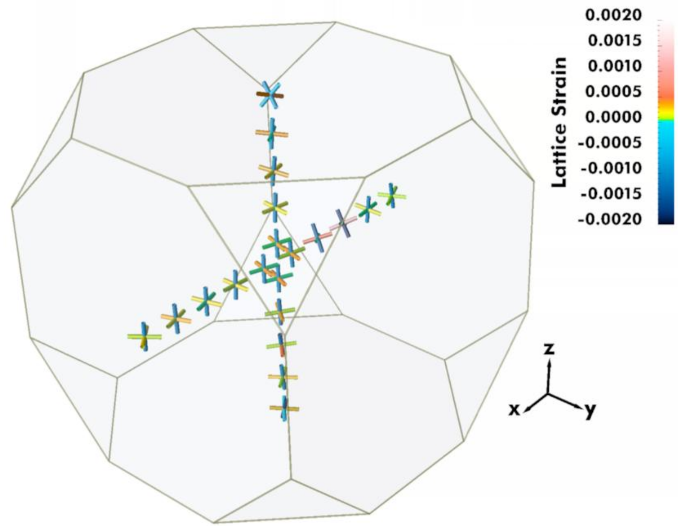
Principal Strains along Fibers

Stress Direction Evolution

Macro Stress = 158MPa



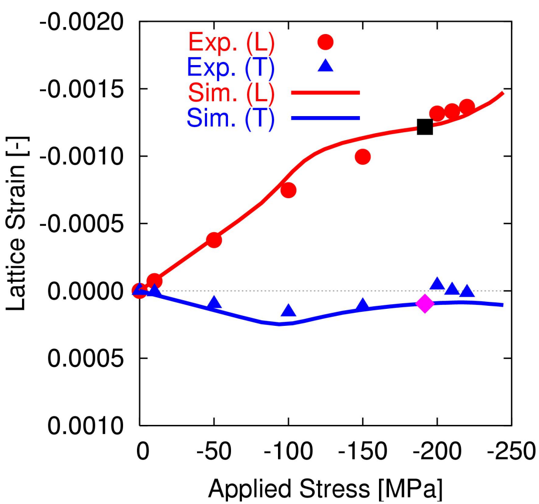
Average Fiber Lattice Strain



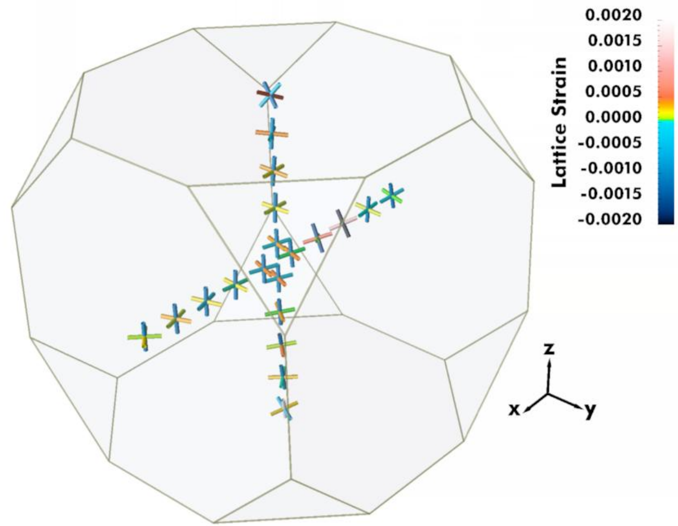
Principal Strains along Fibers

Stress Direction Evolution

Macro Stress = 192MPa



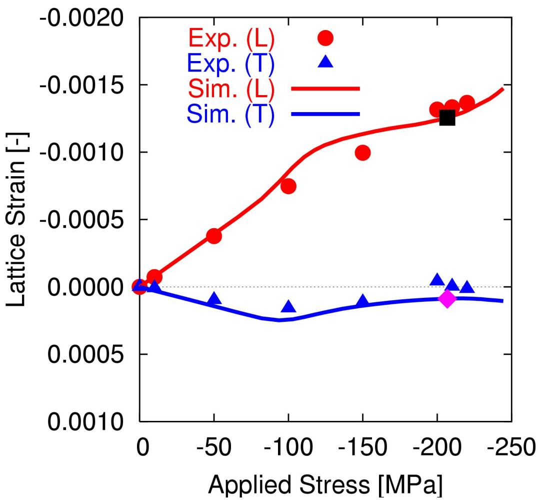
Average Fiber Lattice Strain

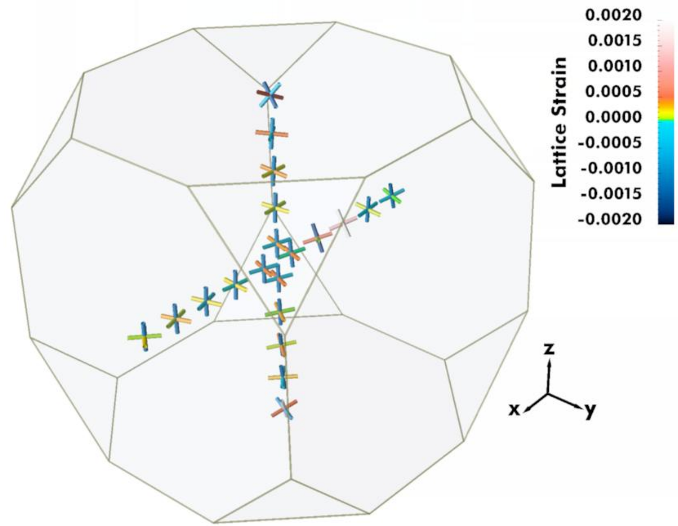


