Self-consistent Modeling of Polycrystal Plasticity

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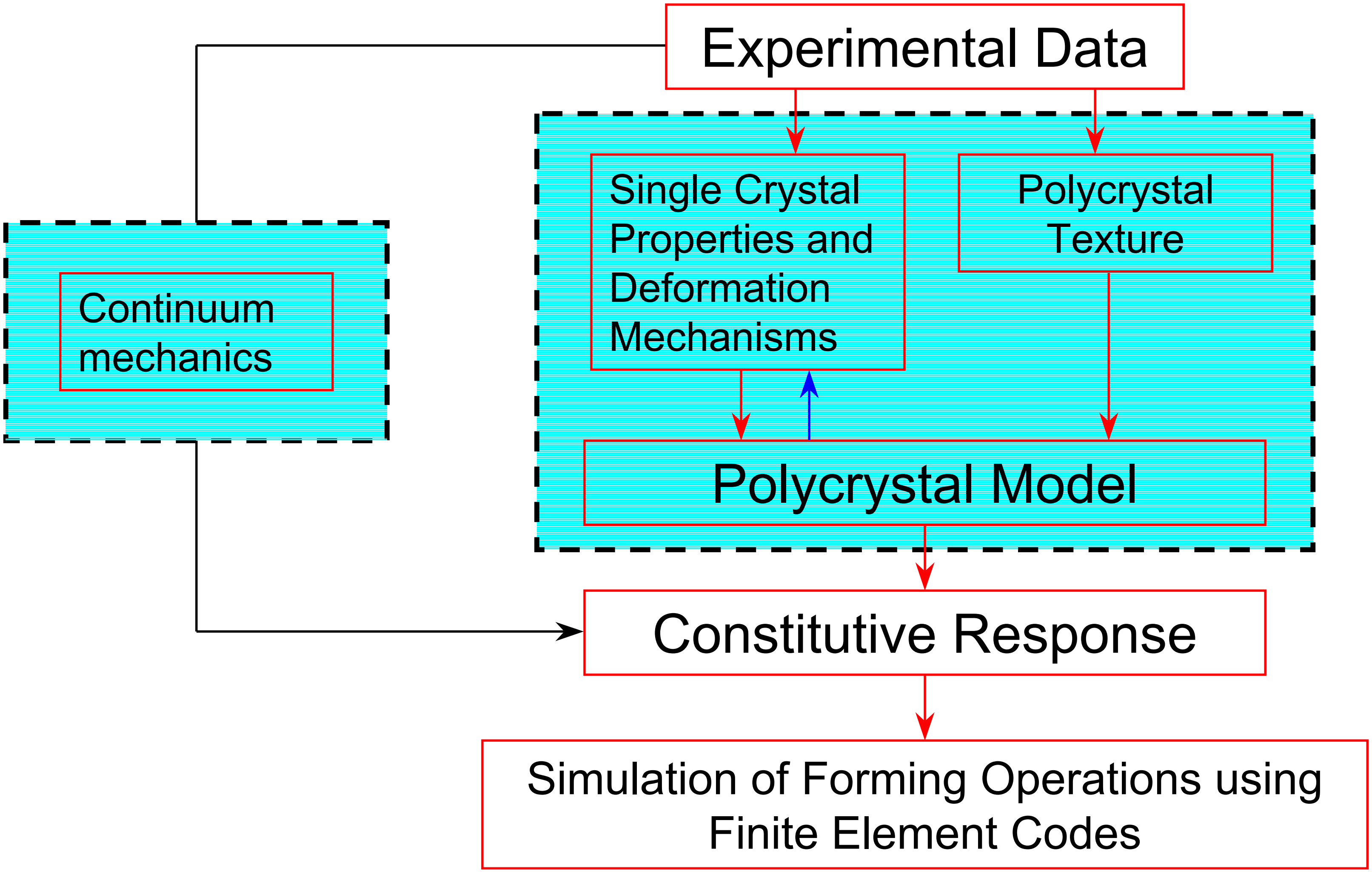
Polycrystal versus Continuum Constitutive Description



