Elastic-Plastic Self-Consistent Model Including Grain Reorientation Due to Twinning

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Motivation

- Developing polycrystal deformation models
  - Predict forming processes
  - Need physically based model
- Why do we need sophisticated models?
  - Industrial example
    - Use of magnesium in auto manufacturing
    - Investigate lack of room temperature ductility
    - Design microstructure that maximizes ductility
  - Science
    - Bridging the gap between micro and macro level
    - The models act as the medium for bringing together experimental and theoretical research on many levels

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Self-consistent Polycrystal Deformation Models

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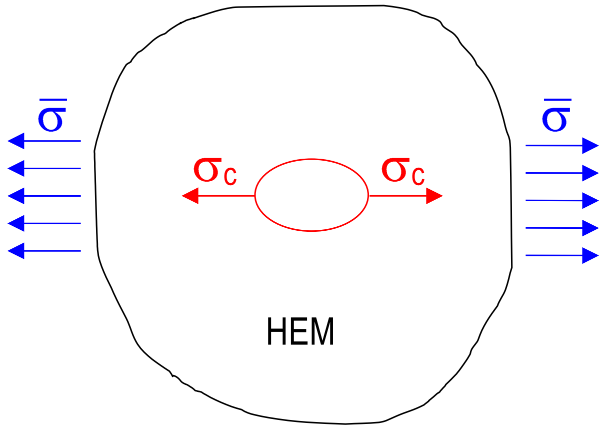
Self-consistent Polycrystal Deformation Models

- The polycrystal is regarded as an agglomerate of single crystal grains
  - Properties of each grain is given by single crystal elastic constants, possible plastic deformation mechanisms and their hardening behavior
- No direct grain-to-grain interactions
  - Eshelby theory used to describe interaction between single grain and a homogeneous equivalent medium (HEM)



- The properties of the HEM is found as the weighted average over all the grains – hence the name “self-consistent”

Self-consistent Polycrystal Deformation Models

- **EPSC** – Elastic-plastic Self-consistent Model
  - Small strain model; Texture development not included

$$\dot{\boldsymbol{\sigma}}_c = \boldsymbol{L}_c \dot{\boldsymbol{\varepsilon}}_c \qquad \boldsymbol{L}_c = \mathcal{L}_c \left(\boldsymbol{I} - \sum_m \boldsymbol{\alpha}^m \otimes \boldsymbol{f}^m \right)$$

$$\boldsymbol{f}^i = \sum_k Y^{ik} \mathcal{L}_c \boldsymbol{\alpha}^k \qquad Y^{ij} = \left[X^{ij} \right]^{-1} \qquad X^{ij} = h^{ij} + \boldsymbol{\alpha}^i \mathcal{L}_c \boldsymbol{\alpha}^j$$

  - Keep stresses in equilibrium
    - Very small increments

- Model validation
  - Macroscopic properties and diffraction measurements of internal elastic strains

Turner and Tomé, *Acta Metall.*, vol. 42(12), pp. 4143-4153, 1994

Self-consistent Polycrystal Deformation Models

- **VPSC** – Visco-plastic Self-consistent Model
  - Large strain model; Texture included, Elasticity is not included

$$\dot{\boldsymbol{\varepsilon}}^c = \boldsymbol{M}^c \boldsymbol{\sigma}^c \qquad M_{ij}^c = \dot{\gamma}_0 \sum_s \frac{\alpha_i^s \alpha_j^s}{\tau^s} \left(\frac{\alpha_k^s \sigma_k}{\tau^s} \right)^{n-1}$$

  - Reference state is ‘reset’ at each step
    - Large strain steps are possible
- Model validation
  - Measured macroscopic properties and texture

Lebensohn and Tomé, *Acta Metall.*, vol. 41(9), pp. 2611-2624, 1993

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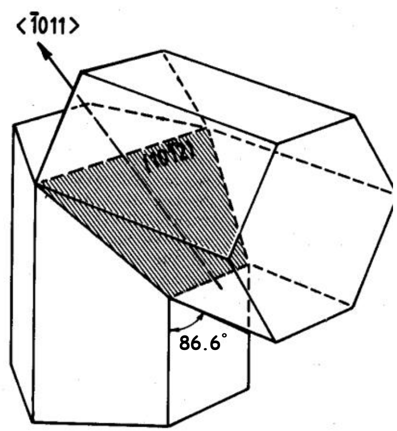
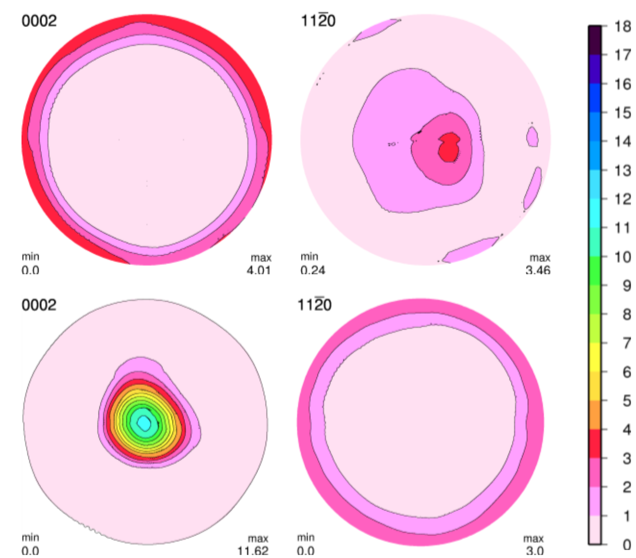
Self-consistent Polycrystal Deformation Models

- Missing link
  - Materials deforming primarily by twinning exhibits *significant* texture development at small strains (<10% strain)
  - Example:
    - Magnesium twins very easy on the tensile twin system
    - Twin volume fraction about 70% after 10% strain $\Rightarrow$ Major texture change



As extruded

10% compression



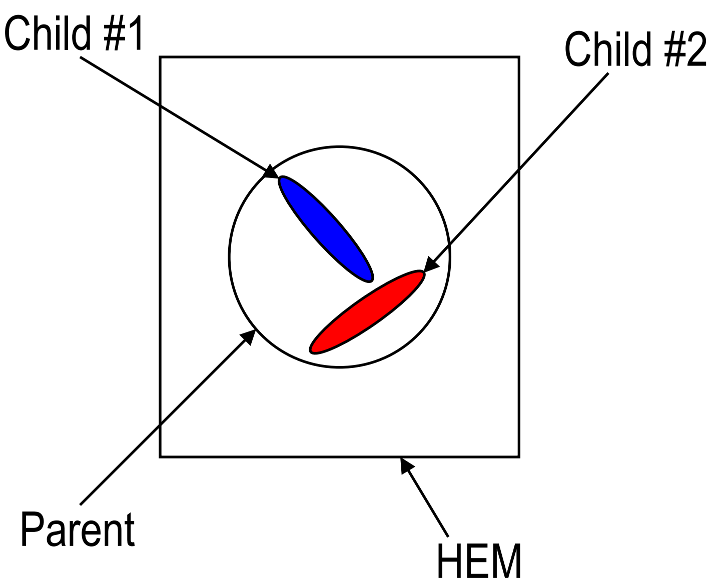
Tensile Twin: $\langle 10\bar{1}1\rangle \; \{10\bar{1}2\}$

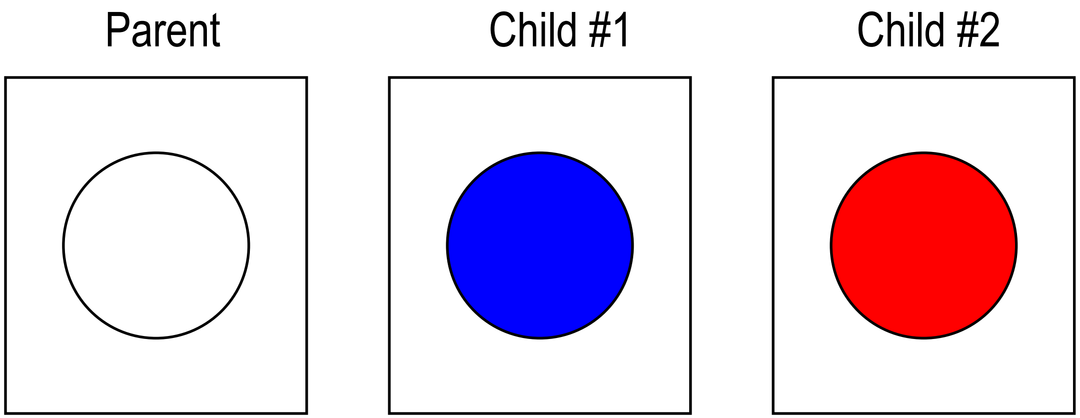
Motivation

- Need a model for predicting behavior of materials that deform primarily by twinning
- Must account for
  - Internal stresses and strains
  - Texture development
  - Initial state of twin grains
  - Stress relaxation due to twinning