Principal Strains along Fibers

Stress Direction Evolution

Macro Stress = 207MPa



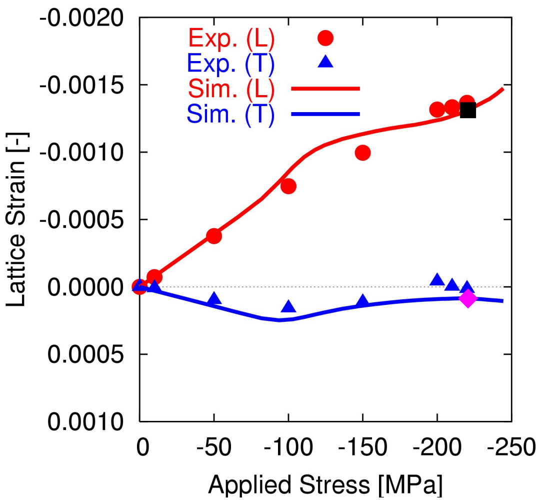


Average Fiber Lattice Strain

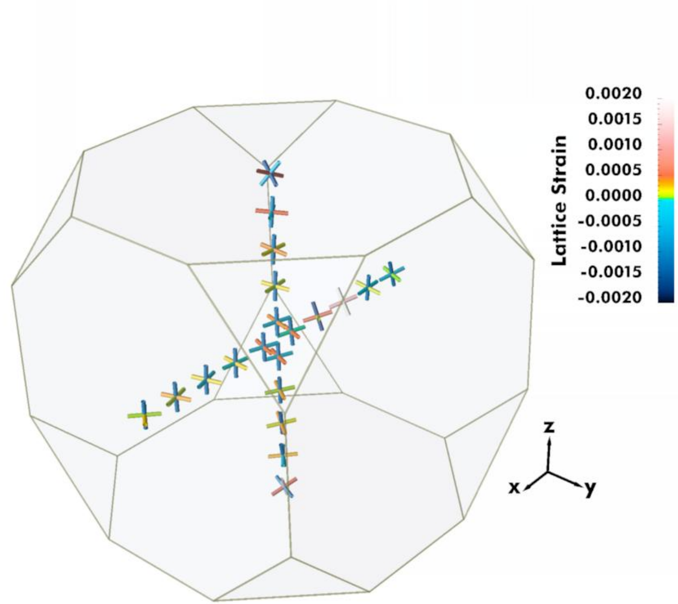
Principal Strains along Fibers

Stress Direction Evolution

Macro Stress = 221MPa



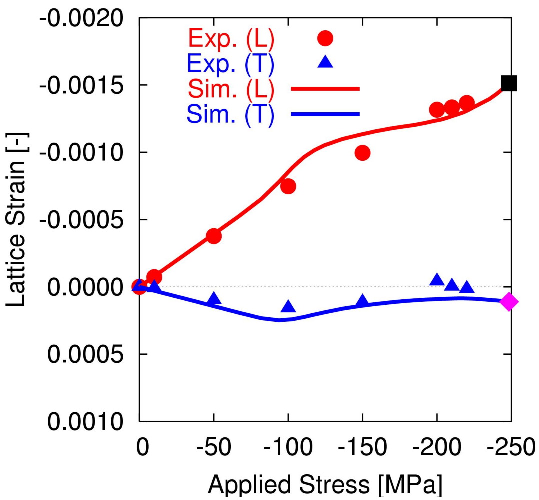
Average Fiber Lattice Strain



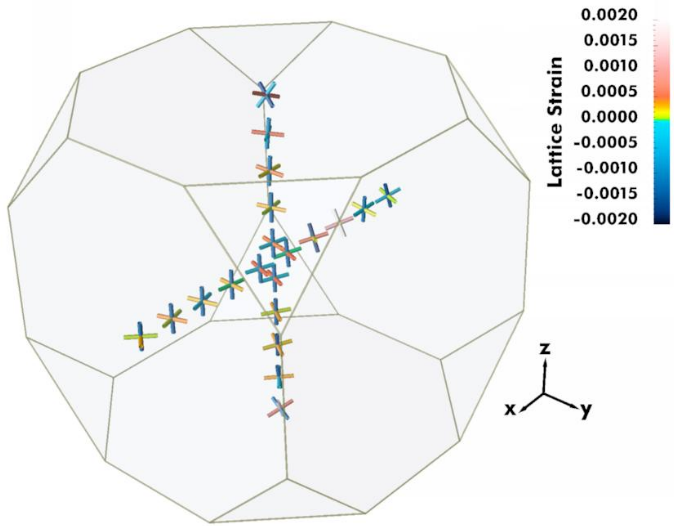