Outline

- Self-consistent model (SCM)
  - Input, assumptions, output
- Internal and residual strain development (EPSC)
  - Tensile testing of stainless steel
- Influence of deformation modes on texture development (VPSC)
  - Clock rolled Zircaloy
- Incorporating SCM into FEM formulation
  - Bending of highly textured zirconium bars
- Conclusions

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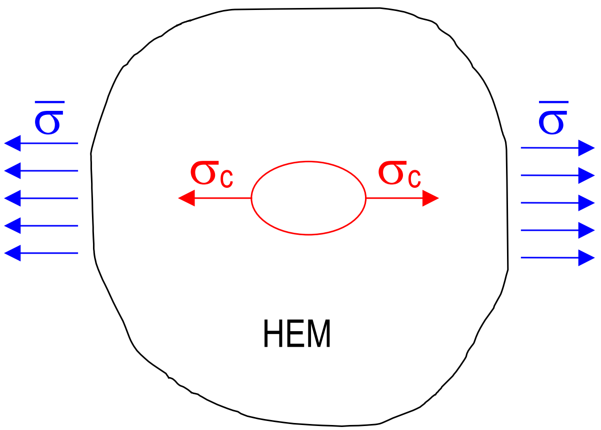
Self-consistent model (SCM) - EPSC

- Material parameters
  - Single crystal stiffnesses and coefficients of thermal expansion
  - Description of texture with discrete set of grain orientations
  - Crystal structure, slip (and twinning) systems
  - CRSS and hardening law
- Model Assumptions
  - Eshelby inclusion theory
  - HEM properties equal to weighted average of the grains
- Output
  - Direct comparison with neutron diffraction measurements
  - Averages over grains sets representing reflections



Self-consistent model (SCM) - basic equations

$$\dot{\varepsilon}_c^P = \sum_i \boldsymbol{\mu}^i \dot{\gamma}^i$$

$$\sum_j \dot{\gamma}^j X^{ij} = \boldsymbol{\mu}^i \boldsymbol{\mathcal{L}}_c \dot{\boldsymbol{\varepsilon}}_c \,, \quad X^{ij} = h^{ij} + \boldsymbol{\mu}^i \boldsymbol{\mathcal{L}}_c \boldsymbol{\mu}^j$$

$$\dot{\gamma}^i = \boldsymbol{f}^i \dot{\boldsymbol{\varepsilon}}_c \,, \quad \boldsymbol{f}^i = \sum_k Y^{ik} \boldsymbol{\mathcal{L}}_c \boldsymbol{\mu}^k, \quad Y^{ij} = \left(X^{ij}\right)^{-1}$$

$$\boldsymbol{L}_c = \boldsymbol{\mathcal{L}}_c \left(\boldsymbol{I} - \sum_m \boldsymbol{\mu}^m \boldsymbol{f}^m\right)$$

$$\dot{\boldsymbol{\varepsilon}}_c = \boldsymbol{M}_c \dot{\boldsymbol{\sigma}}_c, \quad \boldsymbol{M}_c = \left(\boldsymbol{L}_c\right)^{-1}$$

$$\boldsymbol{A}_c = \left(\boldsymbol{L}_c + \tilde{\boldsymbol{L}}\right)^{-1} \left(\boldsymbol{L} + \tilde{\boldsymbol{L}}\right)$$

$$\boldsymbol{L} = \langle \boldsymbol{A}_c \boldsymbol{L}_c \rangle$$

$$\tilde{\boldsymbol{L}} = \left(\boldsymbol{I} - \boldsymbol{S}\right)^{-1} \boldsymbol{S} \boldsymbol{L}$$

EPSC (small strain)

$$\dot{\varepsilon}_c^P = \sum_s \boldsymbol{\mu}^s \dot{\gamma}^s$$

$$\dot{\gamma}^s = \dot{\gamma}_0 \sum_s \boldsymbol{\mu}^i \left(\frac{\boldsymbol{\mu}^{s}:\sigma'}{\tau_c^s}\right)^n$$

$$\boldsymbol{M}_c = \dot{\gamma}_0 \sum_s \frac{\mu_i^s \mu_j^s}{\tau_c^s} \left(\frac{\mu_k^s \sigma'_k}{\tau_c^s}\right)^{n-1}$$

$$\dot{\boldsymbol{\varepsilon}}_c = \boldsymbol{M}_c : \boldsymbol{\sigma}'_c$$

$$\boldsymbol{B}_c = \left(\boldsymbol{M}_c + \tilde{\boldsymbol{M}}\right)^{-1} \left(\boldsymbol{M} + \tilde{\boldsymbol{M}}\right)$$

