

# Engineering

Using diffraction to  
measure strain

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# Introduction

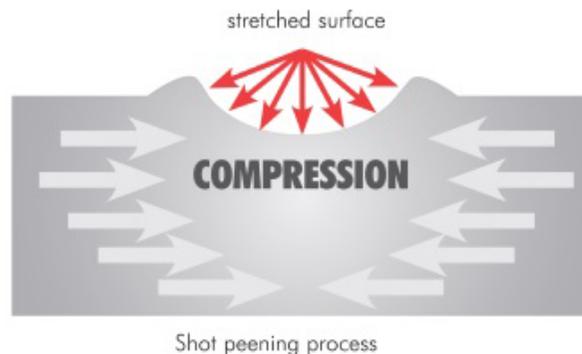
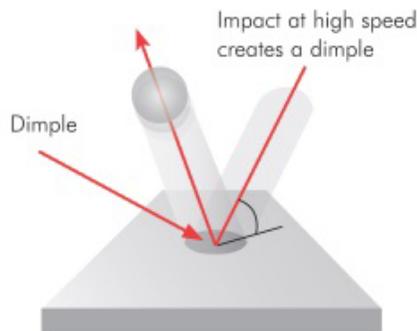
- What are residual stresses
- The principle of measuring strain
- Intragranular strain development
- Neutron and Synchrotron X-ray diffraction
  - Properties
  - Facilities
- Case Studies / Questions
- From Engineering to Physical Metallurgy – Understanding plasticity
- Conclusions

# Introduction

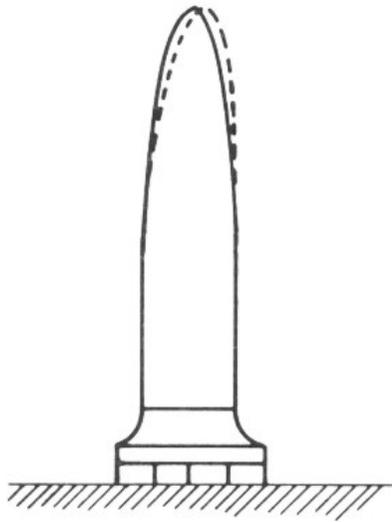
- Residual stresses in materials
- Principles of measuring residual stresses by diffraction
- Neutron and Synchrotron X-ray diffraction
  - Properties
  - Facilities
- Case Studies / Questions
- From Engineering to Physical Metallurgy – Understanding plasticity
- Conclusions

# What are residual stresses?

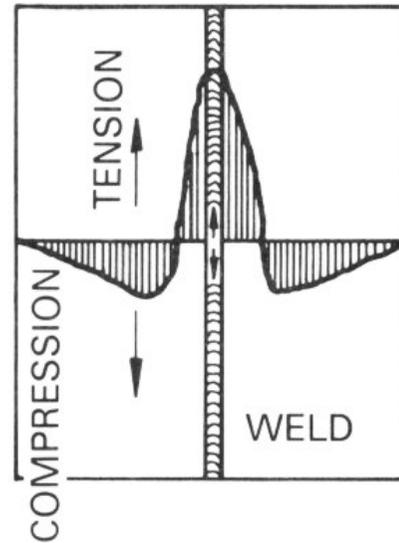
- Stresses that exist in a body without applying any external load
- Stresses are caused by a misfit
  - result of uneven deformation and/or
  - thermal expansion/shrinkage at different times