EPSC with Grain Re-Orientation due to Twinning

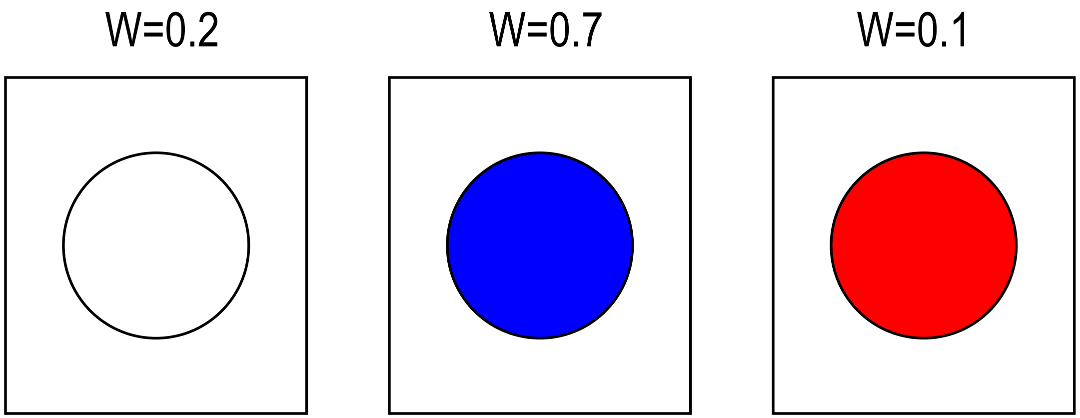
- Add a new grain for each active twin system in Parent grains
  - Possible multiple Child grains for each Parent grain
  - No direct interaction between Parent and Child after conception
    - The Child grains are "just another grain in the polycrystal"





EPSC with Grain Re-Orientation due to Twinning

- Weight fraction shifted from Parent to Child grains
  - Amount determined from twin shear in Parent and the characteristic shear for the twin system
  - A parent grain can fully disappear
    - Total weight of Parent and Child grains is always equal to the initial weight of the Parent grain
    - No initial waiting period as in the Predominant Twin Reorientation scheme used in VPSC

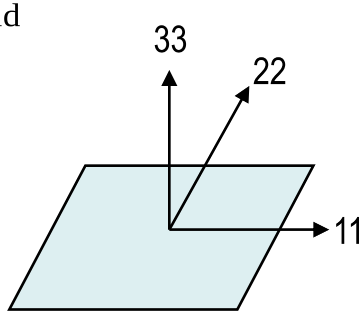


EPSC with Grain Re-Orientation due to Twinning

- Initial stress and strain state in the Child grains?
  - Continuity of tractions and displacements across the twin plane
    - Using the shear direction as the 11 direction and the twin plane normal as the 33 direction we find that:

$$\varepsilon_{11}^{\text{E, Parent}} = \varepsilon_{11}^{\text{E, Child}}, \varepsilon_{22}^{\text{E, Parent}} = \varepsilon_{22}^{\text{E, Child}} \text{ and } \varepsilon_{12}^{\text{E, Parent}} = \varepsilon_{12}^{\text{E, Child}}$$

$$\sigma_{33}^{\text{Parent}} = \sigma_{33}^{\text{Child}}, \sigma_{23}^{\text{Parent}} = \sigma_{23}^{\text{Child}} \text{ and } \sigma_{13}^{\text{Parent}} = \sigma_{13}^{\text{Child}}$$

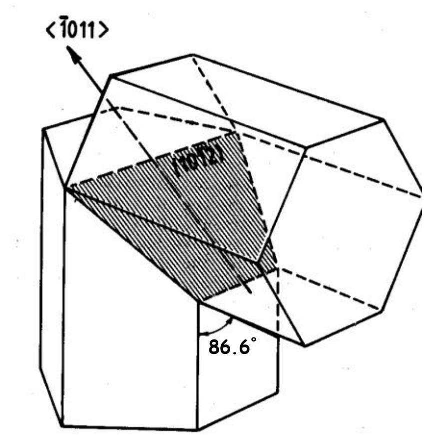


    - The stiffness tensor of the twin is needed to determine the unknown stress and ***elastic*** strain components within the twin
    - The ***plastic*** strain of the twin is assumed equal to the plastic strain in the parent

Compressive Loading of Extruded Magnesium

Compressive Loading of Extruded Magnesium

- Magnesium twins very easily on the tensile twin system
  - It is call a tensile twin system as it is activated when the c-axis is subjected to tension



Tensile Twin: $\langle 10\bar{1}1\rangle \ \{10\bar{1}2\}$

Compressive Loading of Extruded Magnesium

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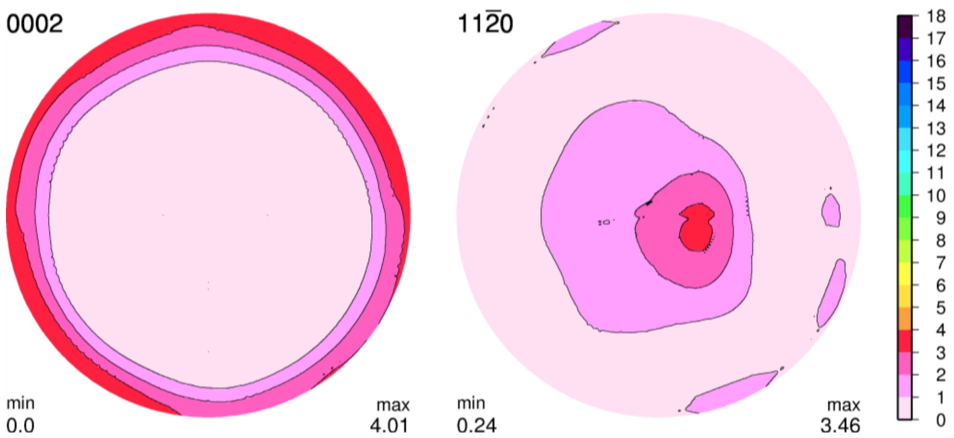
- In extruded magnesium all basal poles are perpendicular to the extrusion direction