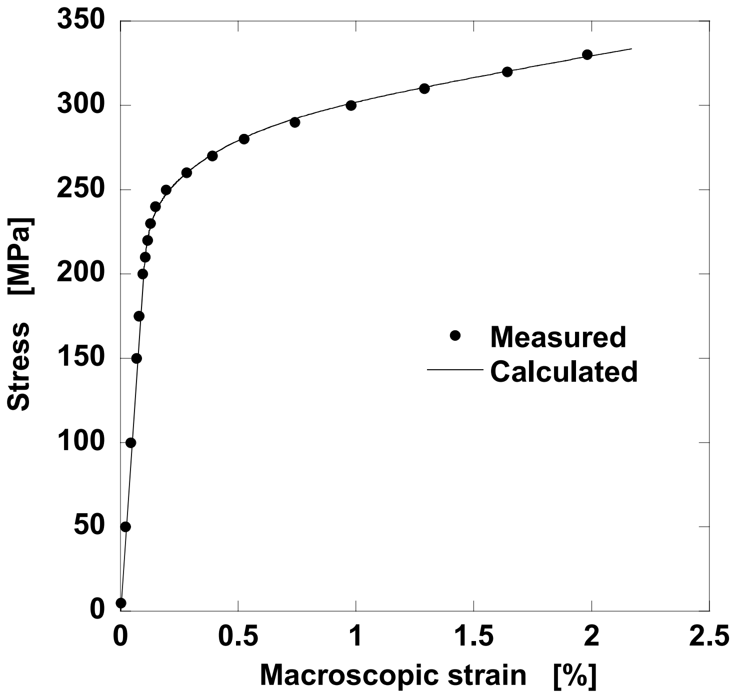
$$\boldsymbol{M} = \langle \boldsymbol{B}_c \boldsymbol{M}_c \rangle$$

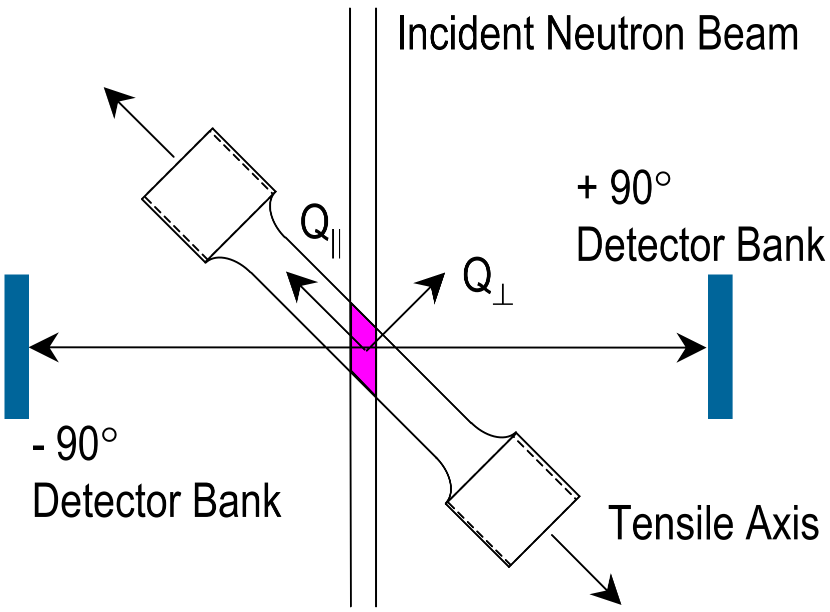
$$\tilde{\boldsymbol{M}} = n \left(\boldsymbol{I} - \boldsymbol{S}\right)^{-1} \boldsymbol{S} \boldsymbol{M}$$