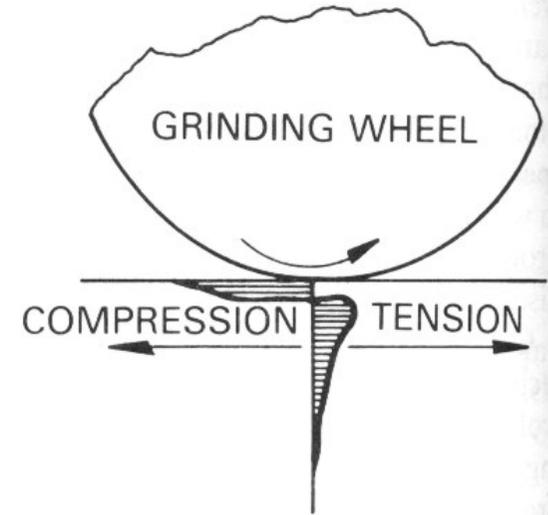
# Examples of Residual Stresses



(A) Thermal Distortion in a Structure Due to Solar Heating



(B) Residual Stresses Due to Welding

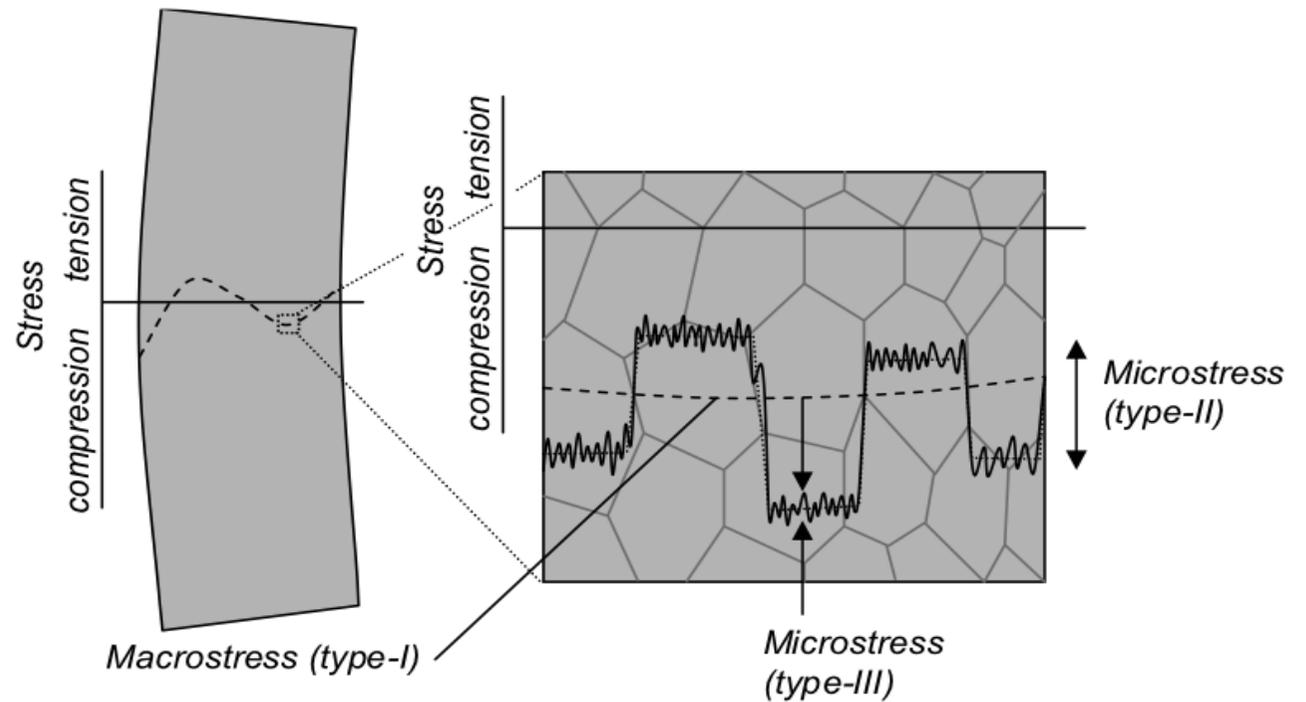


(C) Residual Stresses Due to Grinding

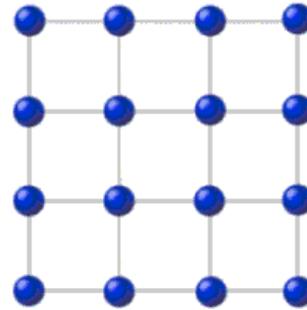
# Residual Stresses

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

## Bent bar:



# Effect of elastic strain on diffraction signal

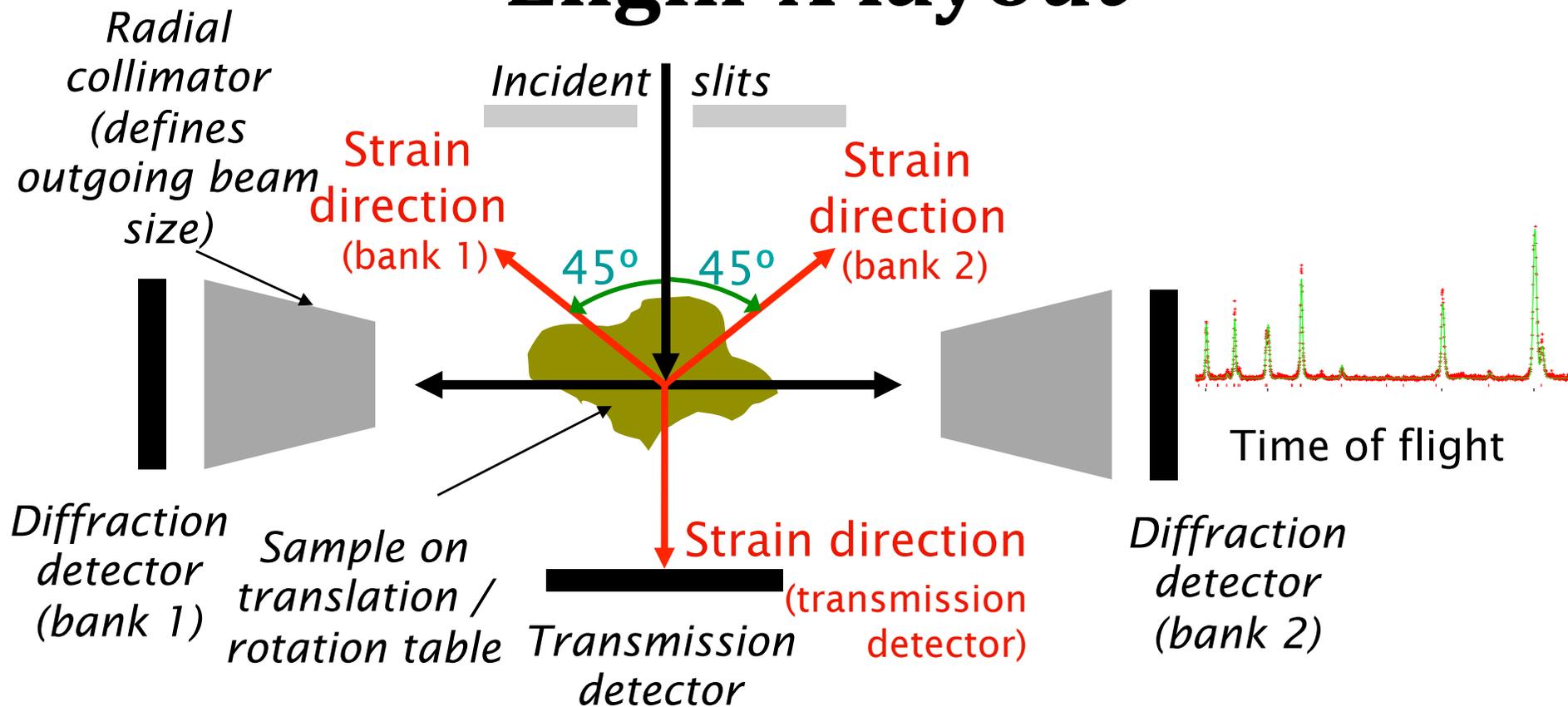


$$\lambda = 2d \sin \theta$$

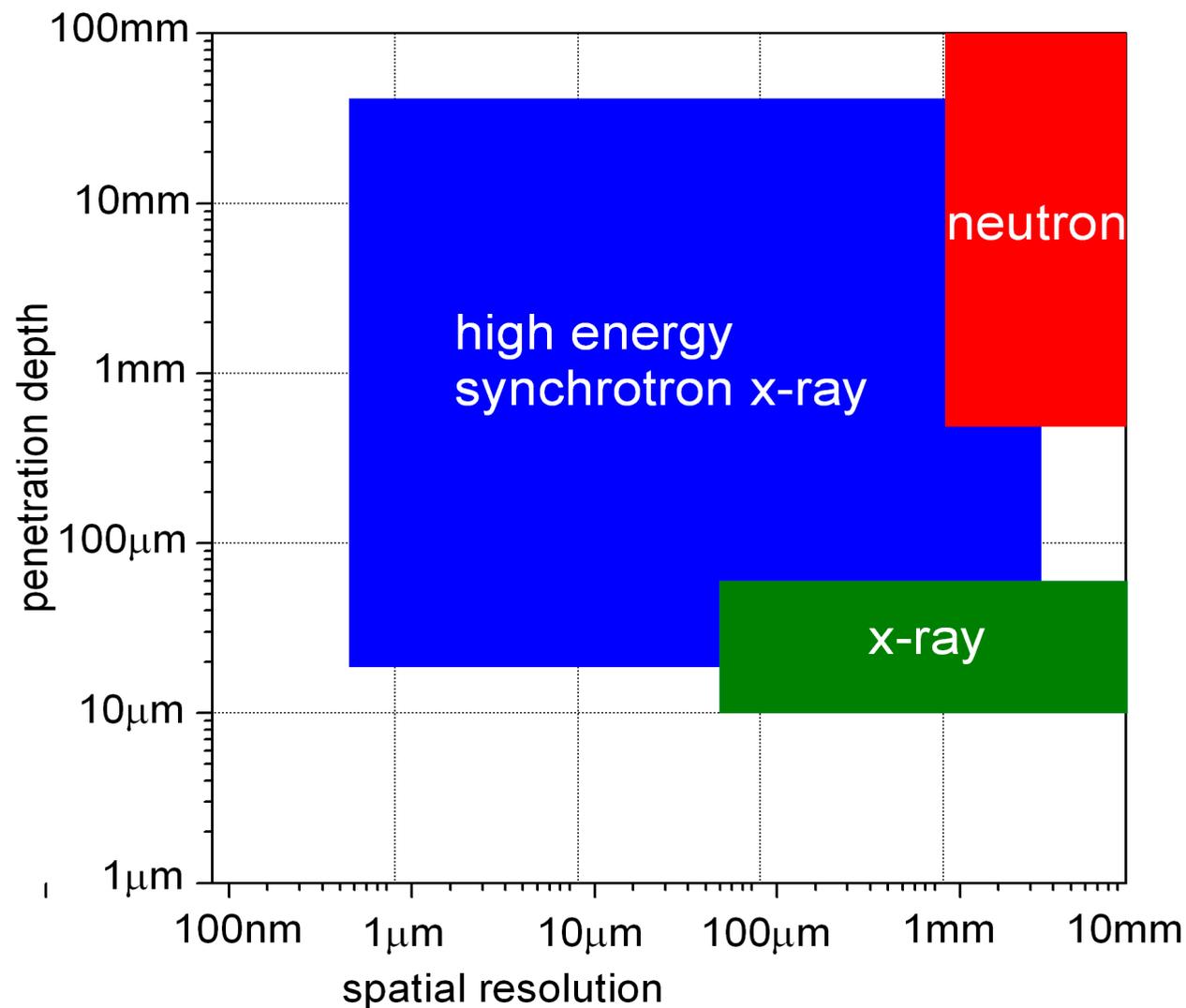
- Diffraction measures elastic lattice strain as peak shifts
- Uses the poly-crystalline lattice planes as internal strain gauges

# Set up of Engineering Instrument

## Engin-X layout



# General Overview: Diffraction methods available



# 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 diagram shows a yellow rectangular element in a 3D coordinate system with axes x, y, and z. On the right face (normal to x), there is a normal stress  $\sigma_{xx}$  and shear stresses  $\tau_{xy}$  and  $\tau_{xz}$ . On the front face (normal to y), there is a normal stress  $\sigma_{yy}$  and shear stresses  $\tau_{yx}$  and  $\tau_{zy}$ . On the bottom face (normal to z), there is a normal stress  $\sigma_{zz}$  and shear stresses  $\tau_{zx}$  and  $\tau_{yz}$ . A callout for  $\tau_{xy}$  shows a dashed line indicating it acts in the x-direction on the y-face. A note states: "The stress acts in the x-direction 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:

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

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

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

To calculate a stress direction:

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

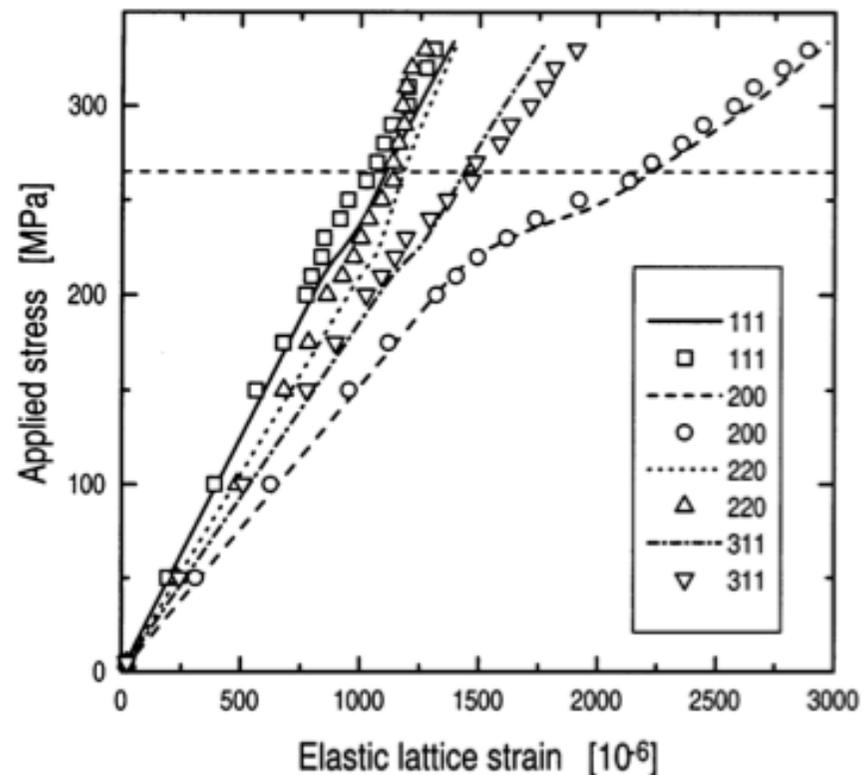
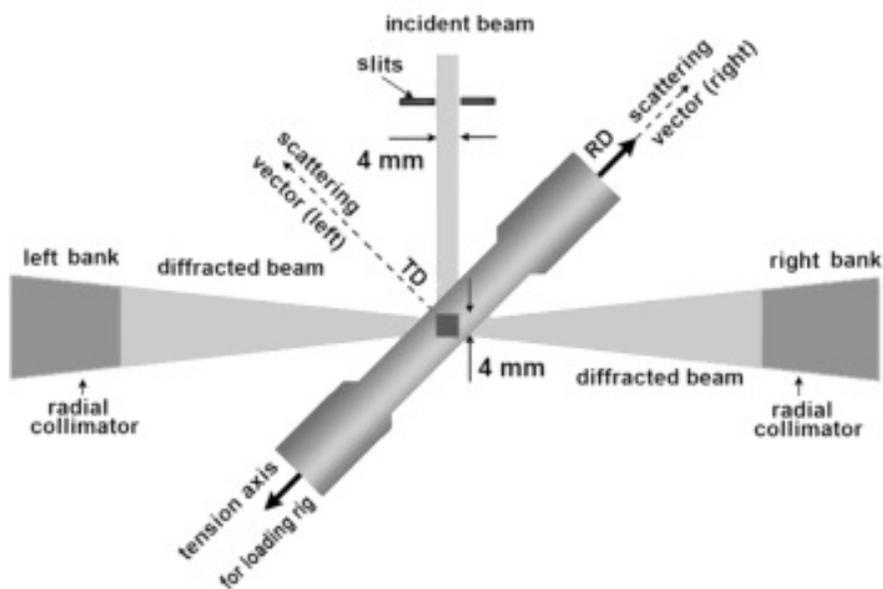
**(Attention: not always this simple!)**

# Response of diffraction planes during mechanical loading

- Measuring individual reflections

In-situ Loading

Austenitic Stainless Steel



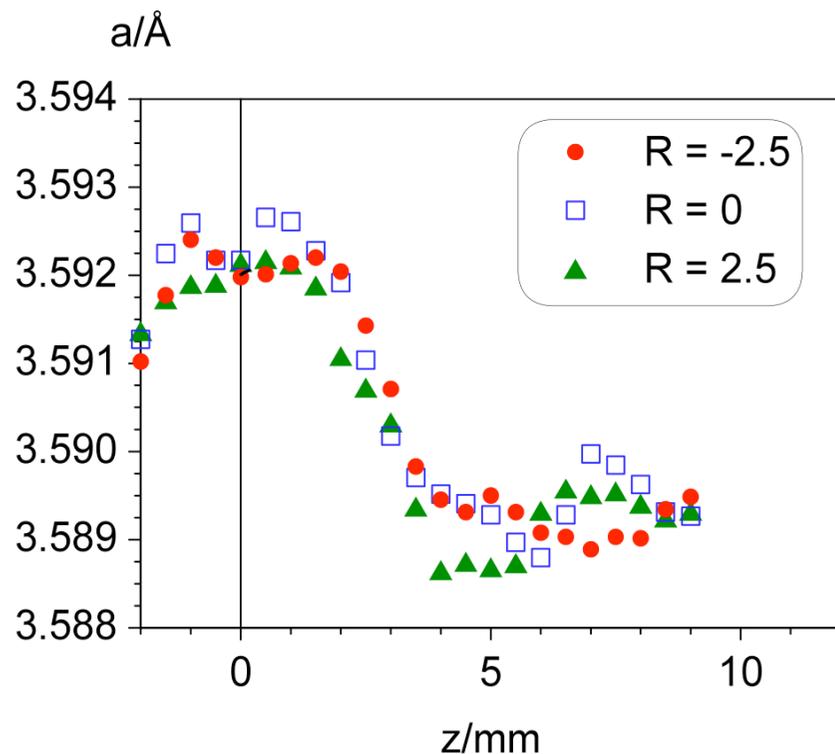
# Which reflection should be used ?