Measured Initial Texture



Compressive Loading of Extruded Magnesium

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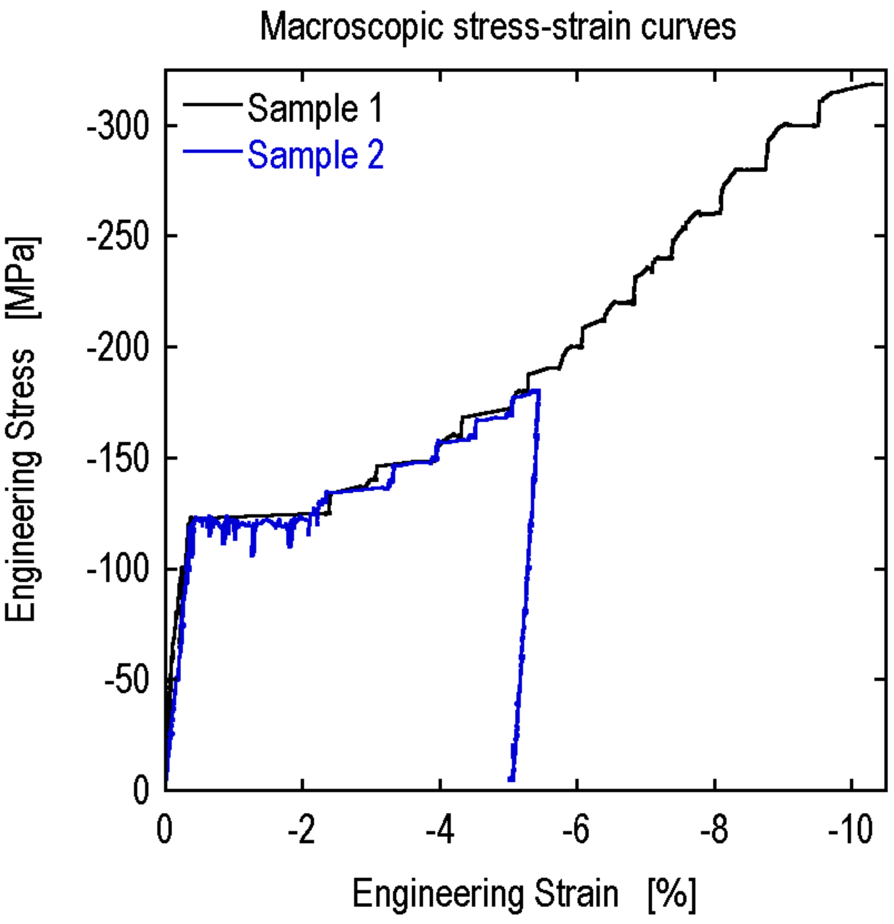
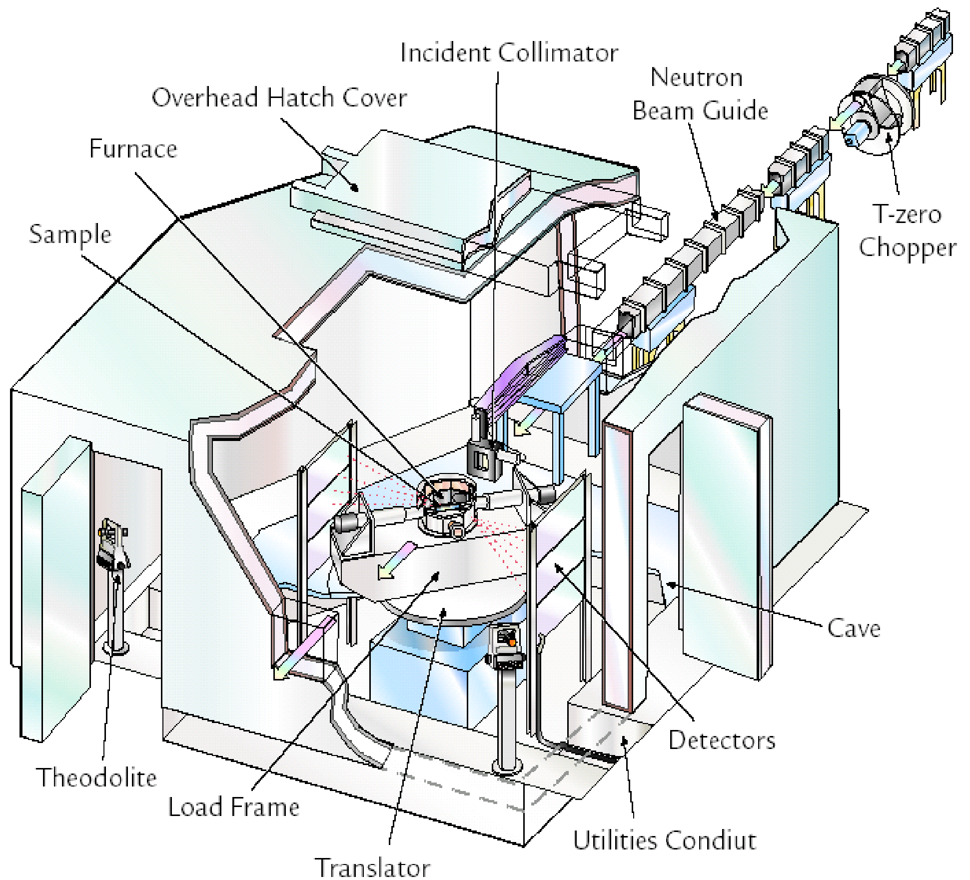
- In extruded magnesium all basal poles are perpendicular to the extrusion direction
- Plateau in macroscopic stress-strain curve



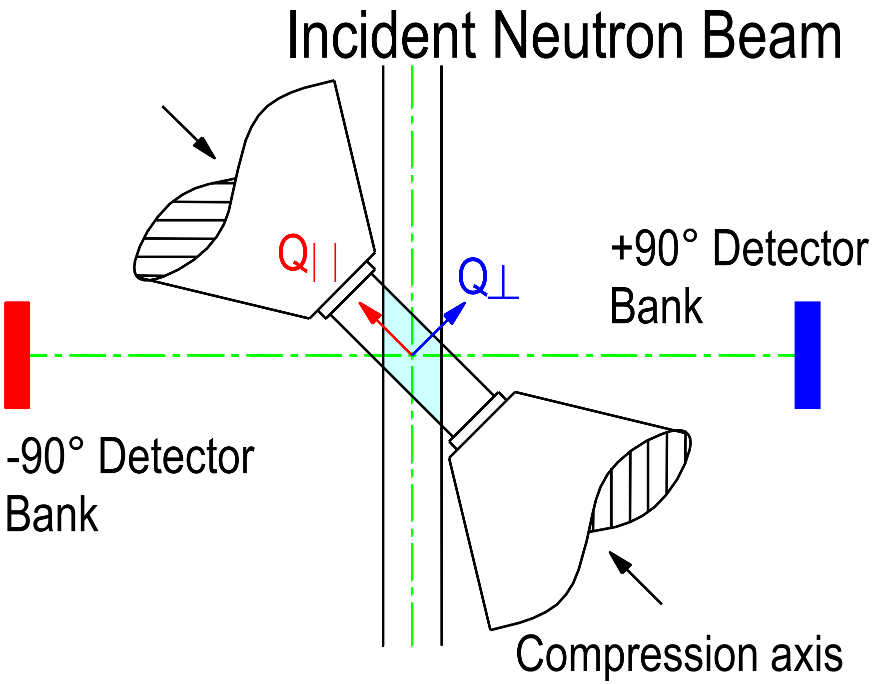
SMARTS

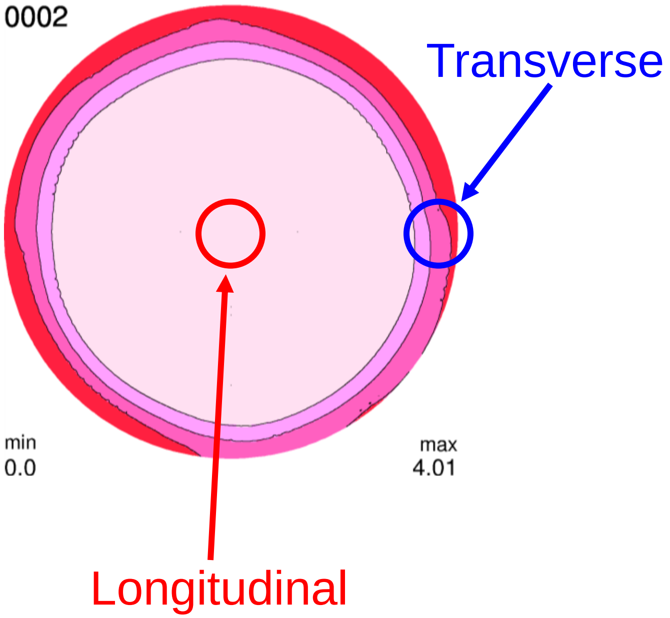
- **S**pectrometer for **MA**terials **R**esearch at **T**emperature and **S**tress

- Spatially resolved measurements
  - Residual strains in components
- *In situ* measurements
  - Strains as a function of stress, temperature, environment, …
- Instrument Scientists:
  - Donald W. Brown
  - Bjørn Clausen

