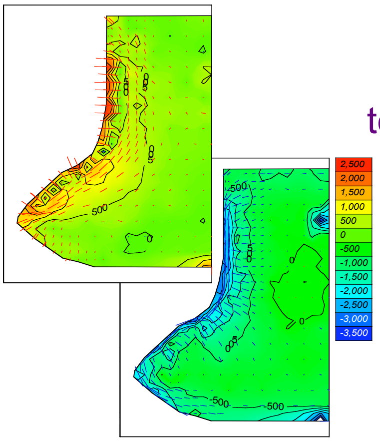

Engineering

Advanced diffraction techniques for Residual Stress determination

Michael Preuss
University of Manchester

Introduction

- Residual stresses in materials
- Principles of measuring residual stresses by diffraction
- Neutron and Synchrotron X-ray diffraction
  - Properties
  - Facilities
- Case Studies / Questions
- From Engineering to Physical Metallurgy – Understanding plasticity
- Conclusions

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What are residual stresses

Deformation mismatch

Example: Welding

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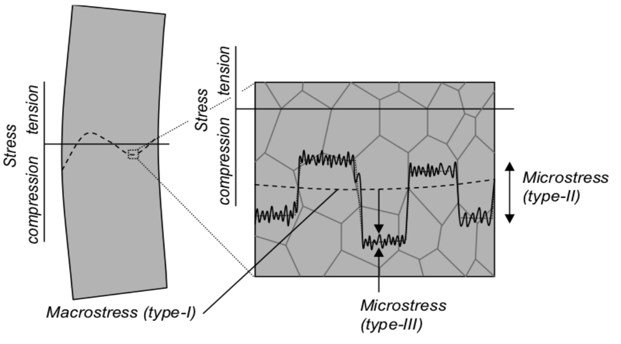
Residual Stresses

- Internal stresses
- Caused by misfit
  - Type I
  - Type II
  - Type III

Bent bar:



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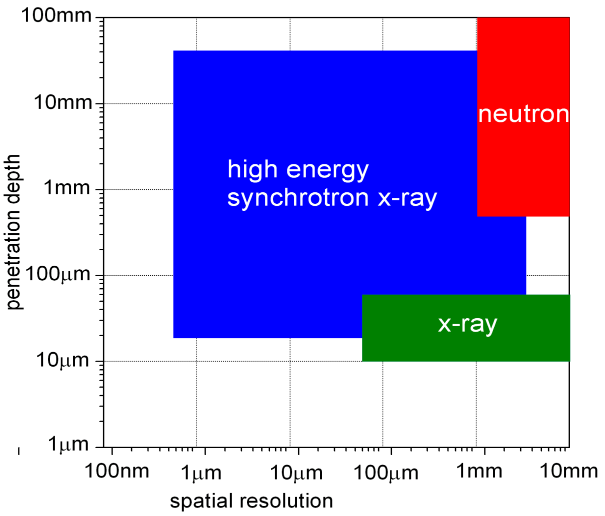
General Overview: Diffraction methods available



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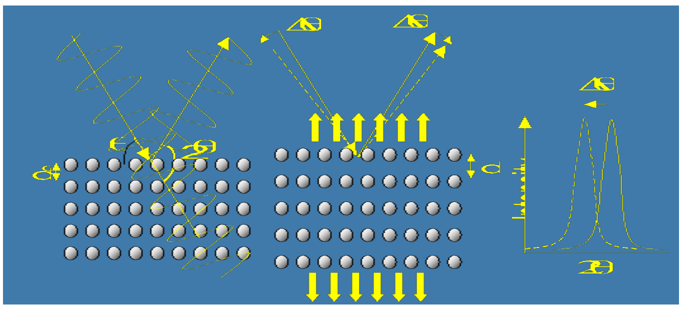
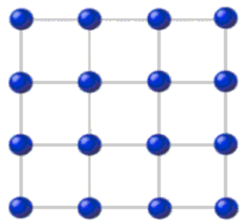
General Overview: Basic Principles: diffraction



$$\lambda = 2d\sin\theta$$

- Diffraction measures elastic lattice strain as peak shifts
- Uses the poly-crystalline lattice planes as internal strain gauges

Basic Principle



Bragg scattering angle

wavelength: $\lambda = \frac{hc}{E} = \frac{12.39}{[keV]}$

Bragg's law: $\lambda = 2d\sin\theta$

$$\frac{12.39}{[keV]} = 2d\sin\theta$$

Scattering Angle

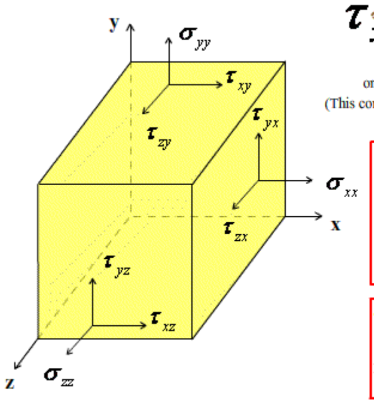
$$\theta = \arcsin\left(\frac{12.39}{2d[keV]}\right)$$

General Overview: Basic Principles

- Measured strains have to be converted into stresses! (Hooke’s law)

$$\varepsilon = \frac{a - a_0}{a_0} = \frac{d - d_0}{d_0}$$

The 9 components of a stress tensor:



The stress acts in the x-direction

τ_{xy}

on the plane with a normal in the y direction
(This convention maybe vice versa in some books.)

$$\sigma_{ij} = \begin{pmatrix} \sigma_{xx} & \tau_{xy} & \tau_{xz} \\ \tau_{yx} & \sigma_{yy} & \tau_{yz} \\ \tau_{zx} & \tau_{zy} & \sigma_{zz} \end{pmatrix}$$

Tensor Equation: $\sigma_{ij} = C_{ijkl}\varepsilon_{kl}$

Matrix Equation: $\sigma_p = C_{pq}\varepsilon_q$

General Overview: Basic Principles

- Measured strains have to be converted into stresses! (Hooke’s law)

$$\varepsilon = \frac{a - a_0}{a_0} = \frac{d - d_0}{d_0}$$

e.g. isotropic triaxial along principal directions:

$$\varepsilon_{11} = \frac{1}{E}\left[\sigma_{11} - \upsilon(\sigma_{22} + \sigma_{33})\right]$$

$$\varepsilon_{22} = \frac{1}{E}\left[\sigma_{22} - \upsilon(\sigma_{33} + \sigma_{11})\right]$$

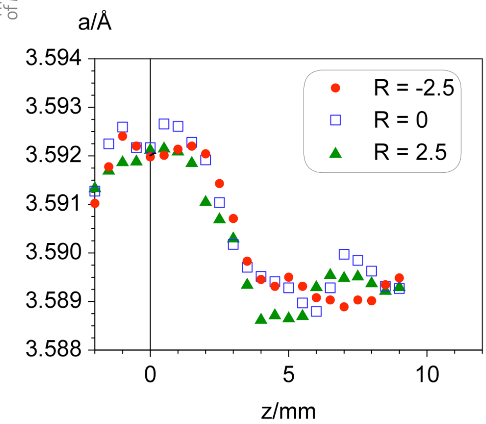
$$\varepsilon_{33} = \frac{1}{E}\left[\sigma_{33} - \upsilon(\sigma_{11} + \sigma_{22})\right]$$