- When using single reflections particular peaks are least prone to intergranular strain development
  - Requires use of diffraction elastic constants to convert strain to stress
- TOF instruments offer possibility to measure lattice parameter rather than d-spacing
  - Young modulus and Poisson number can be used to convert strain to stress

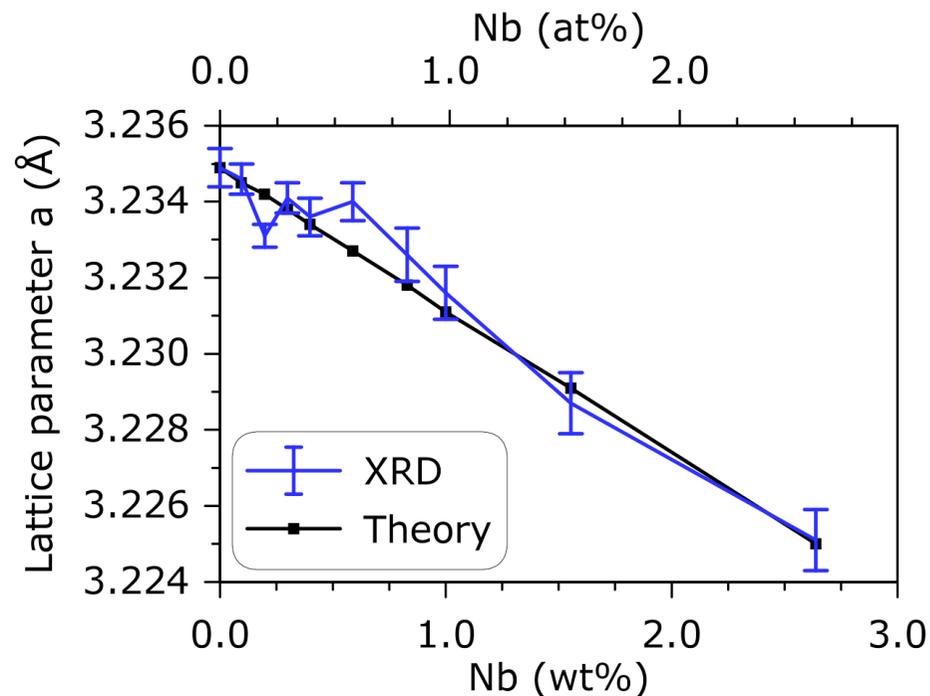
# $d_0$ variation

Accurate strain analysis relies on accurate determination of  $d_0$

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



Example of  $d_0$  variation across a tubular Nickel weld



The Vegard Law  
Example: Nb in Zr

# 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  $1\text{mm}^3$  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**

# Why do we like neutrons ?

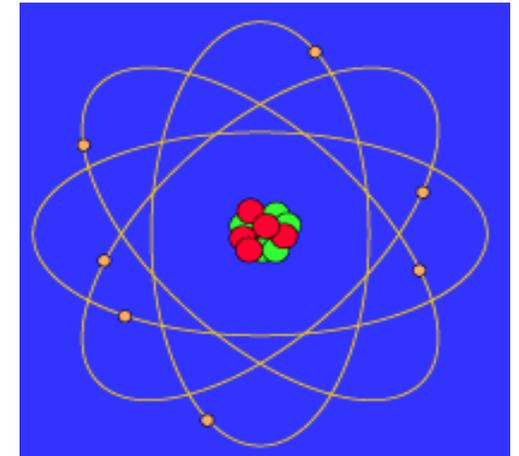
- Part of the nucleus
- Same mass as protons
- Interesting wavelength/mass relationship:

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

← 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 !!