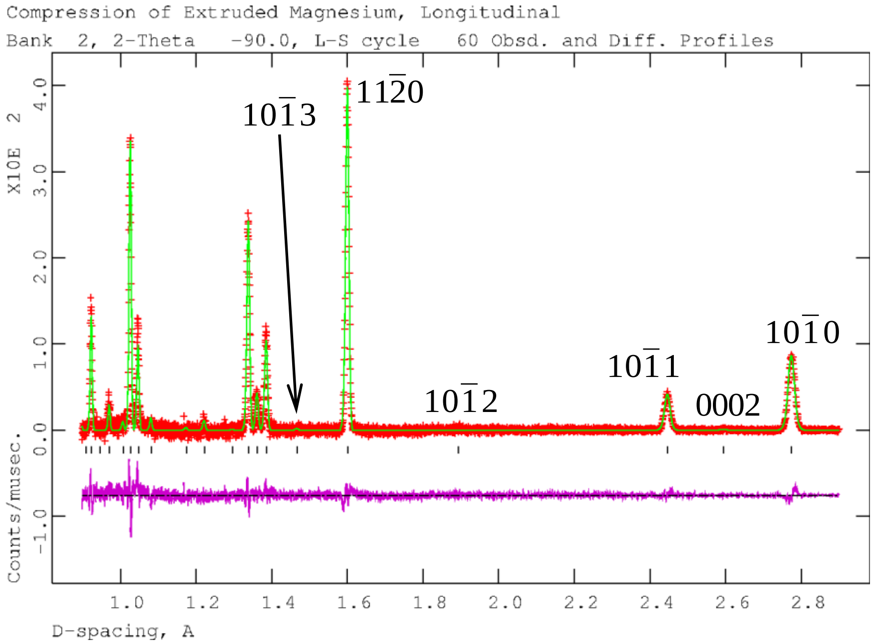


Geometry: Scattering Vectors

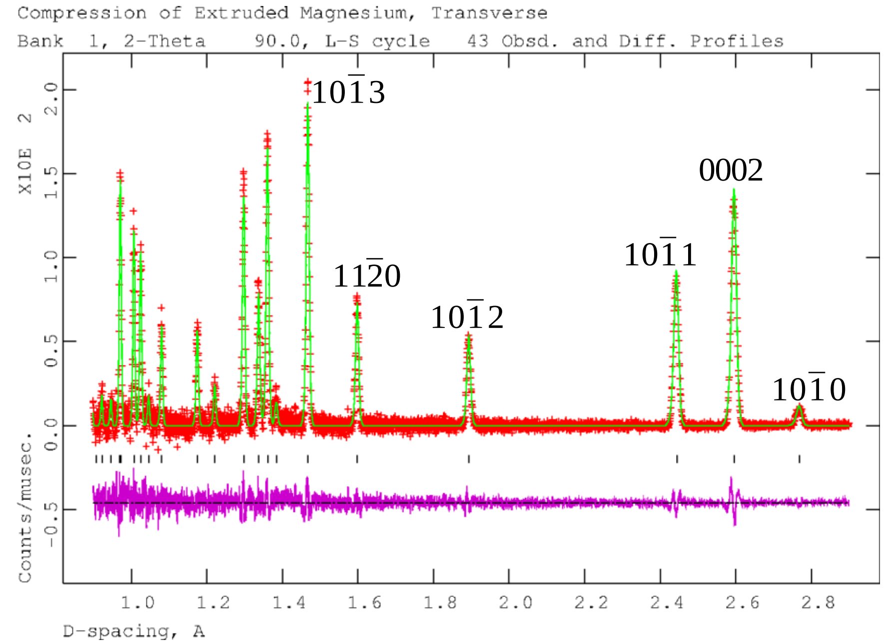




Texture



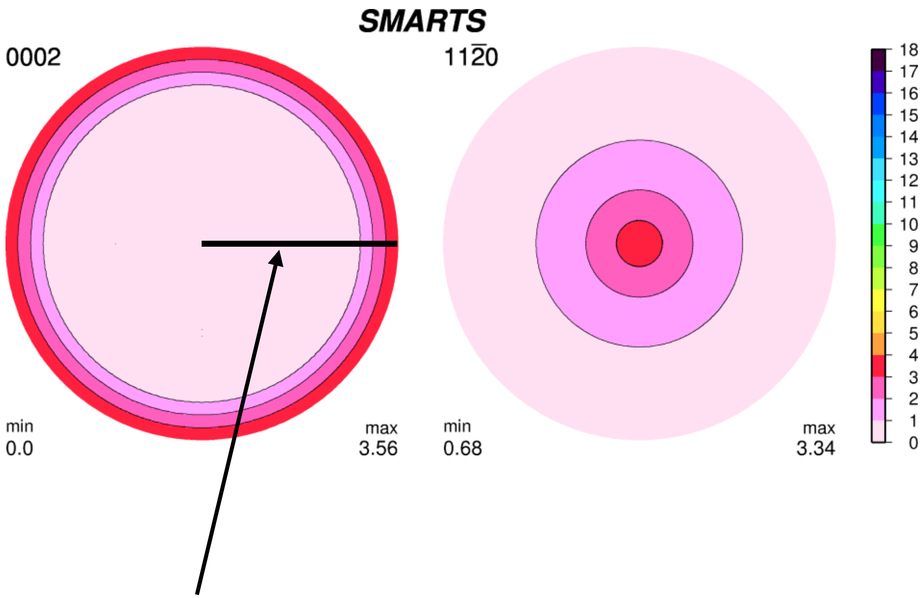
Longitudinal



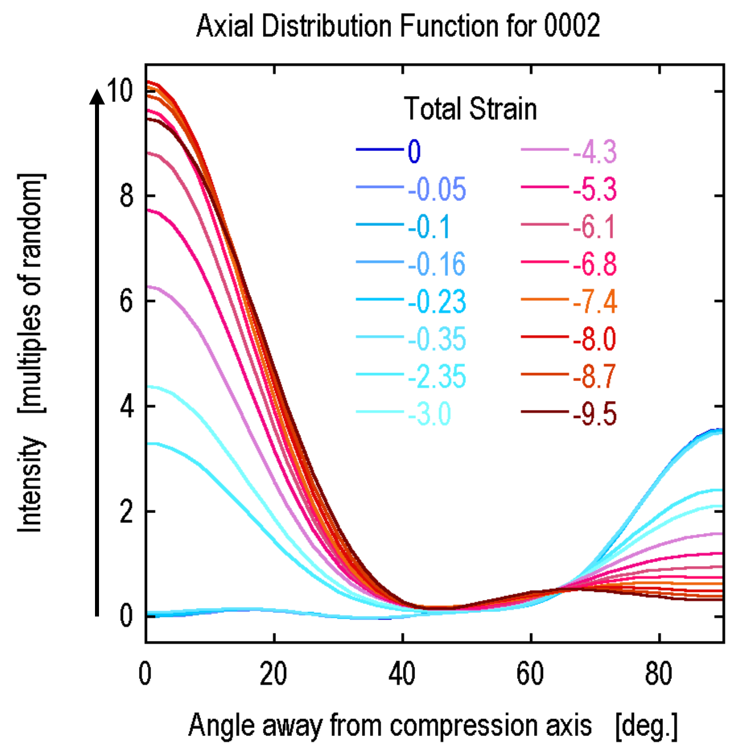
Transverse

- Strong initial texture

Texture

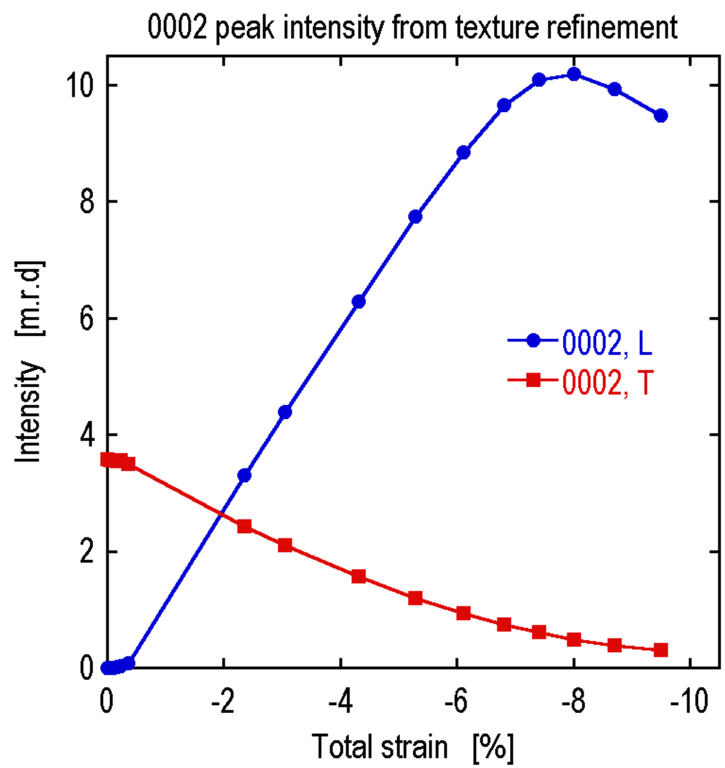


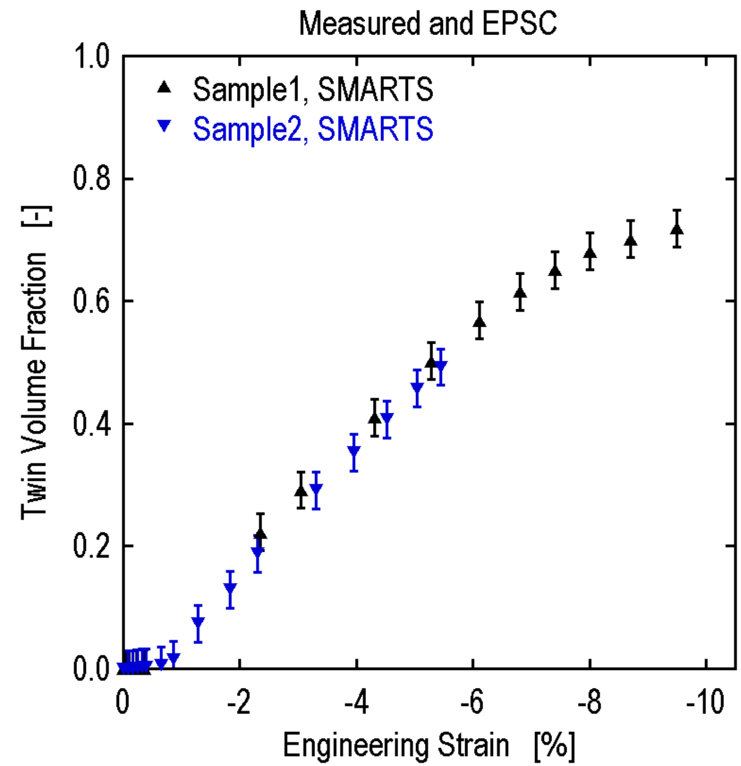
Axial distribution function



- The texture is axisymmetric