Principal Strains along Fibers

Stress Direction Evolution

Macro Stress = 248MPa



Average Fiber Lattice Strain



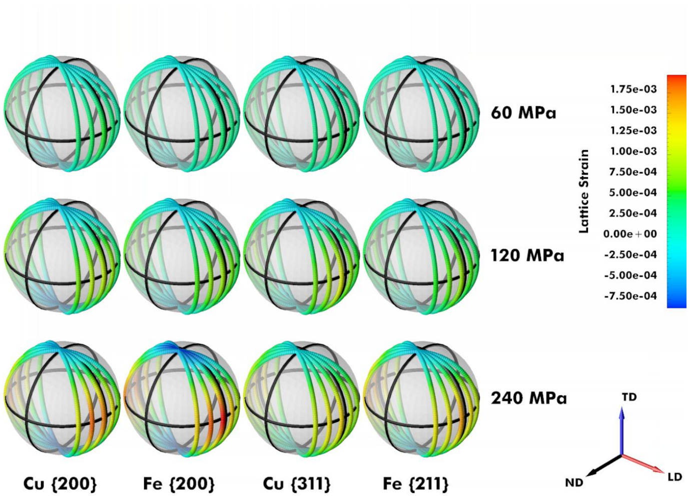
Principal Strains along Fibers

Comparisons of Neutron and X-ray Strains

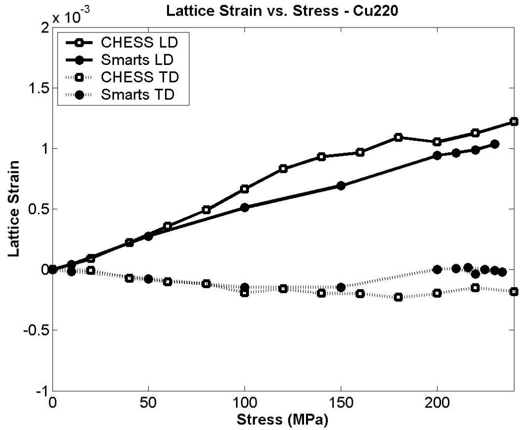
Comparions:

- Neutrons → SMARTS
- X-rays → CHESS
- Tension tests; elastic regime

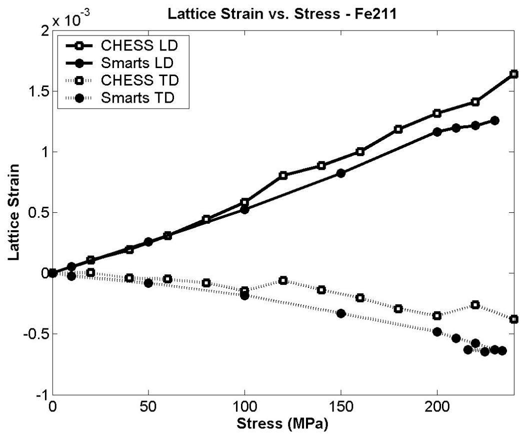
Strain pole figures:



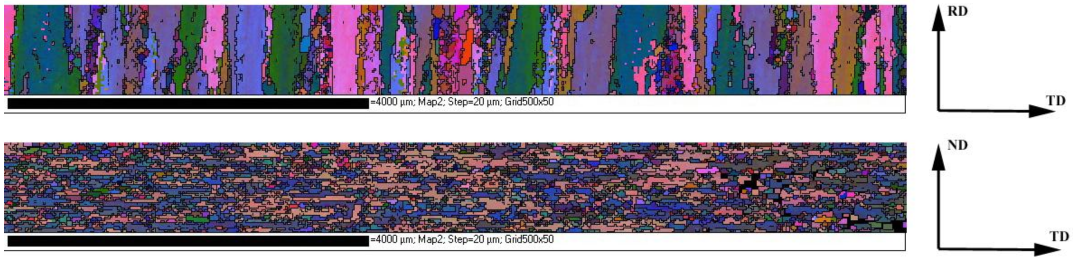
Copper 220 lattice strains



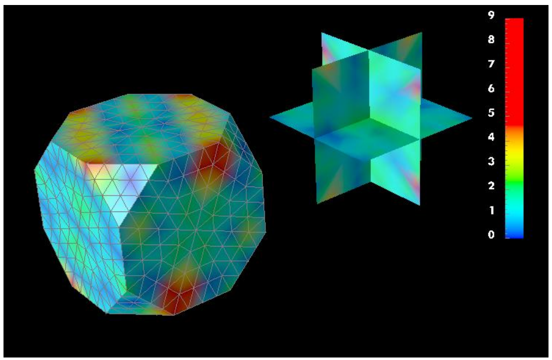
Iron 211 lattice strains



Fatigue Failure in Aircraft Alloys
AA7075-T6 Aircraft Plate

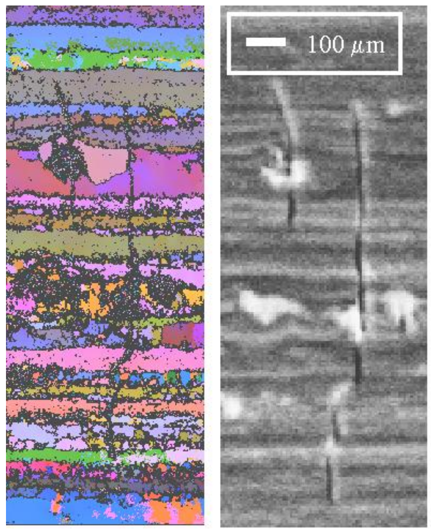


EBSD Scans (Loge)



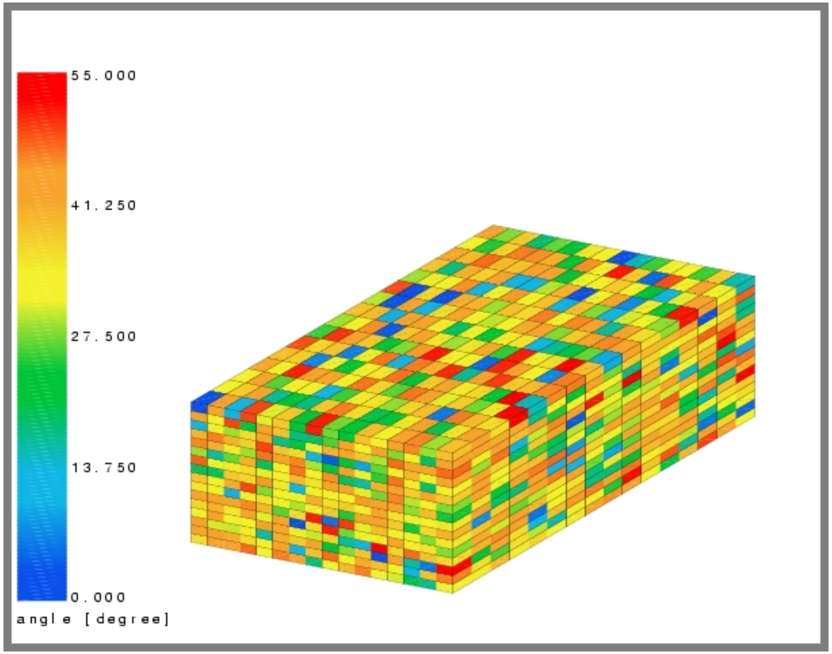
ODF

Observations:
Cracks form quickly at particles
Some grow, others don't
Driven by intracrystalline stress
Local environment is critical