VPSC (large deformations)

- Basic equations for the EPSC and VPSC formulations
- Solve last two sets of equations iteratively

Comparison to neutron diffraction data - EPSC





- Uniaxial tensile loading of austenitic stainless steel
- ND measurements made at load levels marked by the symbols
- Schematic set-up of the NPD at LANSCE. Measurement time is about 2-3 hours
- Measure elastic strains in two directions simultaneously

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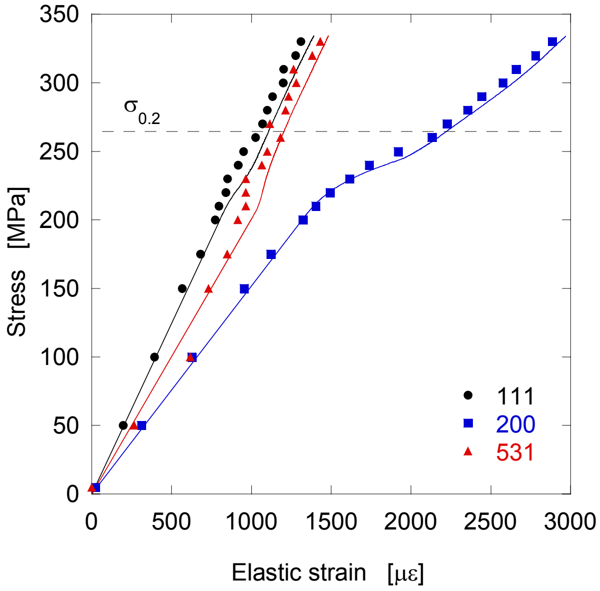
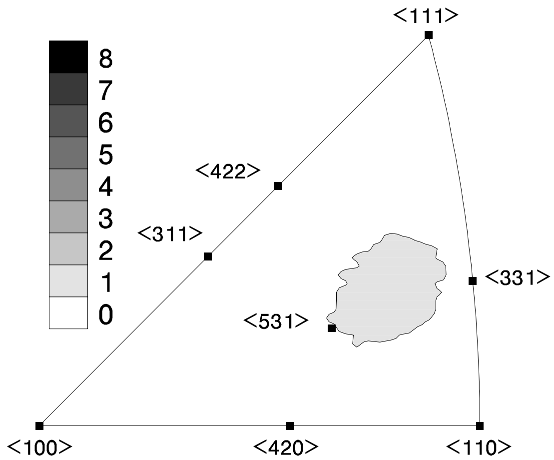
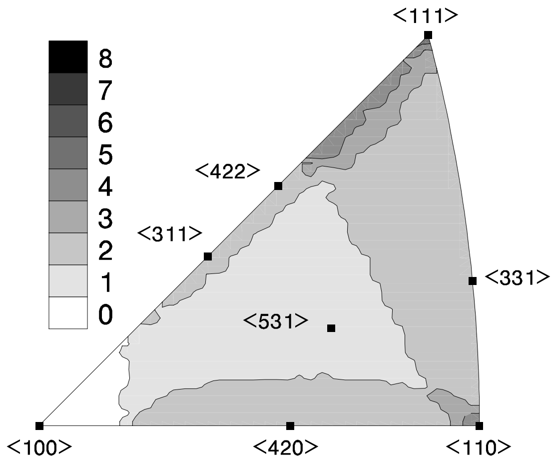
Comparison to neutron diffraction data - EPSC





Active slip systems after 10 $\mu\varepsilon$ plastic strain



Active slip systems after 100 $\mu\varepsilon$ plastic strain

- Applied stress versus measured elastic lattice strain
- ND measures lattice spacing changes and thereby only elastic strains
- Symbols are measurements, lines are model predictions

- The reflections carry different amount of the load
- Plasticity starts around the <531> orientation
  - => the <531> reflection deflects to the left
- The <100> orientation stays elastic the longest
  - => the <200> reflection deflects to the right