  - We can make a full texture measurement on SMARTS

Twin Volume Fraction

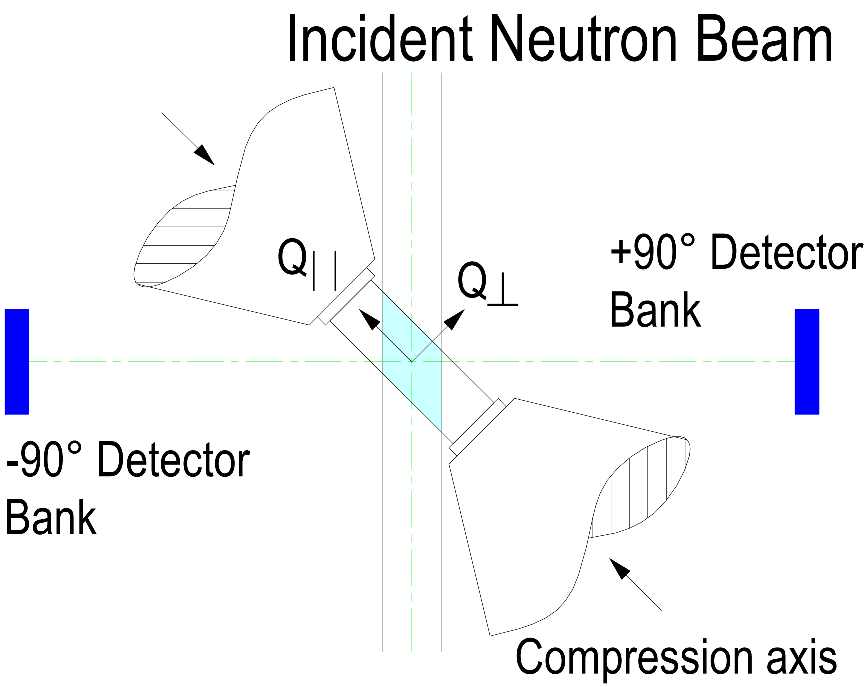


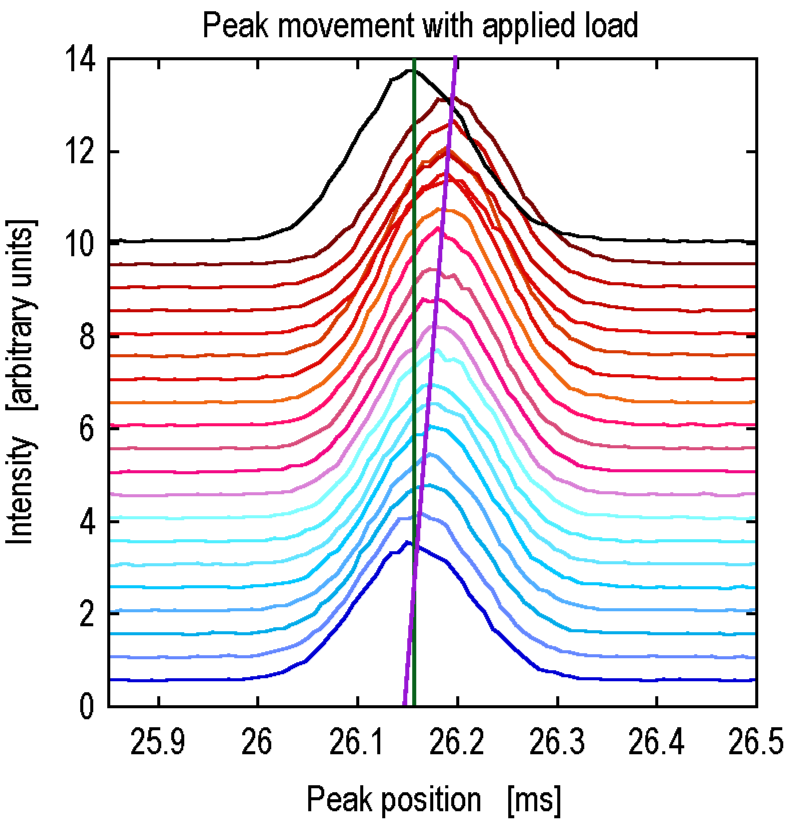


- Initially no 00.2 intensity at center of pole figure
  - Determine the twin volume fraction from the integrated area
  - η > 45: Parents, and η < 45: Twins

Lattice Strains

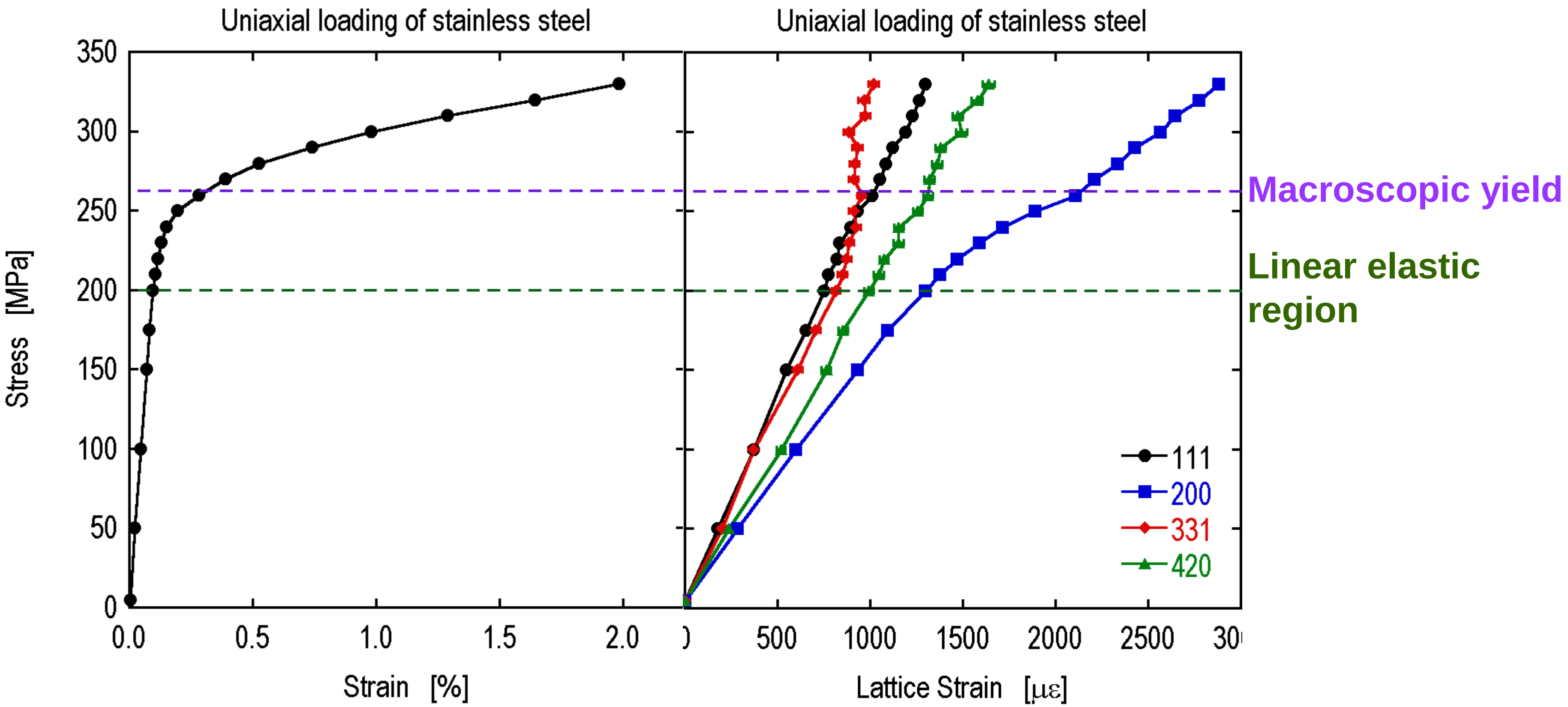
- Elastic lattice strain from position changes in diffraction peaks