To calculate a stress direction:

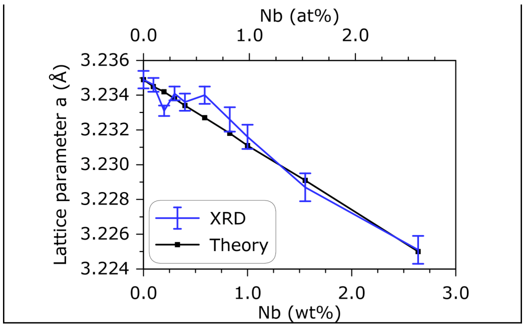
$$\sigma_{11} = \frac{E}{(1+\nu)(1-2\nu)}[(1-\nu)\varepsilon_{11} + \nu(\varepsilon_{22} + \varepsilon_{33})]$$

(Attention: not always this simple!)

d_0 variation



Example of d_0 variation across a tubular Nickel weld



The Vegard Law
Example: Nb in Zr

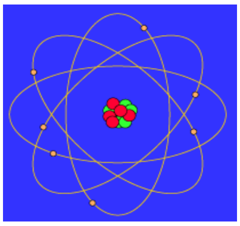
Why do we like neutrons ?

- Part of the nucleus
- Same mass as protons
- Interesting wavelength/mass relationship:

$$\lambda = \frac{h}{p} = \frac{h}{mv}$$

Planck

Mass * Velocity



- “Thermal” neutrons: wavelength similar to those of X-rays 0.5-5Å similar to atomic spacing in solids
- Allows cubic gauge volumes!
- Relatively divergent beam !!

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Neutron and Synchrotron Sources

Neutron:

- Reactor Sources (Fission)
  - Constant wavelength/Single Peak
- Accelerator Sources (Spallation)
  - Time-of-flight / Full Spectra / Rietveld

Synchrotron:

- Monochromatic λ and white beam

ESRF Grenoble, France ILL

ISIS Chilton, UK Diamond

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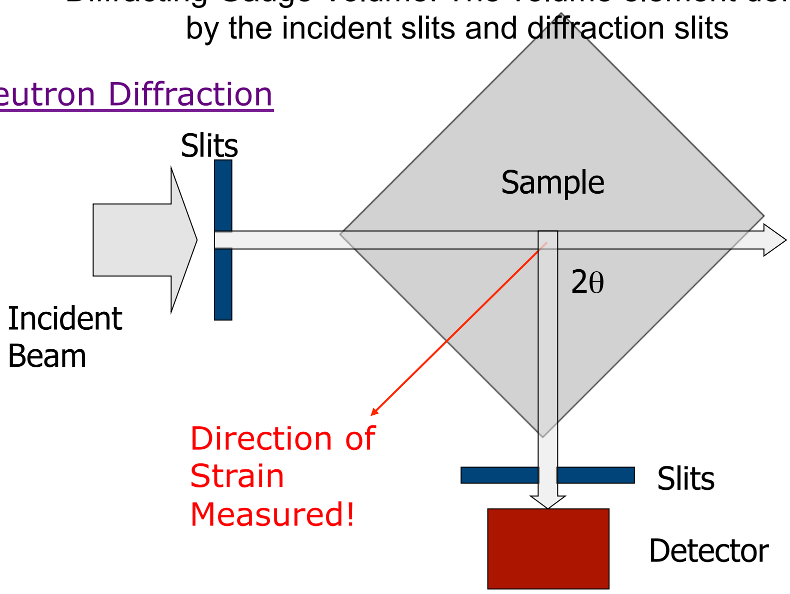
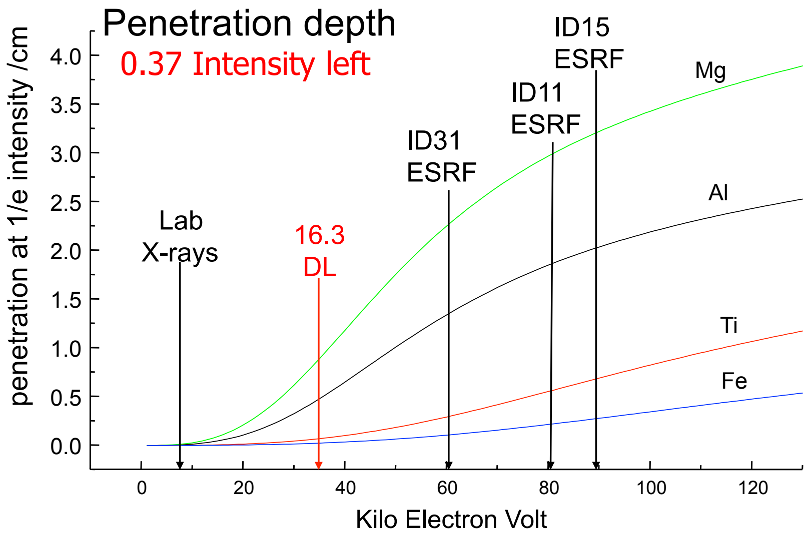
General Overview: Strain Scanning

Diffracting Gauge Volume: The volume element defined by the incident slits and diffraction slits

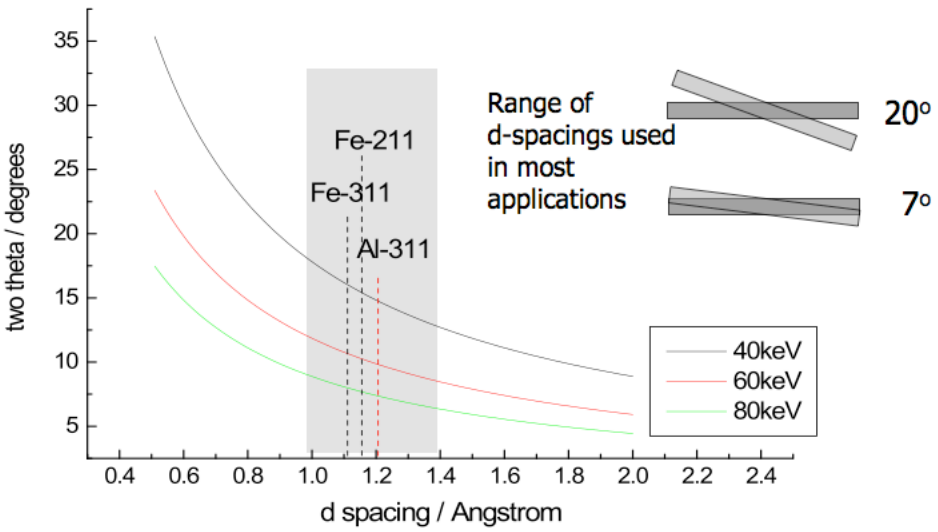
Neutron Diffraction



Synchrotron Diffraction: Penetration depth (monochromatic beam)



Synchrotrons: Scattering Angle 2θ



General Overview: Diffracting Gauge Volume

Volume element of the material in which the recorded scattering takes place

- Results in averaged d-spacing (powder diffraction - many grains)
- Defines the minimum spatial resolution of the method (around 1mm^3 minimum gauge volume when using neutron diffraction)
- and type of residual stress resolved (macro-stress or type-I usually. Type-II for two phase materials).
- Use the largest possible gauge volume for your specific issue in order to minimise counting time

Near surface measurements

Neither peak shift (strain) nor measurement location is correct near a surface!