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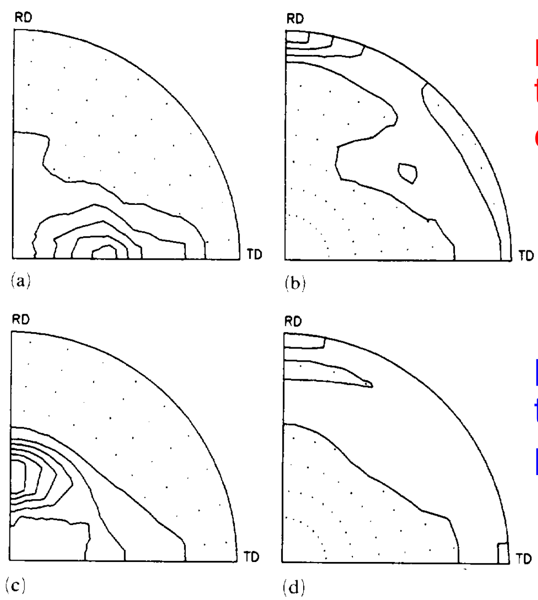
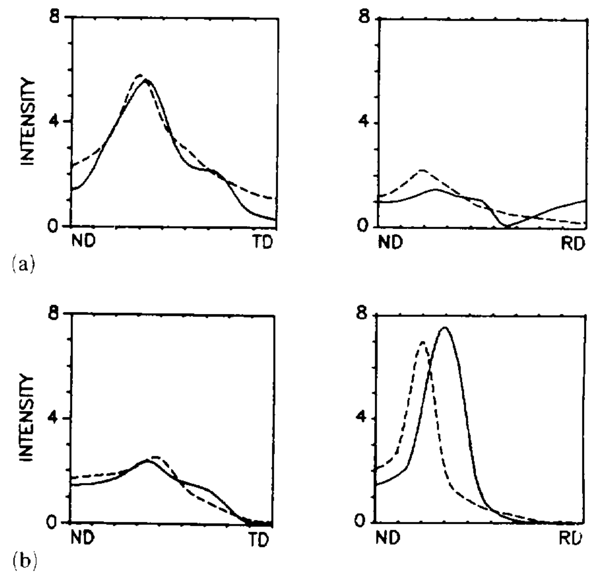
Self-consistent model (SCM) - VPSC



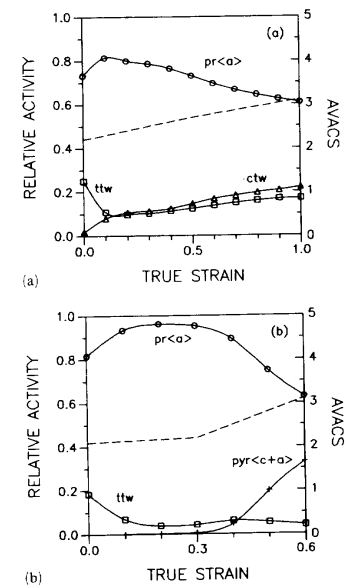
pr
ttw
ctw

pr
ttw
pyr

Predicted <0002> and <10$\bar{1}$0> pole figures



Predicted and measured intensities along ND-TD and ND-RD



Predicted relative activity of the deformation modes

- Prediction of rolling textures for Zircaloy, rolled to a true strain of 1.0
- Two different model assumptions of plastic deformation modes
  - prismatic, tensile twins and compressive twins versus prismatic, tensile twins and pyramidal
- Comparison to measured textures for Zircaloy with two different grain sizes