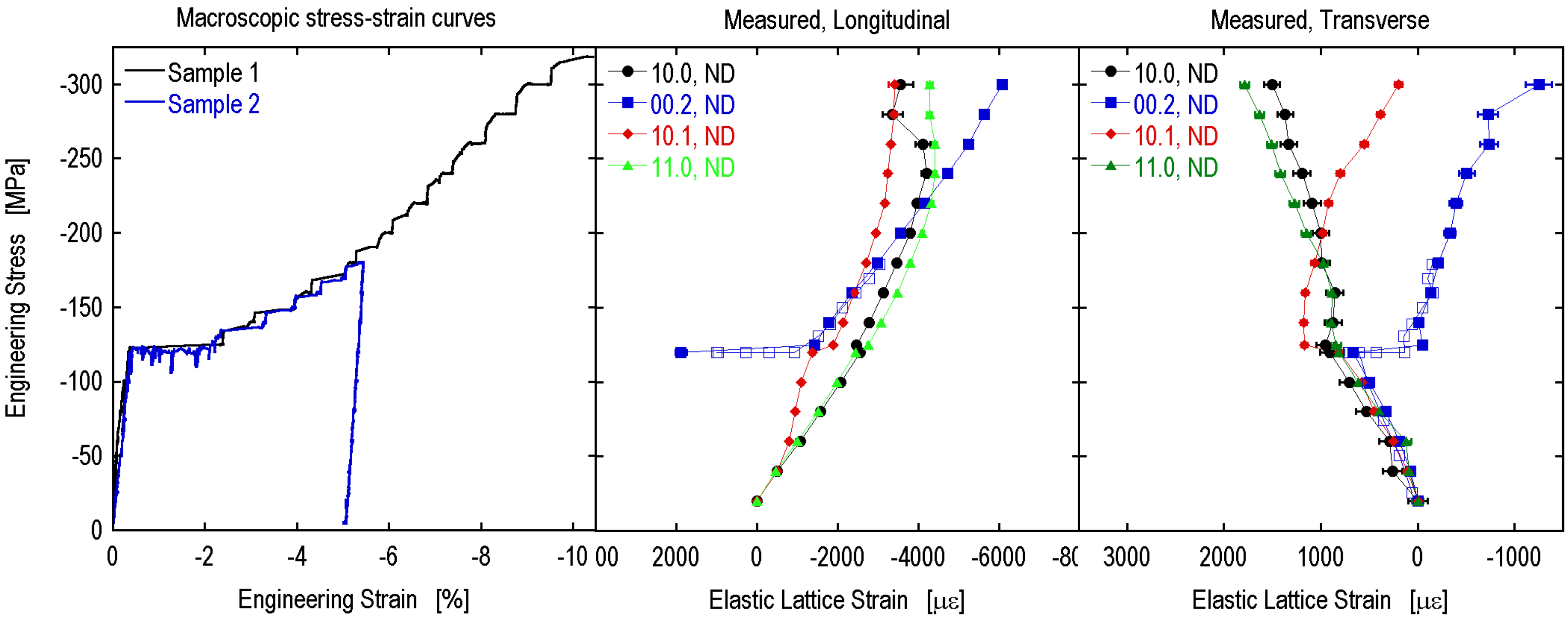
$$\varepsilon_{hkl}^{elastic} = \frac{d_{hkl} - d_{hkl}^{0}}{d_{hkl}^{0}}$$

Lattice Strains – Example: Stainless Steel



- *Elastic lattice strain* is a measure of the average ***stress*** on the grain set

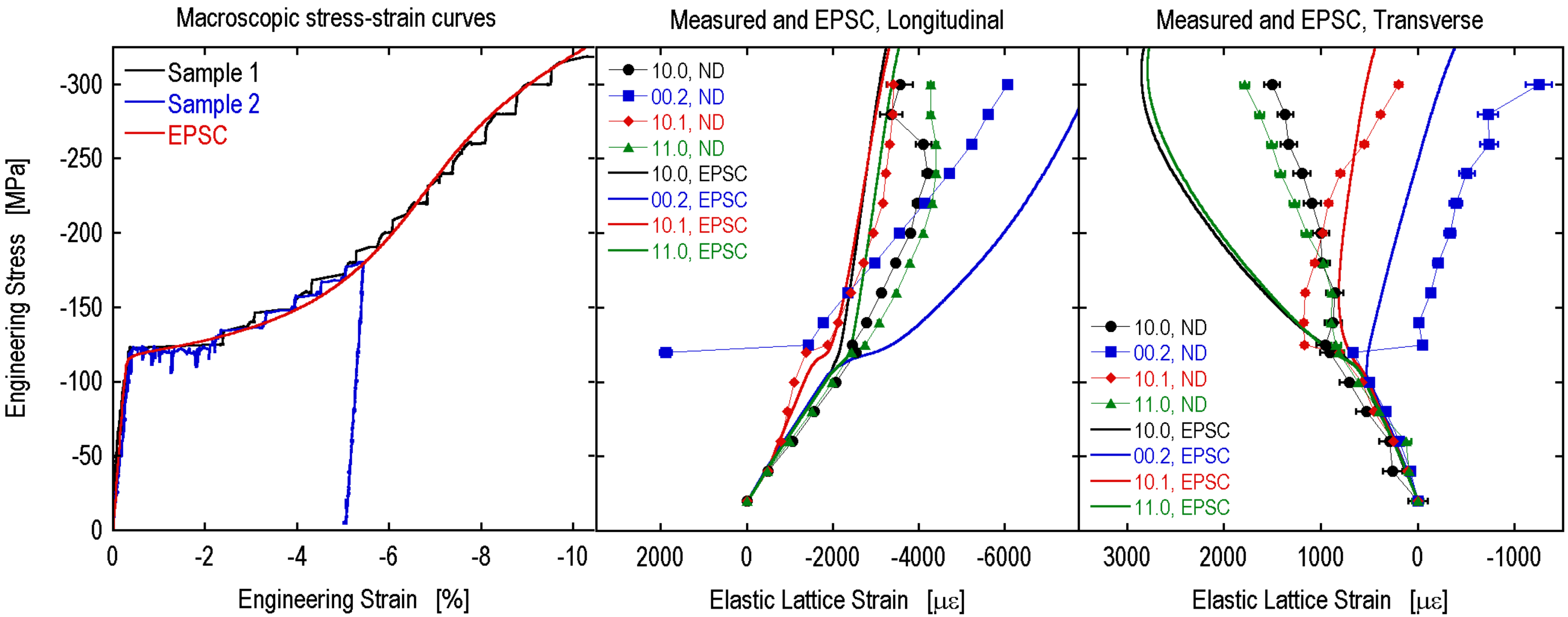
Lattice Strains: Magnesium



- Early non-linearity of the 10.1 reflection
- Large jumps at onset of twinning
- Slope reversal in the transverse direction