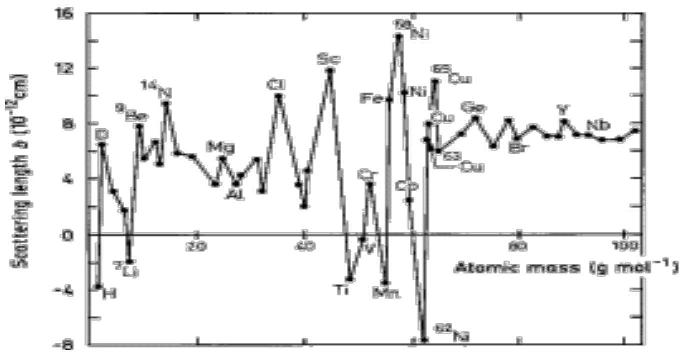
- Partial filling of sampling gauge gives a peak shift - need to correct peak shift
- Translator records centre of gauge which is rarely the centre of gravity of diffracting region
- need to correct gauge position

Neutron Properties

- Neutrons are scattered by atomic nuclei (electrons and X-rays which are scattered by the electron cloud).
- Since the scattering is nuclear process, scattering amplitude varies greatly for different isotopes of same element and in a unpredictable manner from element to element. X-ray and electron scattering increase monotonically with atomic number

Neutron Properties

- Random Scattering length
- Penetration depth independent of energy/wavelength
- Electrically neutral
- Great penetration
- Low flux/intensity



Economic Depth	Al	Steel	Cu	Ti	Ni	SiC
mm	250	37	40	27	24	200

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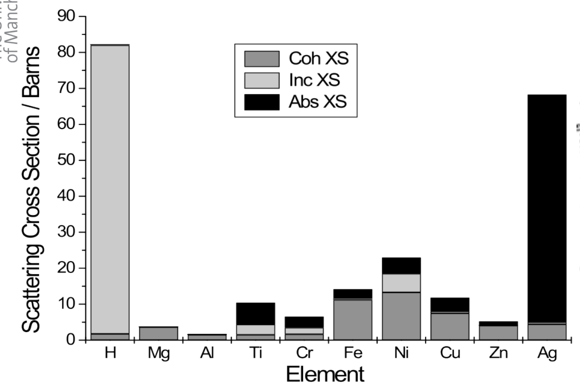
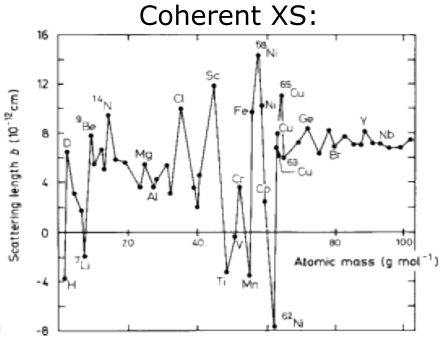
Neutron Scattering



Coherent XS:



$$I_{trans}(t,\lambda) = I_{inc}(\lambda)\, e^{-\Sigma^* t}$$

Coherent XS~ Signal
Incoherent XS~ Background
Absorption XS~1/Intensity

Penetration depth~
1/Sum of Scatt XS

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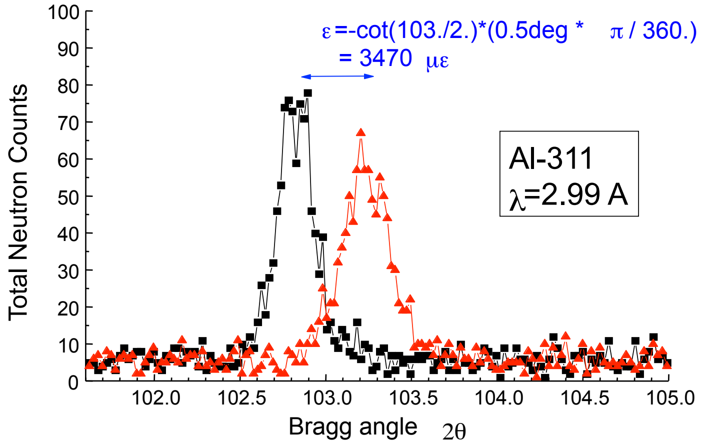
Research Reactors

- Fission in Reactor Core
    - Moderated neutrons
    - Monochromators in guide
- “Constant Wavelength”
- Many Facilities in Europe:
    - ILL, SINQ, FRM-2 (G), Petten (NL), …
    - Generally low flux except ILL and FRM-2

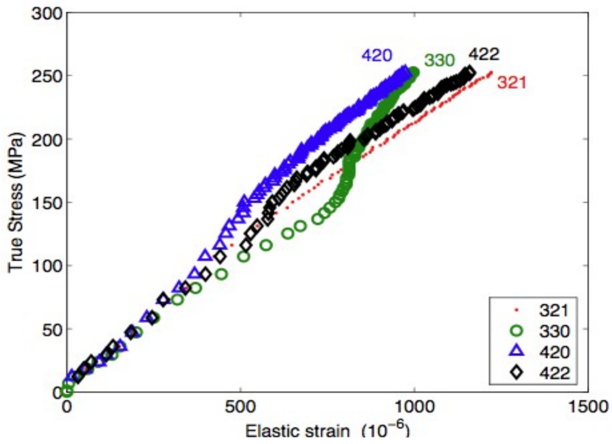
Single Wavelength at Reactor

Single-wavelength instrument: D1A at the ILL
New instrument at ILL: SALSA



Which peak gives us the pure macrostress response ?

In-situ Loading on a neutron diffraction beam line



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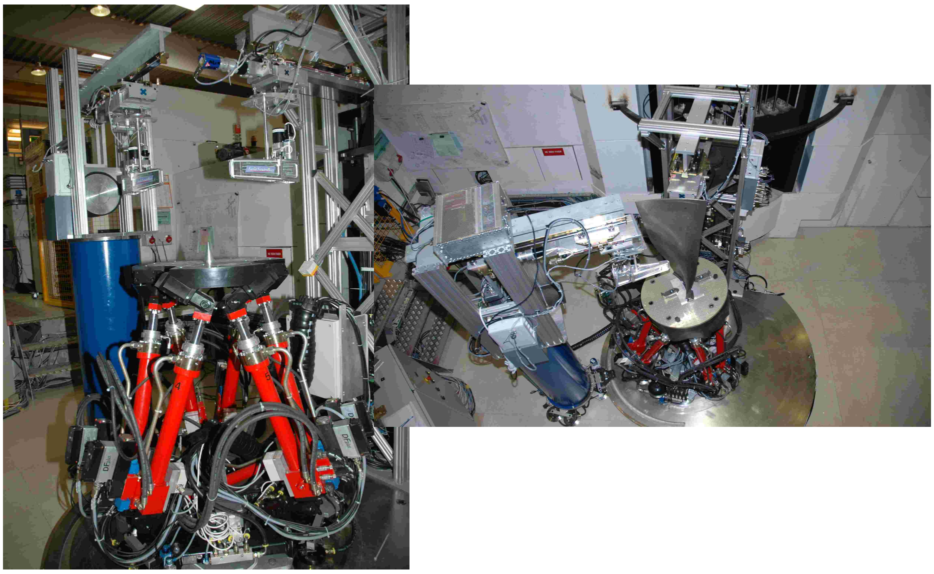
SALSA, ILL