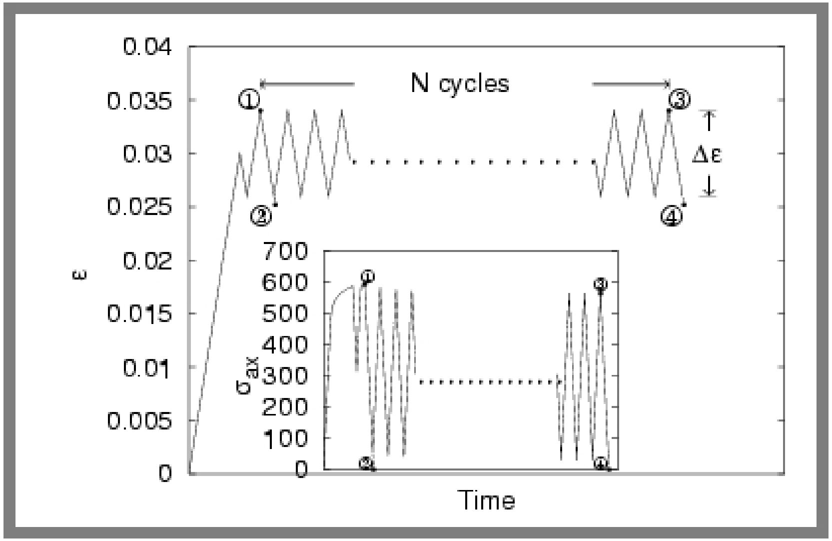
Microcracks

Low Cycle Fatigue of AA7075



Finite Element Polycrystal

Model:
- Element → crystal
- 4096 elements
- Lattice orientations from ODF

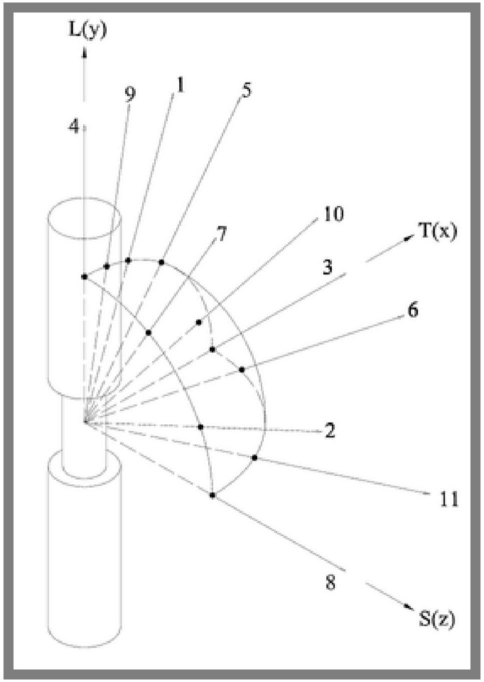


Cyclic Strain History

Simulation:
- 3% prestrain