Model Validation

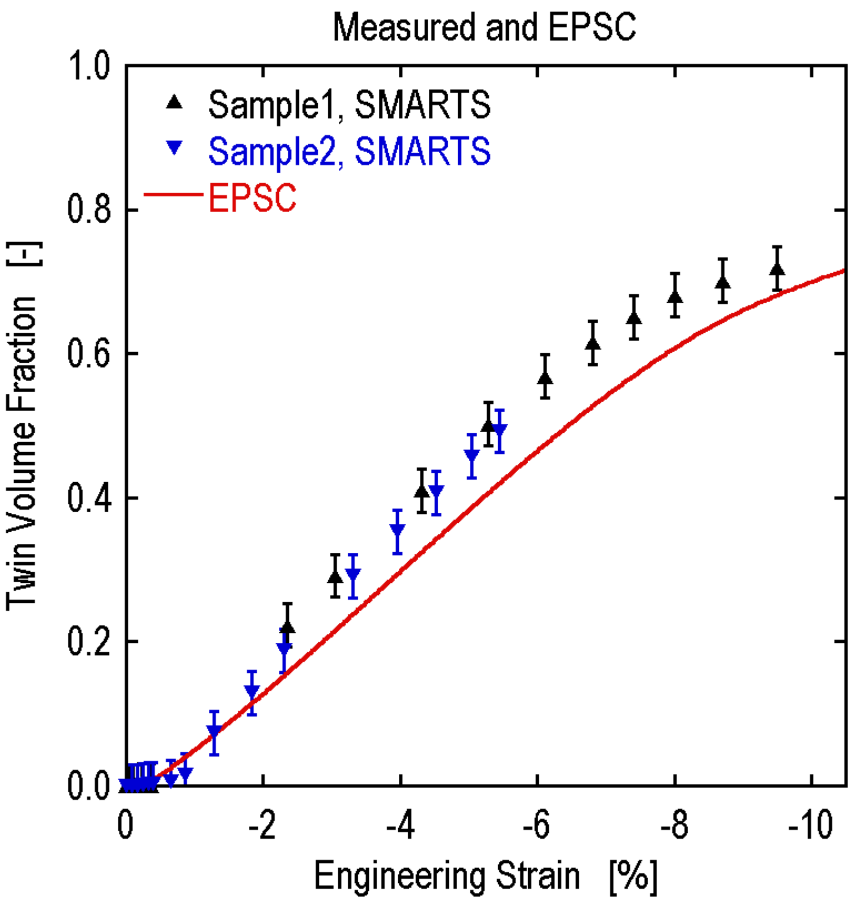
Model Validation



- Strong change in 00.2 grains – slope reversal in transverse direction
- Jump in lattice strain at onset of twinning NOT reproduced
- Prism planes transverse is not in good agreement – but “minority grains”

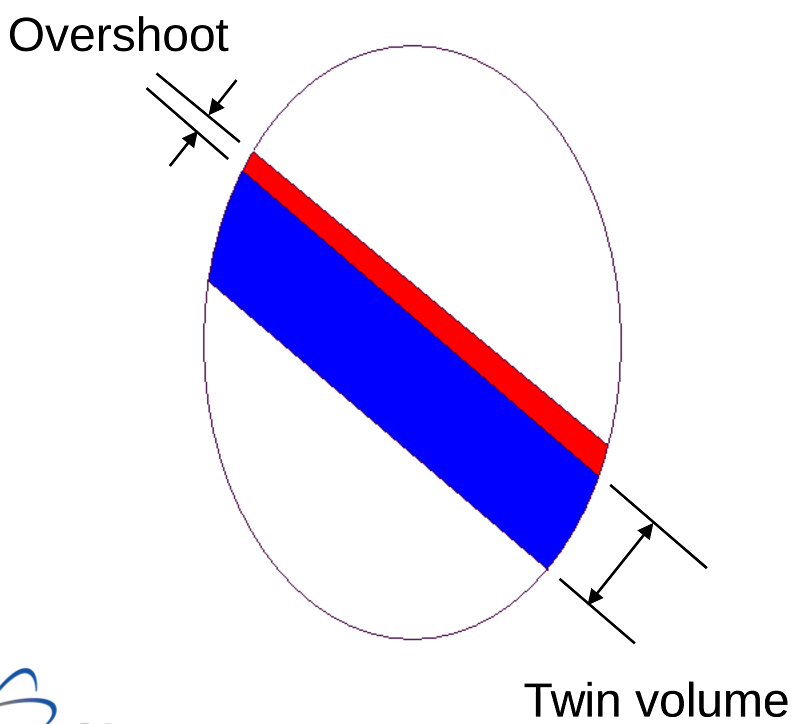
Predicted Twin Volume Fraction

- The predicted twin volume fraction is in qualitative agreement with the measured data



Stress Relaxation

- Stress relaxation due to twinning
  - What is needed to accommodate the strain?
  - What is energetically favorable?



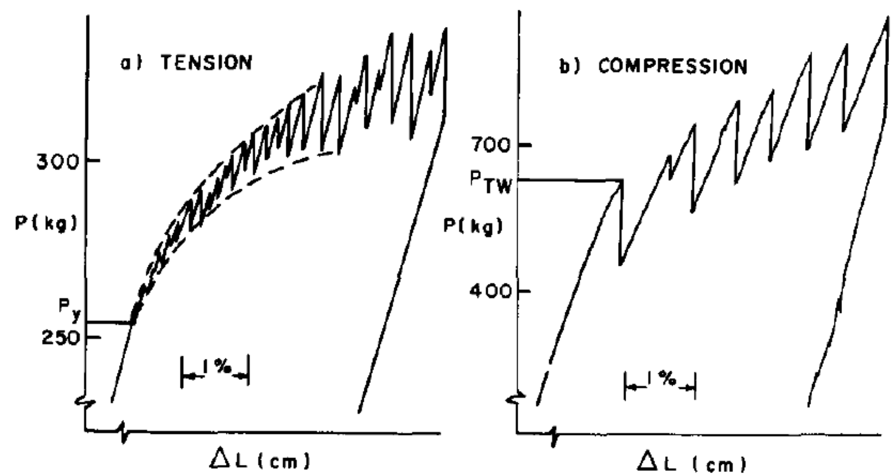


Fig. 2. Typical load - elongation curves observed for UHV-degassed Ta tested at 4.2K in (a) tension and (b) compression. P_y and P_{TW} schematically illustrate the conventions adopted for the CRSS in tension and compression, respectively.

Shields et al., Mat Sci & Eng. Vol. 20 , pp. 71-81, 1975

Twinning Overshoot

- Empirical twinning overshoot in EPSC model
  - We assume twinning overshoot by some fraction of the twin shear
    - The initial overshoot fraction is used as a fitting parameter

$$f = f_0 \frac{w^{Parent}}{w^{Parent} + w^{Child}}$$

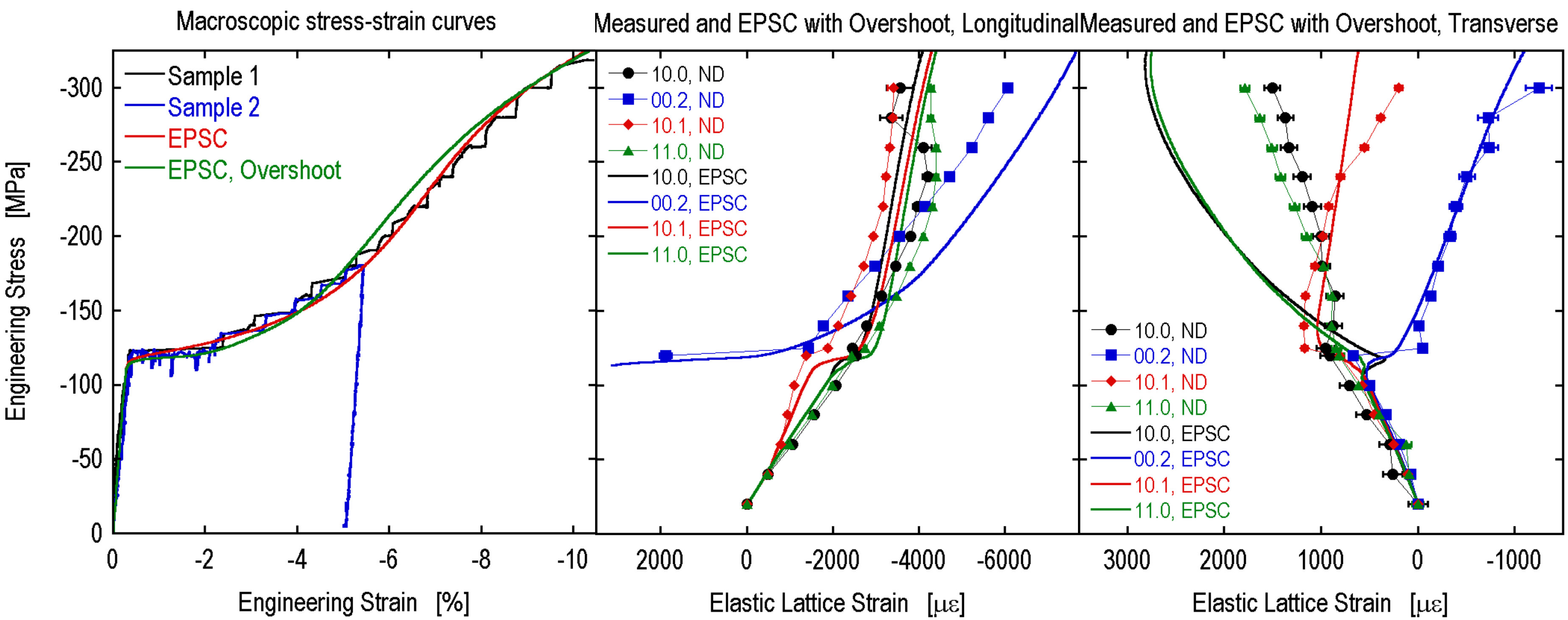
  - The back-stress due to the twinning overshoot is calculated using the twin shear and the elastic stiffness tensor

$$\sigma^{Back-stress} = -f\, L^E \dot{\varepsilon}^{Twin}$$

  - The back-stress is added in each step weighted by the ratio of the Child grain weight fraction and Child weight fraction *increment*

$$\sigma^{Child} = \frac{\sigma^{Child} w^{Child} + \sigma^{Back-Stress} \Delta w^{Child}}{w^{Child} + \Delta w^{Child}}$$