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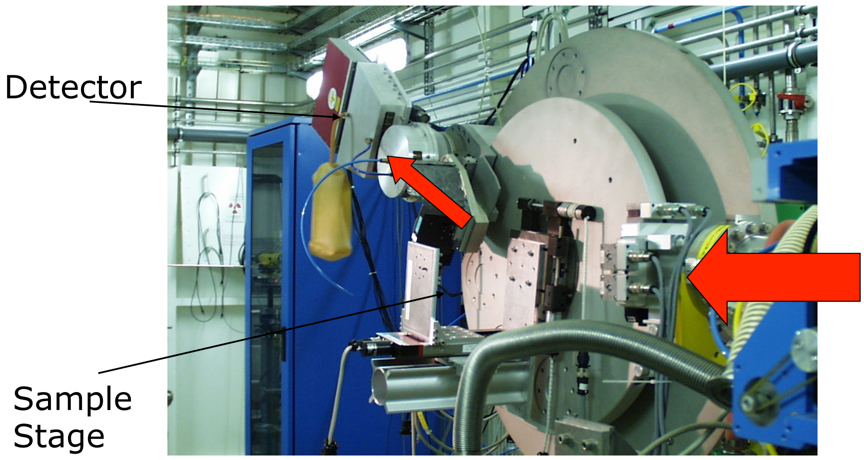
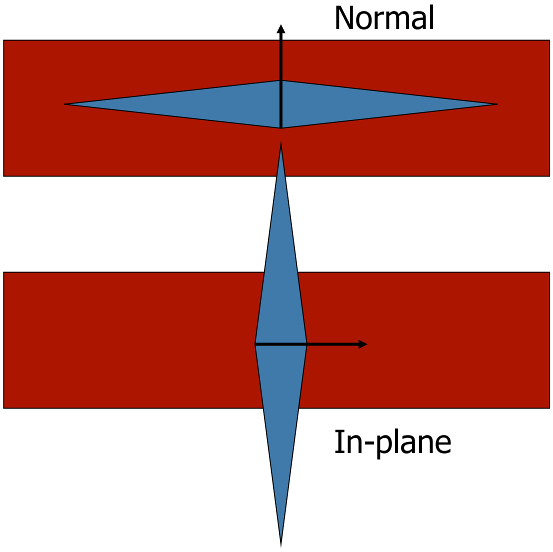
Typical Diffractometer at Synchrotron (here ID31 at the ESRF)



Diamond gauge volume



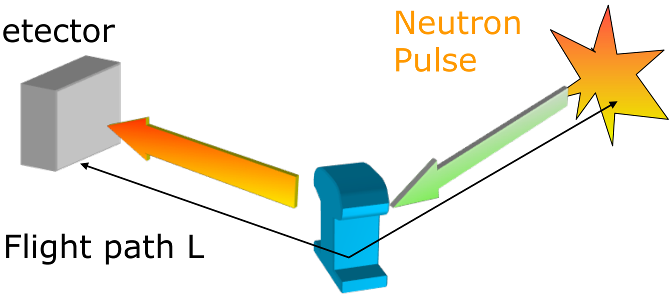
Two orthogonal strain components sample different material volume

Analyser crystal for partly filled Gauge volume necessary!

Time of flight method

- Sharp pulse leaves source
- High energy neutrons (short λ) travel faster and arrive first, low energy (long λ) last $\lambda = ht/ml$ where l is the path length and t time of flight
- a single stationary detector records whole diffraction spectrum as a function of time of flight
- neutrons travel at ~100m/s (speed of sound)
  $\lambda = 2d \sin\theta$ with θ fixed, i.e. λ proportional to d

Spallation Sources: Time of Flight



$$\lambda = \frac{h}{p} = \frac{h}{mv} = \frac{ht}{mL}$$

$+$

$$\lambda = 2d\sin\theta$$

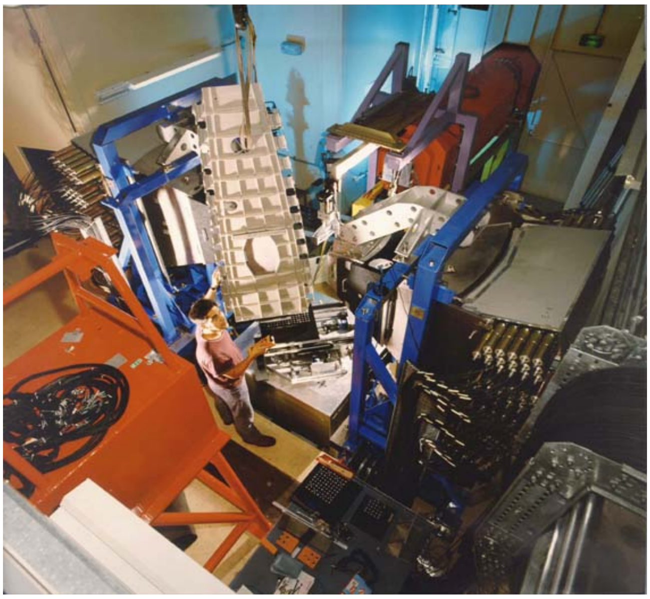
$=$

Time-of-Flight:

$$d = \frac{h}{2mL\sin\theta}\,t$$

Fast neutrons arrive earlier at detector!

ENGIN-X, ISIS

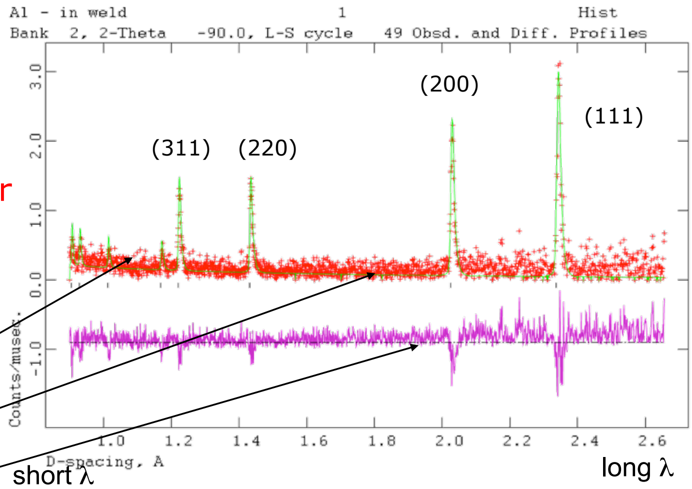


Example of TOF: Rietveld Refinement

TOF: More Information!