- ±0.5% cyclic strain amplitude
- 1000 cycles

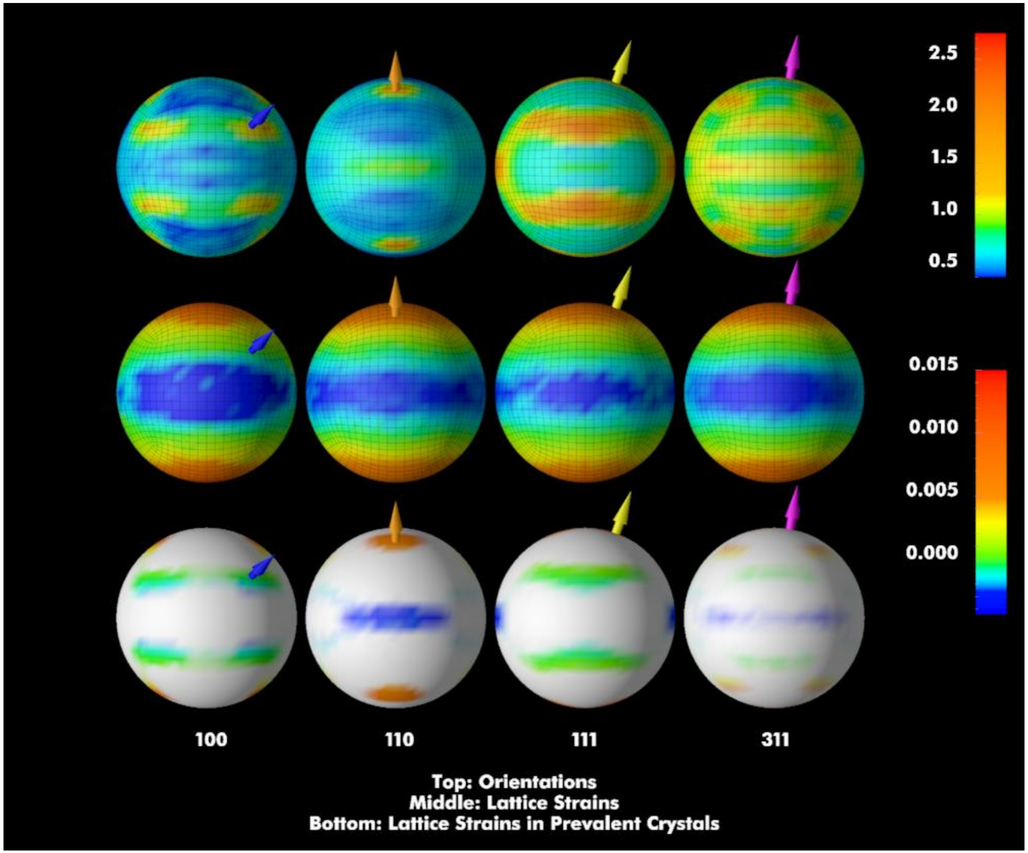
Run time:
- 10 days on 12 processors

Lattice Strain Under Load



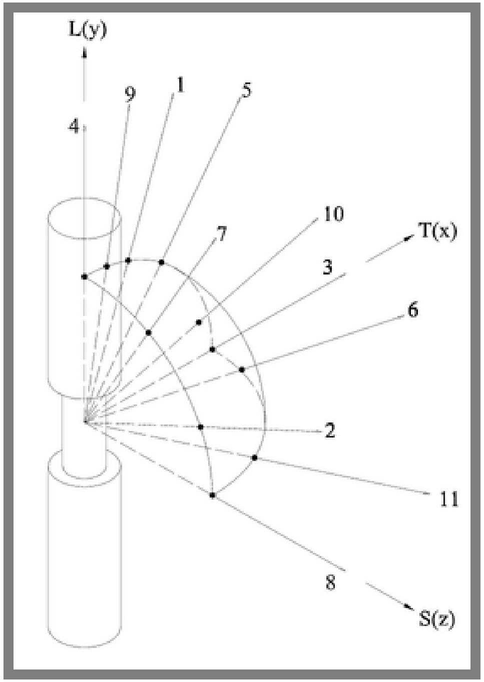
Tensile Specimen

Scattering vectors:
1,2,3 – 111 planes
4,5,6 – 200 planes
7,8 – 220 planes
9,10,11 – 311 planes