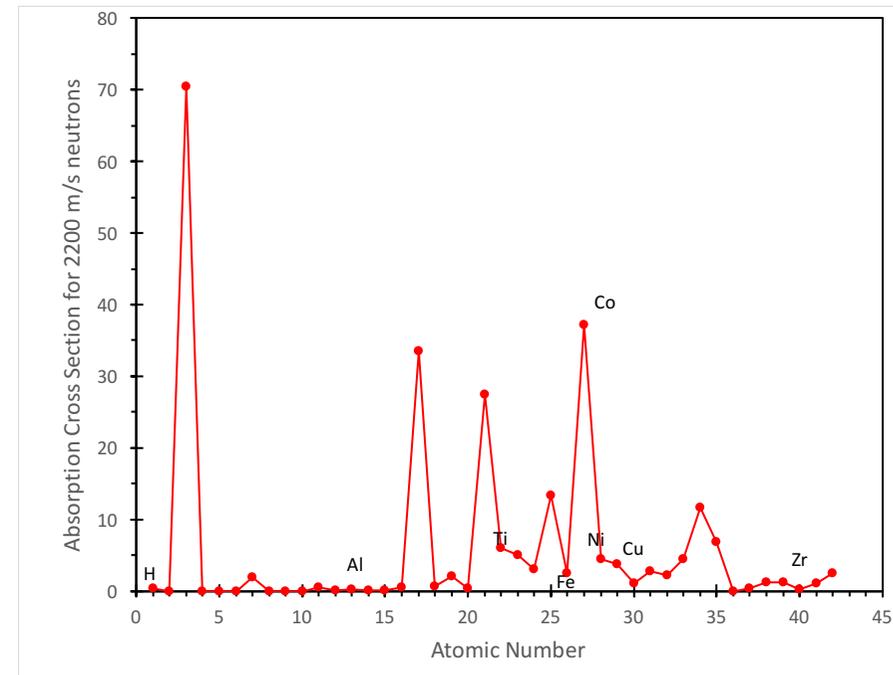
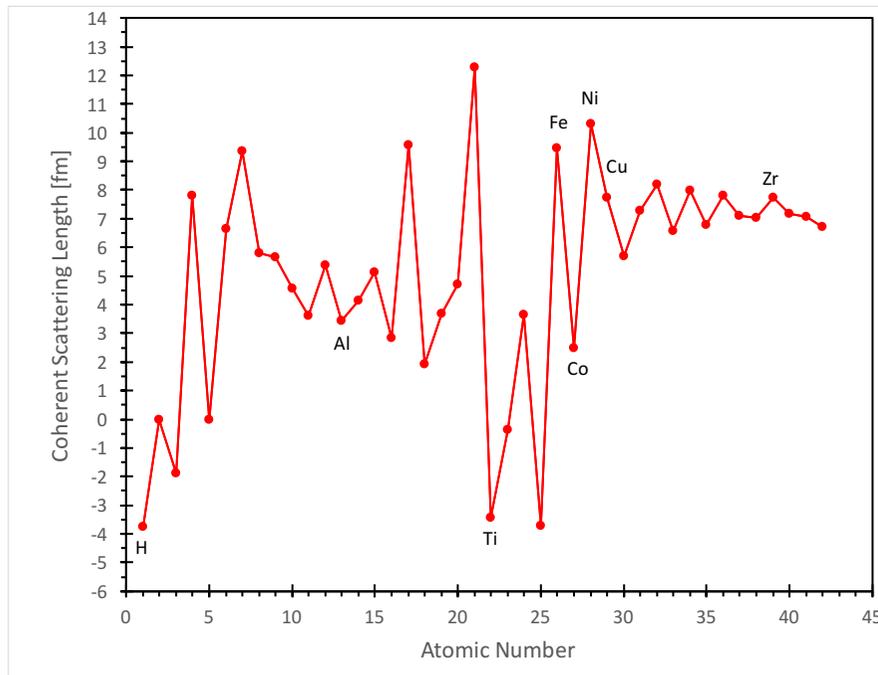


# Neutron Properties

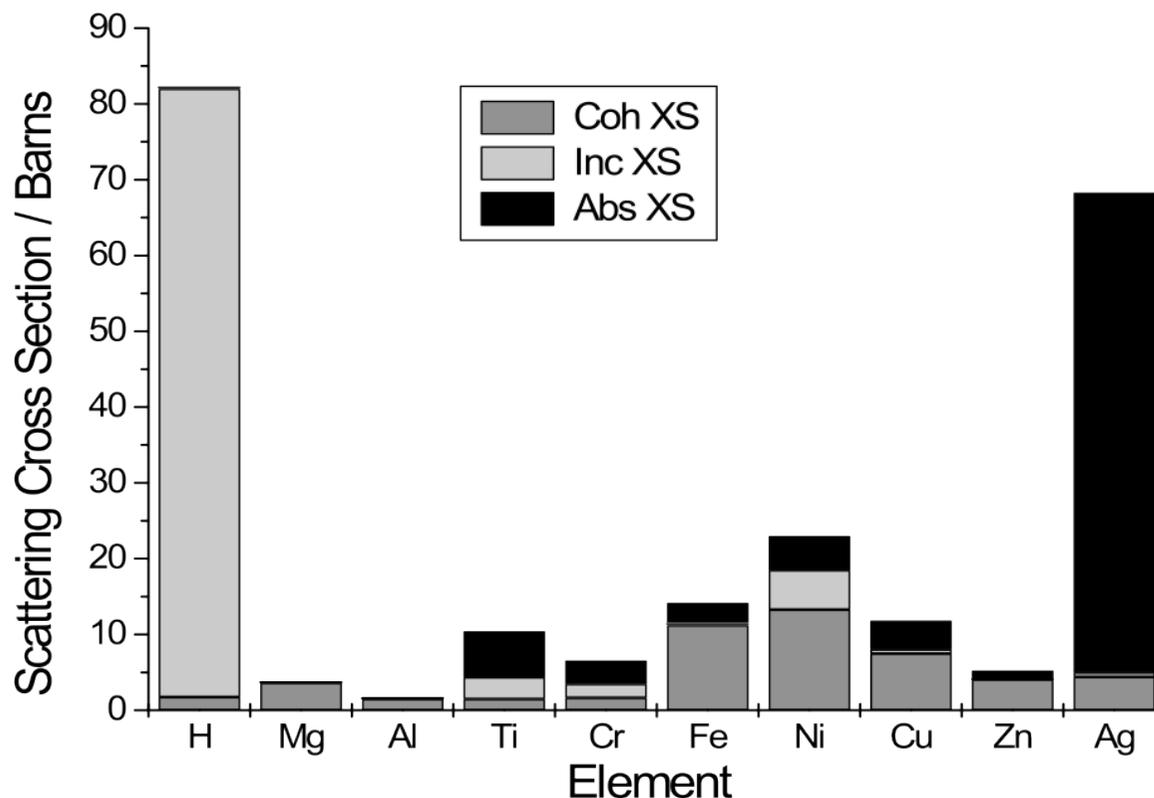
- Neutrons are scattered by atomic nuclei (electrons and X-rays which are scattered by the electron cloud).
- Since the scattering is nuclear process, scattering amplitude varies greatly for different isotopes of same element and in a unpredictable manner from element to element. X-ray and electron scattering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