Rietveld: Fewer Parameters!

$$d_{hkl} = \frac{a_0}{\sqrt{h^2 + k^2 + l^2}}$$



Data

Fitting

Difference

short λ

short times

long λ

long times

Spallation Sources: Measurement of Strain

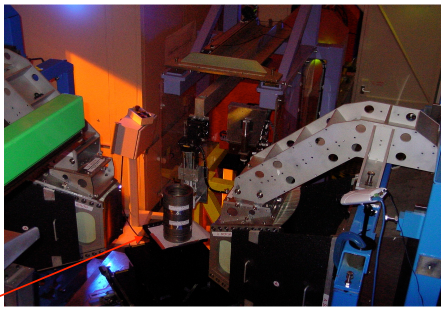
Strain: $\varepsilon = \dfrac{a - a_0}{a_0} = \dfrac{\lambda - \lambda_0}{\lambda_0} = \dfrac{t - t_0}{t_0}$

Cubic gauge volume !

Time-of-Flight:

$$\lambda = \frac{h}{2mL\sin\theta}\, t$$

Fixed



ENGIN-X at ISIS

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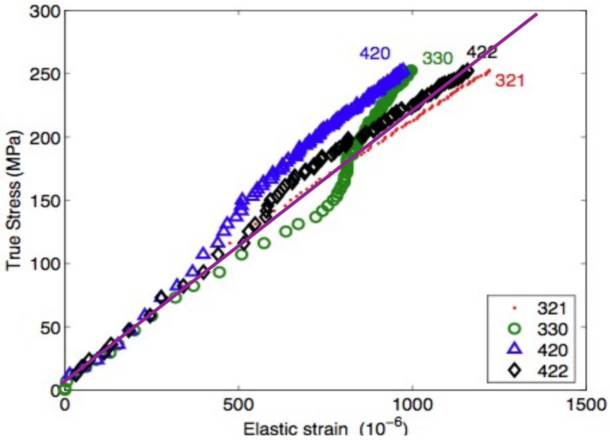
Rietveld vs Single reflection

In-situ Loading on a neutron diffraction beam line



Rietveld analysis generally provides linear stress-strain response with elastic constant equal Young's Modulus

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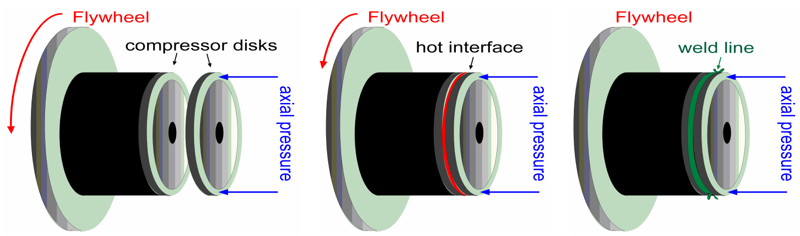
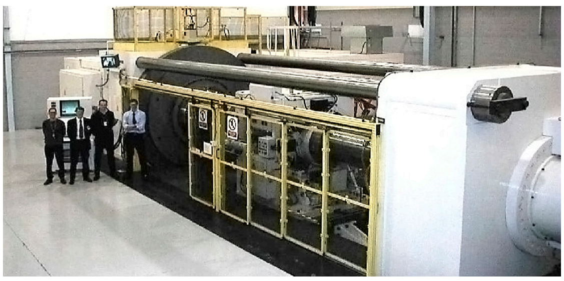
Case Study: Inertia Friction Welding





Solid state joining of compressor, turbine discs and shafts

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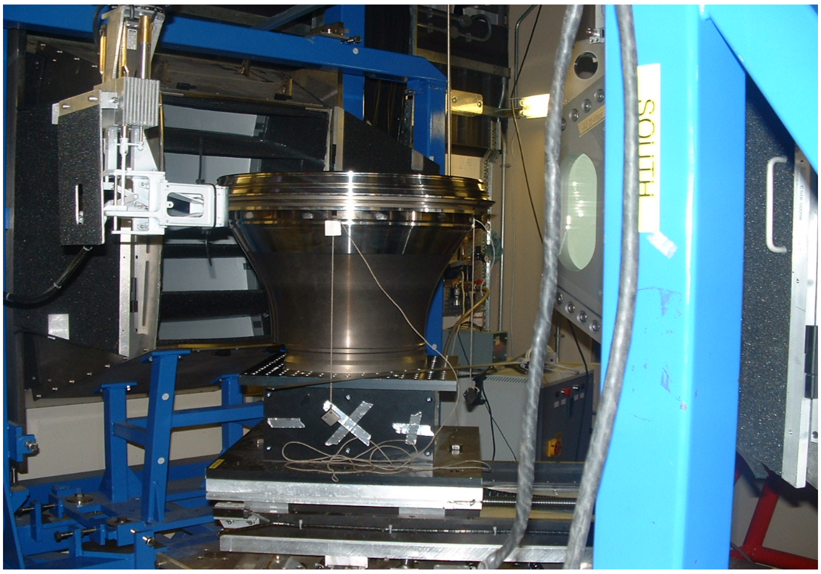
Case Study: Inertia Friction Welding



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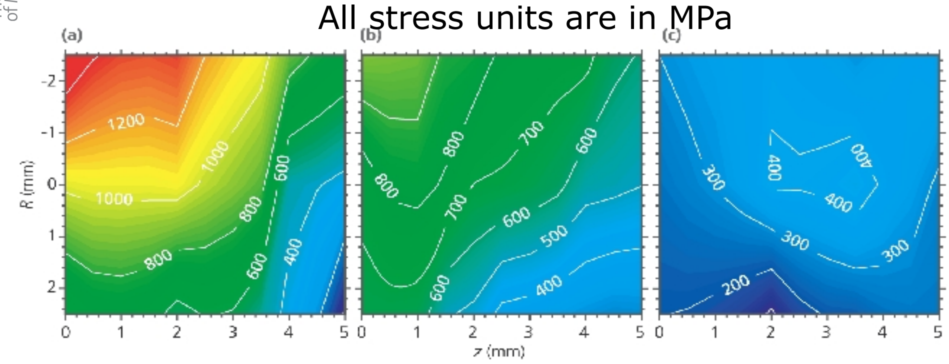
How would you measure such a sample ?