Lattice strains – loaded

Lattice Strains Unloaded



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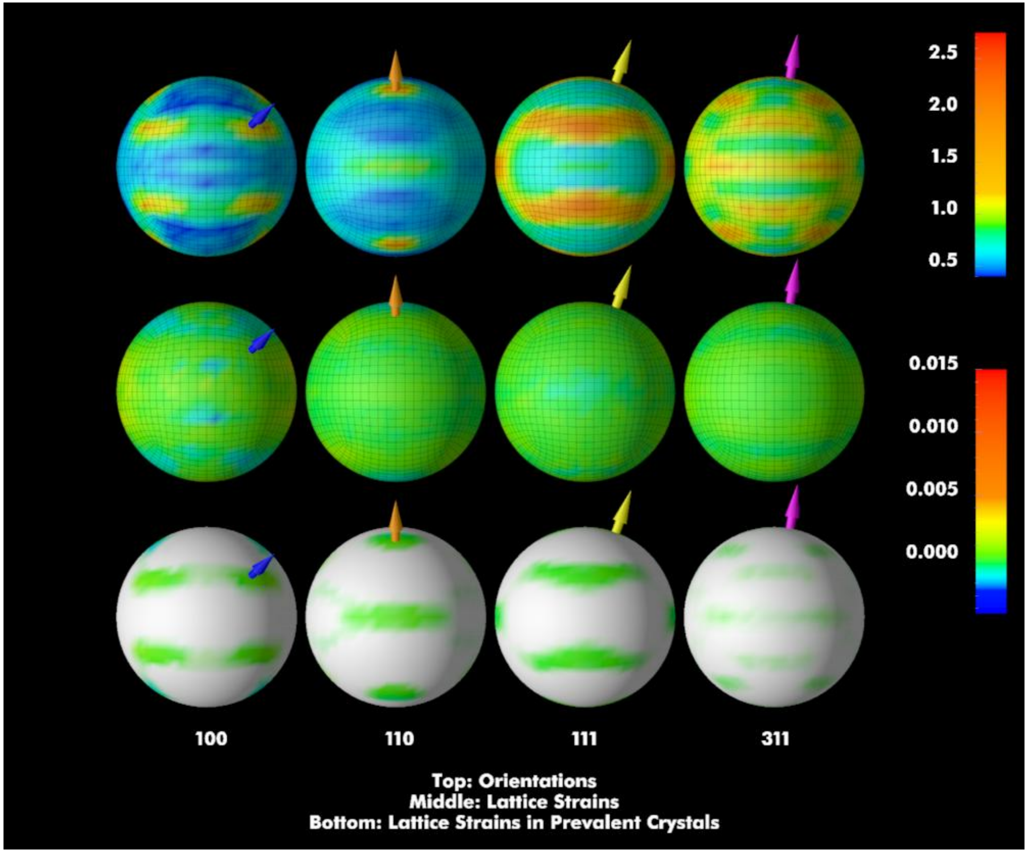
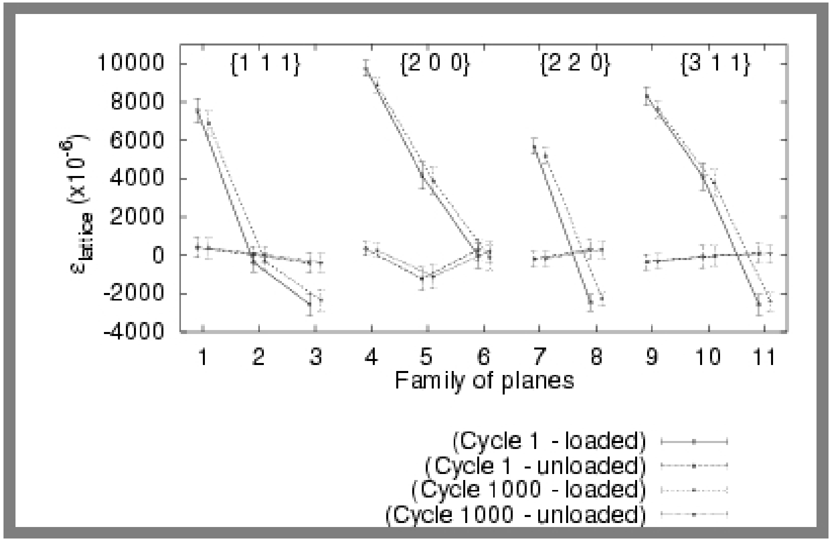
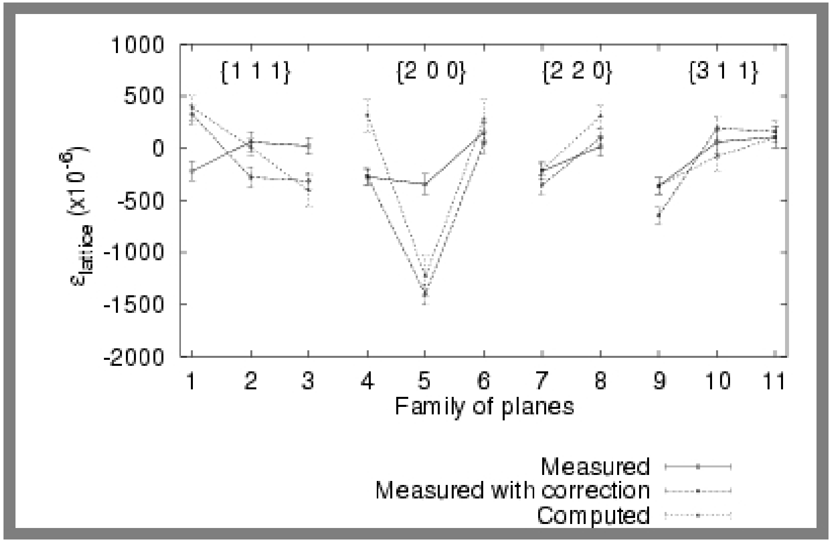