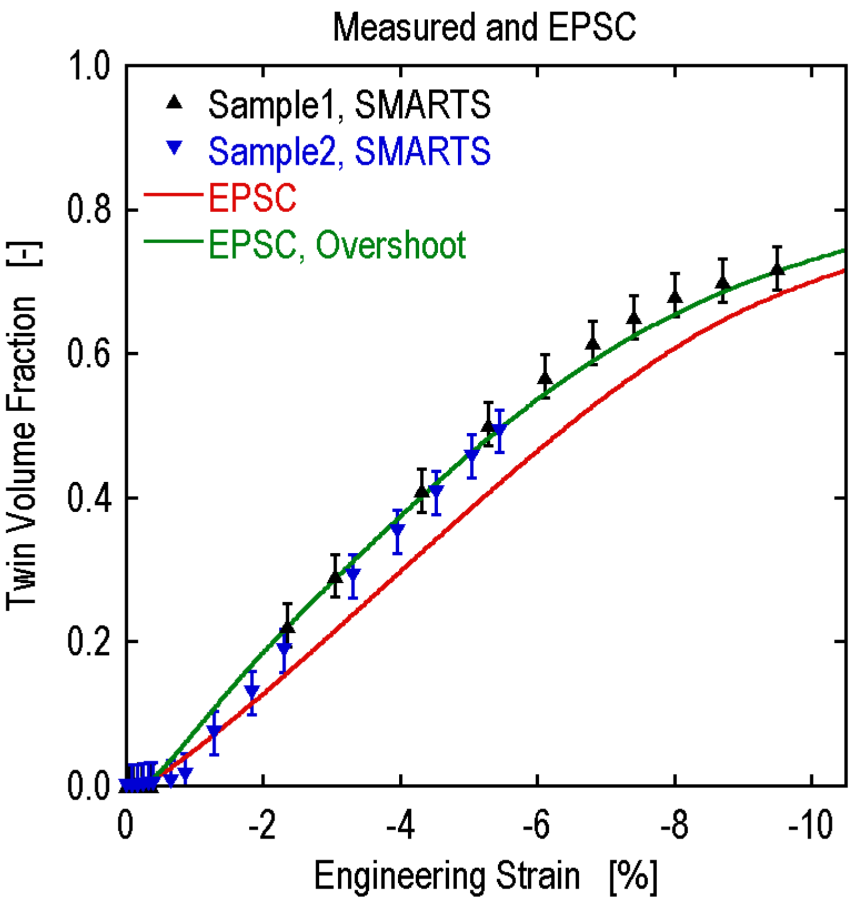
Model Validation



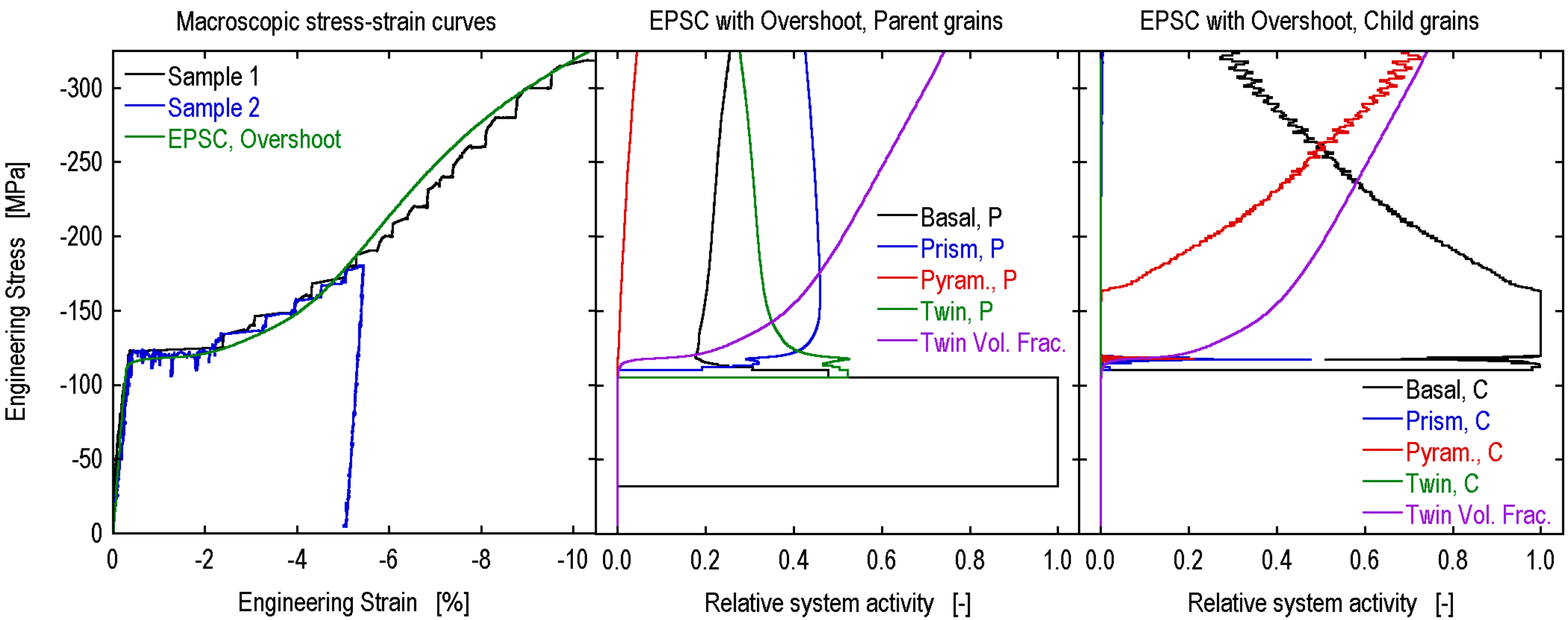
- Jump in lattice strain at onset of twinning is reproduced
- Prism planes transverse are still off

Predicted Twin Volume Fraction

- The predicted twin volume fraction is in **quantitative** agreement with the measured data



Predicted System Activity



- Initial increase in twinning in the Parent grains
- Slight change in system activity in the Child grains due to the updated stress state

Conclusions

Conclusions

- Developed and implemented new version of EPSC
  - Grain reorientation due to twinning
    - Texture development
- Neutron diffraction measurements
  - Internal strains and texture development during compressive loading of extruded magnesium
  - Large jumps in lattice strains at the onset of twinning
  - Strong texture development within 10% strain

Conclusions

- Experimental model validation using diffraction
  - Qualitative agreement in lattice strain and twin volume fraction (texture development)
  - Large jumps in lattice strain at onset of twinning not predicted
- Experimental data gives directions for model improvement
  - Empirical twinning overshoot included
  - Improved agreement with experimental data
    - Macroscopic stress-strain curve
    - Lattice strains: Large jumps are reproduced
    - Quantitative agreement with measured twin volume fraction (texture)

Ongoing Work

- Experimental
  - 3D X-ray Microscope
    - Strain measurements
    - Morphology measurements
  - Load path change measurements (ND)
    - Cyclic tension-compression
    - Cyclic compression-tension
    - Cross-compression
- Modeling
  - Minimum energy determination of twin overshoot fraction
  - Eshelby type calculation of stresses and strains within Parent and Child grains due to overshoot