143mm diameter test inertia friction welds

Hoop stresses in IFW'd nickel-base superalloy

All stress units are in MPa



As-welded

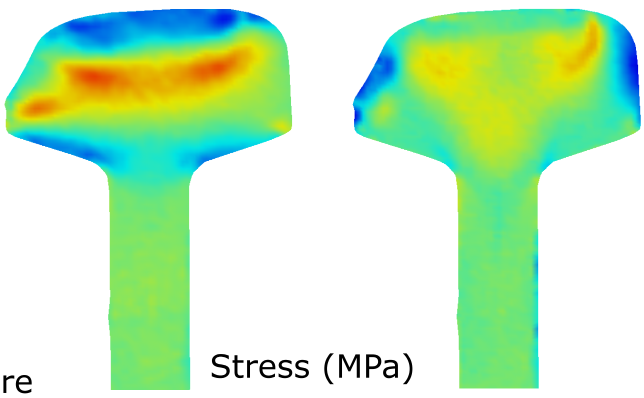
Conventional PWHT

Modified PWHT

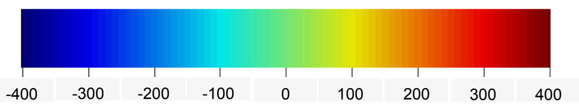
Residual stress measurements were used to develop a new PWHT

Railway Rails

- Slices were cut from the rail to measure the horizontal and vertical stresses. Longitudinal stresses were lost
- Measurements were carried out by using neutron and synchrotron x-ray diffraction



Stress (MPa)



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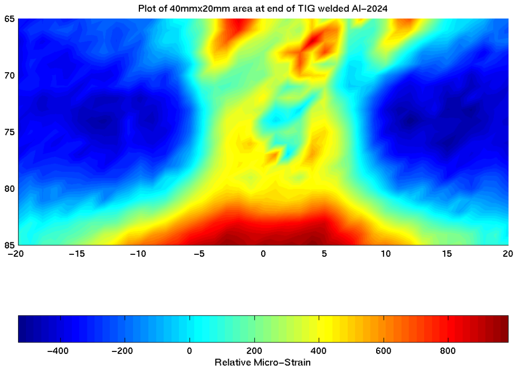
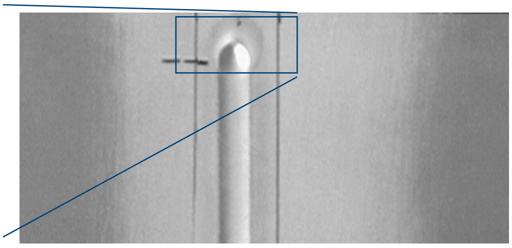
Case Study: Strain Mapping of a TIG weld

2D Map of Residual Strain about the End of a TIG Weld at 100μm Resolution

This map include 20,00 measurements and took 8 hours to acquire





8mm wide Tig Weld in Aluminium Plate

Oxford School on Neutron Scattering 39

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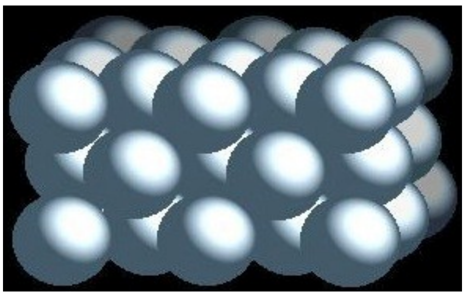
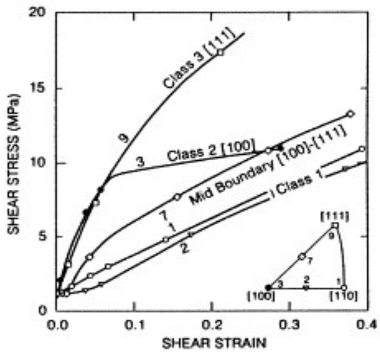
From Engineering to Physical/Mechanical Metallurgy

Single Crystal Anisotropy





Al, fcc

Single Crystal deformation

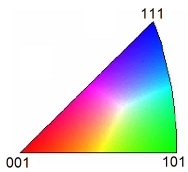
Oxford School on Neutron Scattering 40

What do we know ?

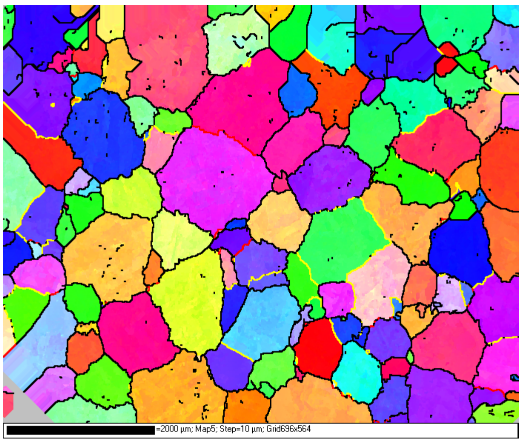
- Deformation of metallic materials happens along most densely packed plane in most densely packed direction
  - For example: in fcc it is the (111) plane and the <110> direction
- Relatively good understanding what happen when a single crystal is deformed

What we struggle with

- How does deformation work in a polycrystalline aggregate



β phase IPF colour key



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Deformation heterogeneity

- Polycrystalline deformation is heterogeneous
- Single crystal elastic and plastic anisotropy
- Grain incompatibility during deformation results in intergranular stresses

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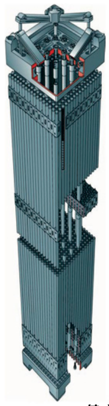
Why do we care ?

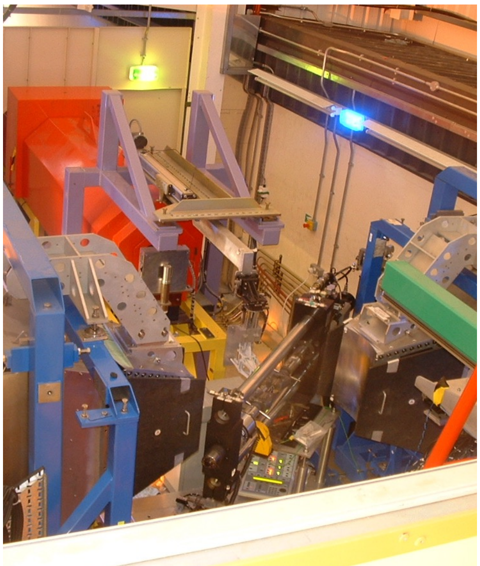
- Deformation mechanisms play a crucial role when material is processed as it affects the microstructure and hence performance of the material that is generated
  - exactly the same alloy can have a strength of 300 or 1000 MPa just by changing the microstructure

Why do we care ?

- Understanding deformation mechanisms is crucial in order to develop a more physical understanding of how materials perform
- Such knowledge is required to predict accurately the life of engineering components
- Particularly important for safety critical components

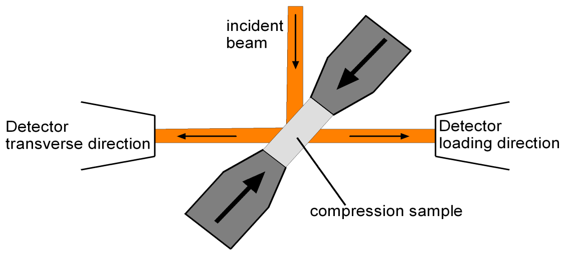


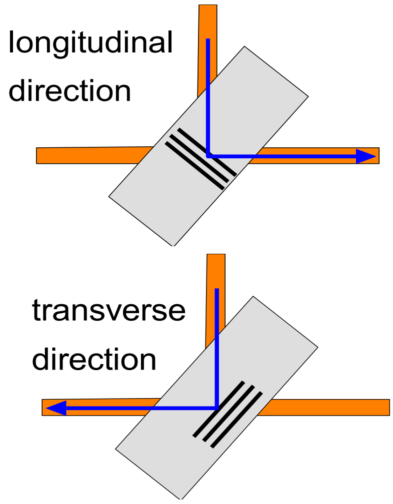
In-situ loading experiments



Experimental Methodologies

- Use of neutron diffraction and high energy synchrotron x-ray diffraction characterising residual stresses, intergranular strains and phase transformation