Lattice strains – unloaded

Lattice Strains



Computed strains

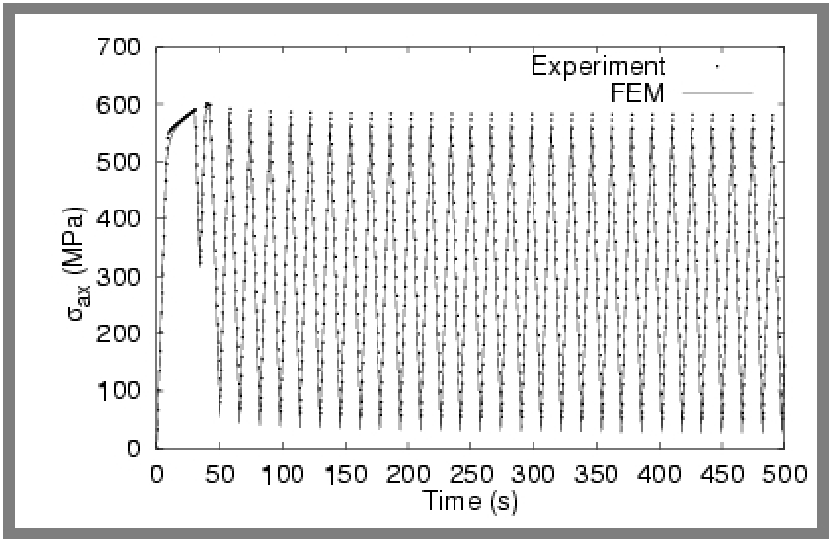


Comparisons

Simulations:
- Loaded and unloaded
- After 1 and 1000 cycles
- Lower loaded strains
- Constant unloaded strains

Comparisons:
- Unloaded strains only
- Experiments adjusted for initial lattice plane spacing

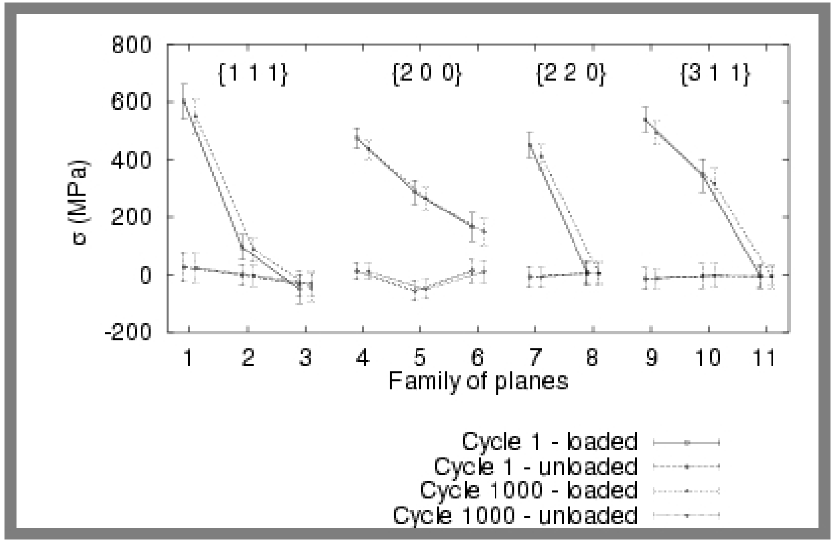
Stress Decay with Loading Cycles



Macroscopic stress

Macroscopic response:

- Stress at peak load diminishes with cycles
- Model and experiments are consistent



Crystal stresses

Microscopic response:

- Lattice stresses diminish with increasing cycles
- 15% standard deviation (compared to peak stress)
- Little evolution of unloaded stress with cycles

Summary Points

Model capability is advancing:

- Rapidly improving polycrystal discretization
  - account for neighborhood
- Capable of better physical fidelity
  - improved models are needed
- Can examine issues around
  - stress variability
  - strain hardening
  - load partitioning among phases
  - mechanisms for failure

Experimental challenges – *In situ* Loading:

- Time-resolved data:
  - phase changes
  - fatigue or fracture
- Spatially-resolved data:
  - load sharing
  - influence of topology
- Statistical confidence:
  - data includes extreme cases
- Profile interpretations:
  - peak width vs structure
  - defect recognition