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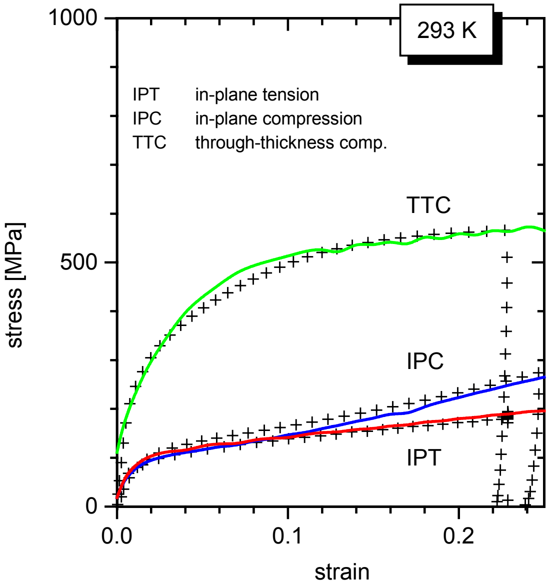
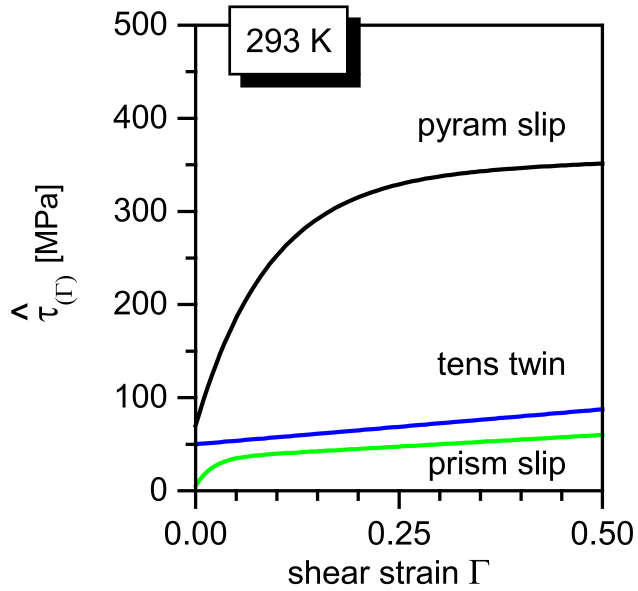
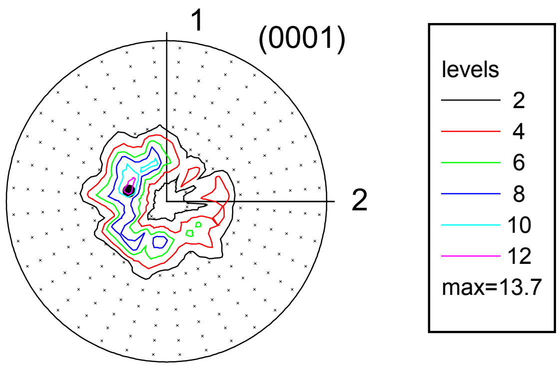
SCM and FEM







- Highly textured “clock” rolled Zirconium
- One set of deformation modes, CRSS and hardening parameters
- Possible to reproduce measured material behavior for all three deformation tests
  - Through thickness compression (TTC), in-plane compression (IPC) and in-plane tension (IPT)