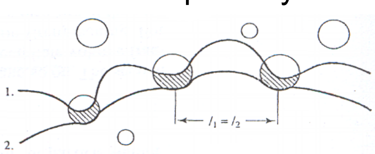


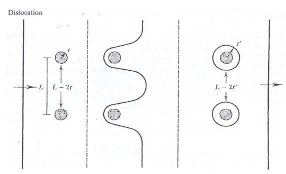


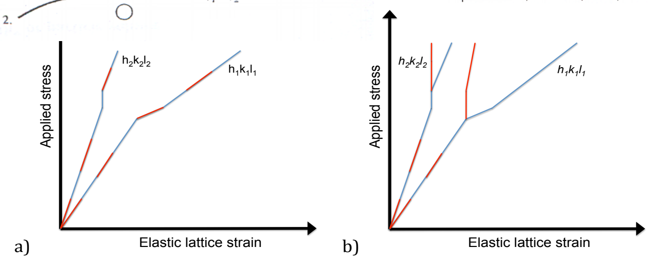
Case Study – Ni base Superalloy

- Use of neutron diffraction and high energy synchrotron x-ray diffraction characterising residual stresses, intergranular strains and phase transformation

Example – Ni base Superalloy



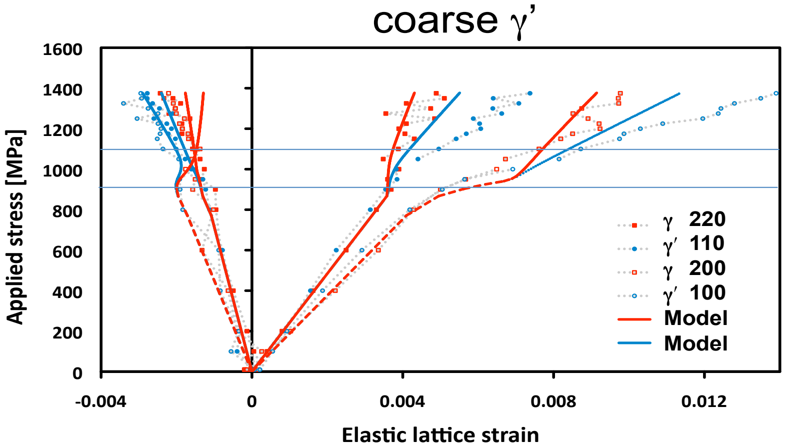




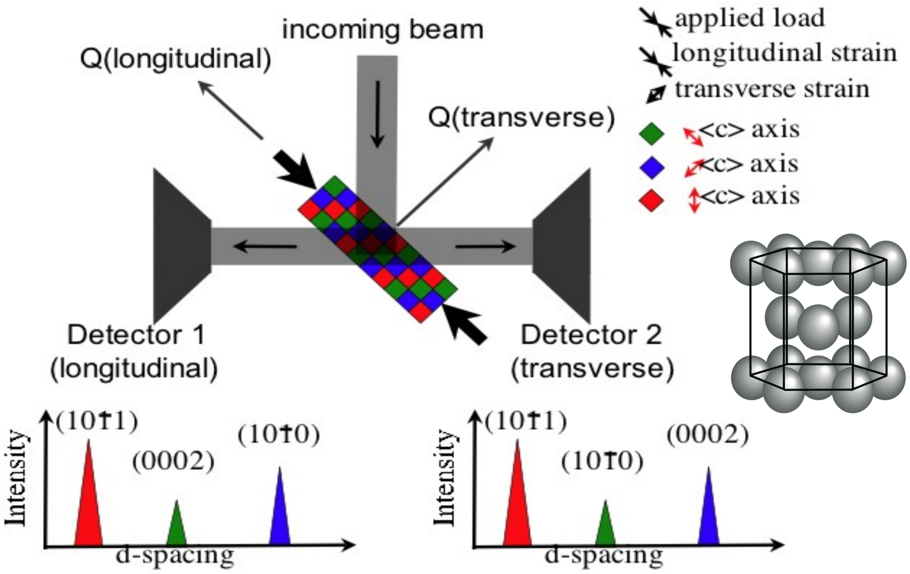
Blue: elastic strain response of γ'
Red: elastic strain response of γ

Case Study – Ni base Superalloy

- Use of neutron diffraction and high energy synchrotron x-ray diffraction characterising residual stresses, intergranular strains and phase transformation

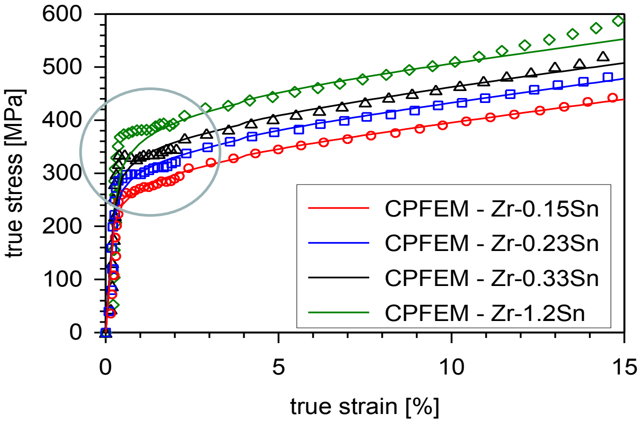


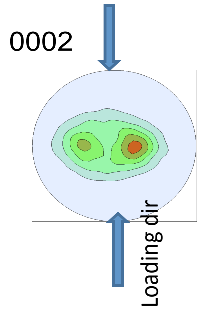
Case Study – hcp metal



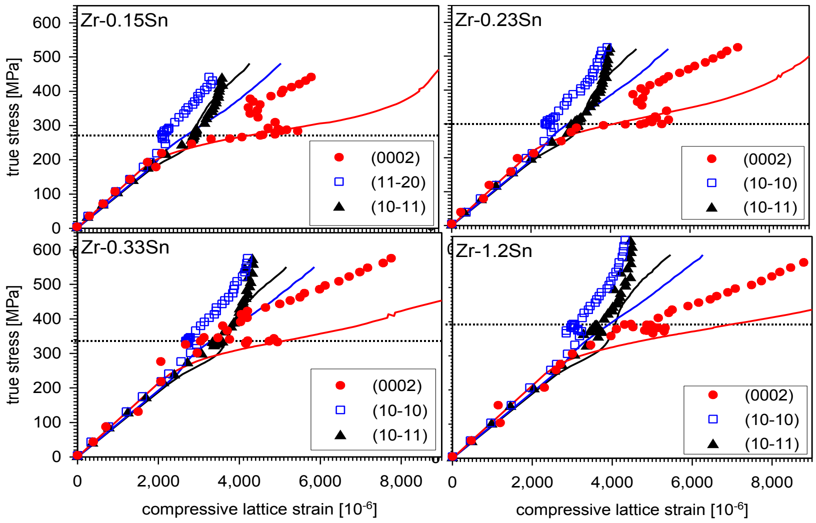
Effect of Sn on twinning in Zr alloys

- Twin nucleation criteria unknown
- Role of alloying elements on twinning unknown



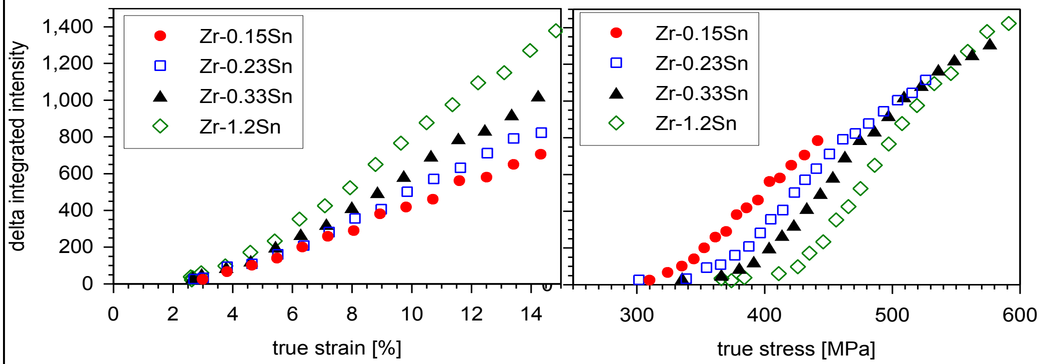


Role of Sn on intergranular strain development



Lattice strain recorded in the loading direction

Critical stress and strain for twinning



(0002) Integrated intensity recorded in loading direction vs. strain

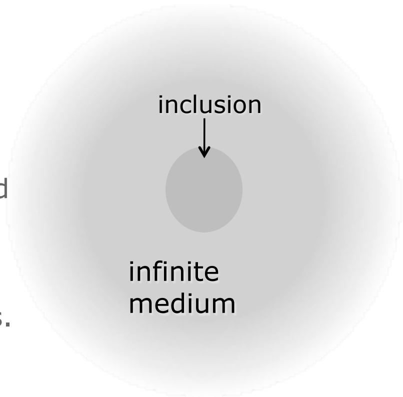
(0002) Integrated intensity recorded in loading direction vs. stress

Modelling deformation

- Micromechanics
  - Dislocations, particles, grain boundaries (grain size), interstitial atoms
- Continuum mechanics:
  - Stresses and strains
  - Intergranular stresses
- Polycrystal plasticity
  - Mean field methods, i.e. every grain has the same matrix
  - Finite element methods
    - Each grain has a characteristic neighbourhood
    - Predict maximum and minimum stresses ?

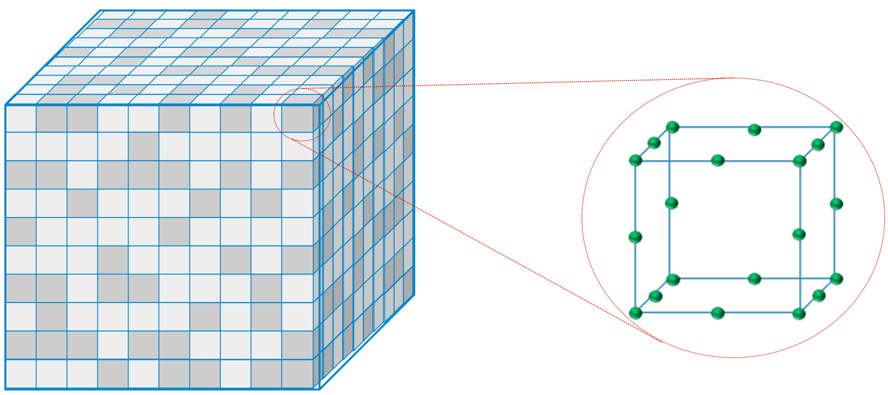
EPSC Modelling

- The elasto-plastic self-consistent model (EPSC), is based on the Eshelby-Hill formulation.
- An elliptical inclusion in an infinite medium.
- The surrounding medium is the average of all orientations.
- The inclusion has uniform stress and anisotropic properties i.e. different orientations have different elastic moduli and plastic deformation is only allowed on specified slip planes.
- The model is capable of simulating multiple thermo-mechanical processes.



CPFEM

- CPFEM is more computer intensive than EPSC modelling, however, it enables the simulation of specified grain structures.



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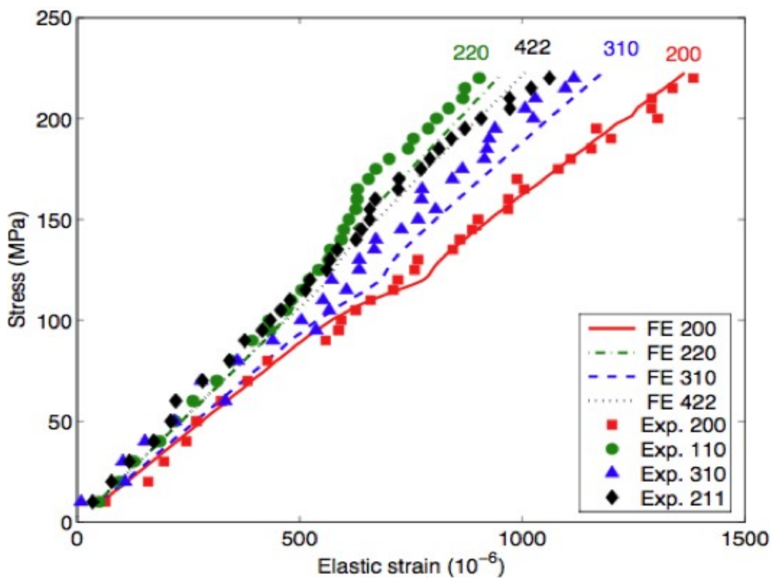
Plasticity Modelling (CPFEM)



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Attempted General Guidelines: Neutrons

Neutrons:

- Non-destructive, full stress analysis because of cubic Gauge Volume (think three directions)
- Good penetration depth due to neutrality
- Big bulky sample with low stress gradients
- Reasonable spatial resolution independent of atomic number
- Steels, aluminium, nickel, copper zinc or related
- Sample in harsh environment: furnace, cryo. etc.
- Phase analysis with Rietveld analysis

Not-so good: near surface or thin materials, titanium, boron cadmium, fast, high-spatial resolution, high instrumental resolution, hydrogenous materials

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Attempted General Guidelines: Synchrotrons

Synchrotrons:

- Non-destructive, fast strain mapping, mostly single peak
- Light alloys (small atomic number)
- High spatial resolution aluminium-titanium (think microns)
- High instrumental resolution (small peak width)
- Near surface measurement because of analyser crystal
- Bulk materials / larger atomic number with energy-dispersive method
- Polymers

Not so good at: Steels and higher, big bulky samples, harsh environments, diamond shaped GV