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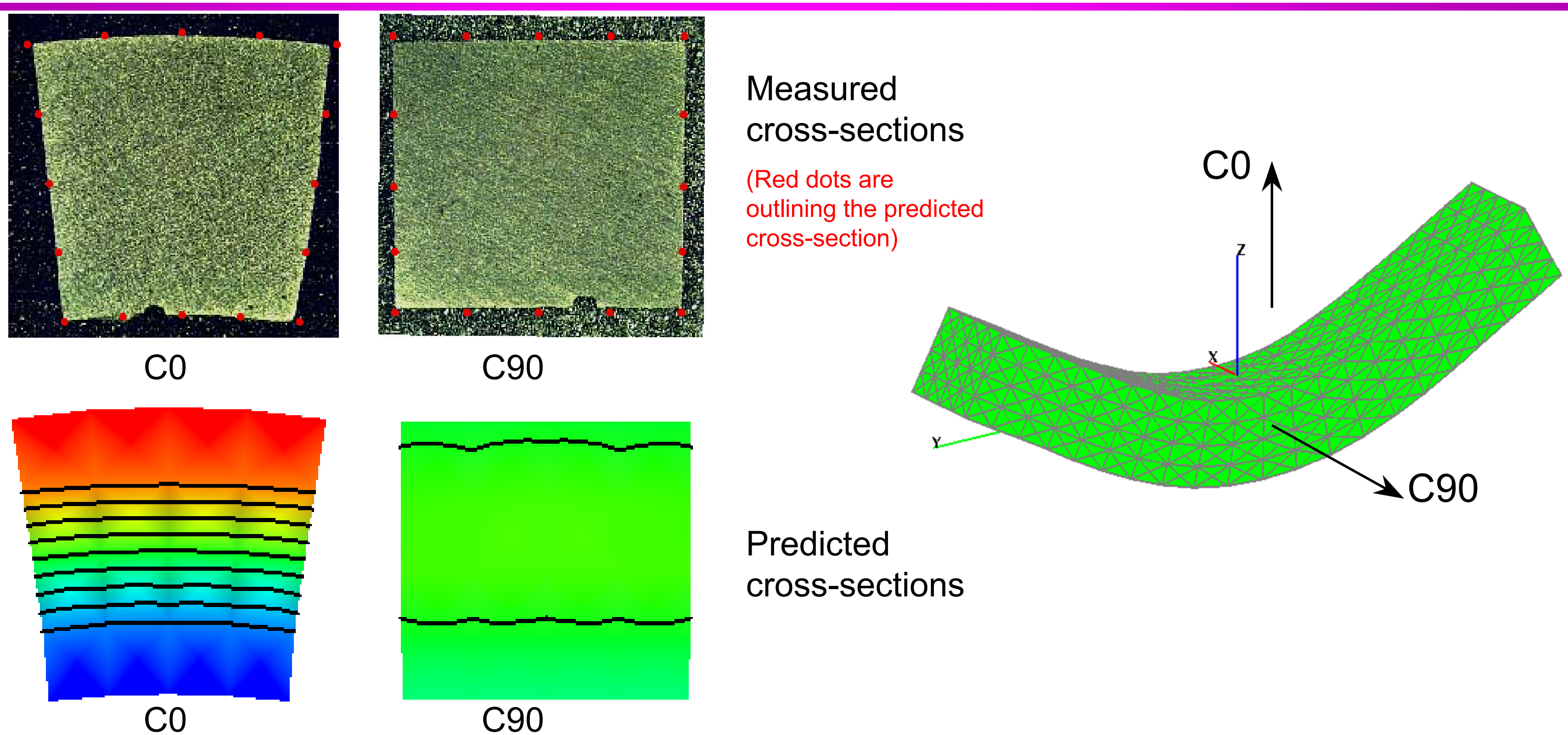
SCM and FEM



- 4-point bending of heavily textured Zirconium bars
- Difference in deformed cross-section depending on orientation of preferred c-axis orientation (C0 or C90)
- 377 grain orientations for each element, 4000 elements
- Good agreement between predicted cross-sections and measured data

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Conclusions

- Self-consistent modeling (polycrystal constitutive model)
  - Very useful tool for interpreting neutron diffraction data
  - Pinpoint active deformation mechanisms
- Prediction of internal and residual stresses and strains (EPSC)
- Prediction of texture development for large strains (VPSC)
- Incorporated SCM into FEM formulation

Self-consistent model (SCM) - EPSC

- Known elastic properties
  - Calculate HEM stiffness using Voigt, Reuss or Hill average
  - Calculate stress and strain increments in all grains for given macroscopic stress or strain increment
    - Requires knowledge of stiffness of HEM and all the grains
    - Determines a new self-consistent average stiffness
  - Compare the new and old average stiffness/compliance
    - Iterate until sufficient convergence is obtained
- Further deformation
  - Yielding in grains (stress exceeds yield criteria)
    - Determine the elastic-plastic stiffness
- "Bookkeeping"
  - Calculate elastic strains for grain sets representing reflections
  - Statistics on; # of slip systems, Taylor factor, plastic strain, etc.

Talk

- Somewhat different length scale - “meso scale”
- Self-consistent polycrystal models
- Tool to predict the macroscopic behavior of a material using microscopic material behavior, such as single X-tal elastic stiffness, inelastic deformation modes like slip and twining, and texture
- Show how we can validate this tool with neutron diffraction measurements of elastic lattice strains and texture measurements

- Start out with describing how we can use the SC models as a constitutive material formulation