# Neutron Properties

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



# Neutron Scattering



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

Coherent XS  $\sim$  Signal  
 Incoherent XS  $\sim$  Background  
 Absorption XS  $\sim$  1/Intensity



Penetration depth  $\sim$   
 1/Sum of Scatt XS

# 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

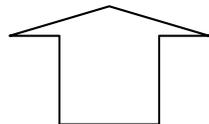
# Time of flight method

- Sharp pulse leaves source
- High energy neutrons (short  $\lambda$ ) travel faster and arrive first, low energy (long  $\lambda$ ) 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  $\sim 100\text{m/s}$  (speed of sound)  
 $\lambda = 2d \sin \theta$  with  $\theta$  fixed, i.e.  $\lambda$  proportional to  $d$

# Spallation Sources: Measurement of Strain

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

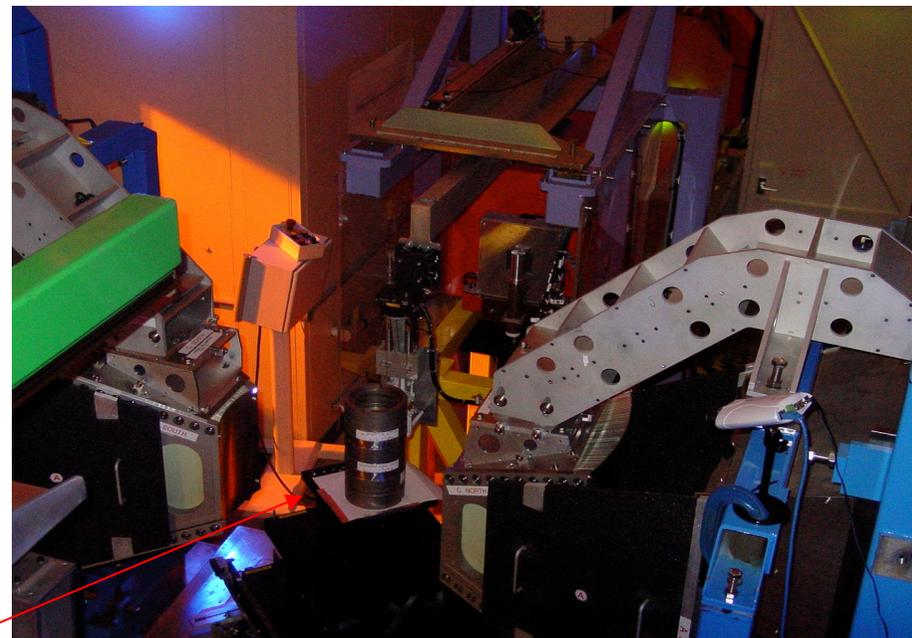
Cubic gauge volume !



Time-of-Flight:

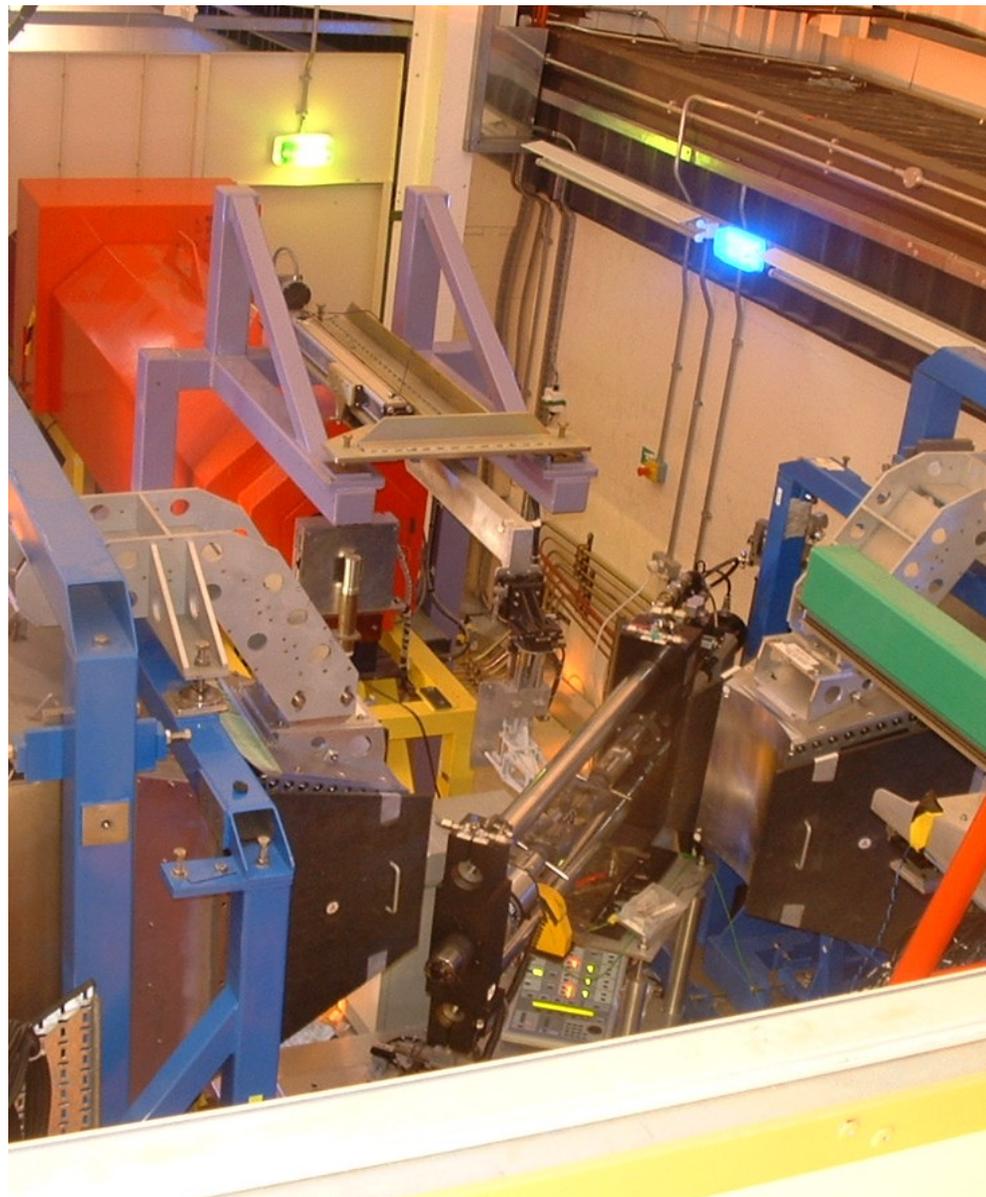
$$\lambda = \frac{h}{2mL \sin\theta} t$$

Fixed



ENGIN-X at ISIS

# In-situ loading experiments

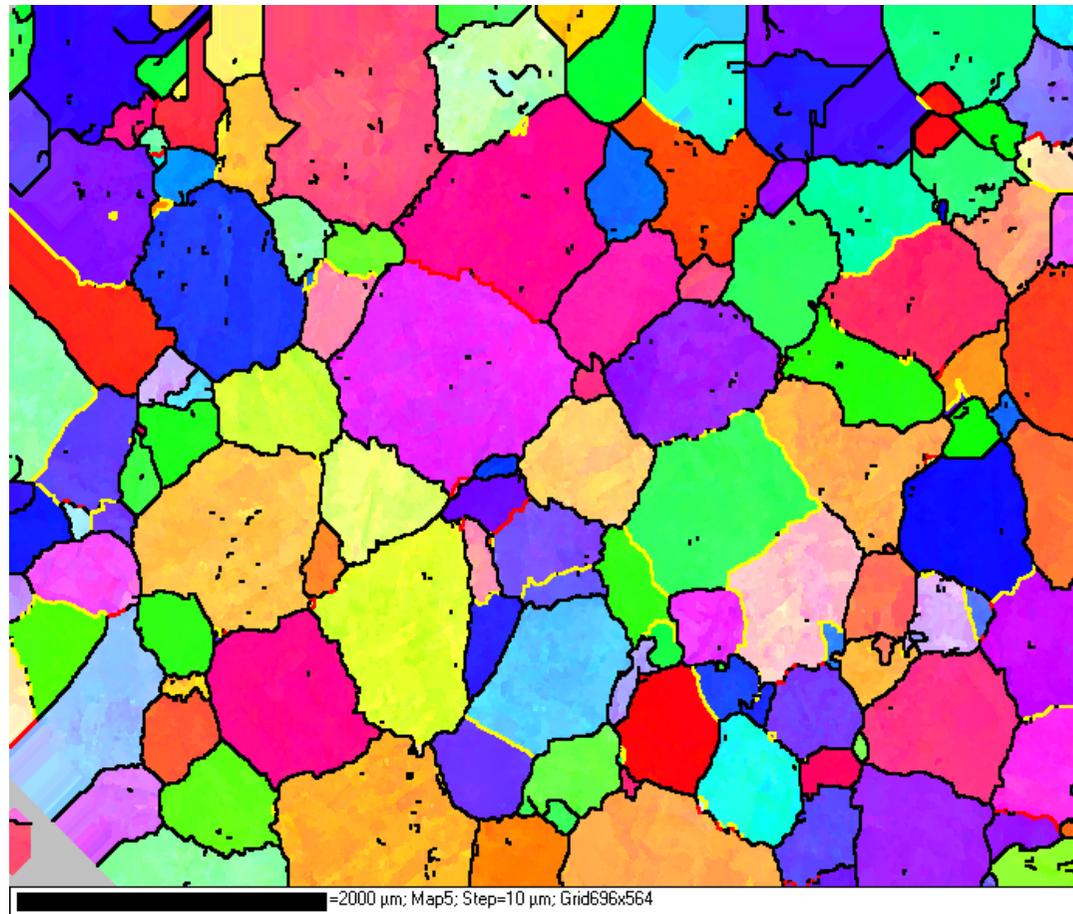


# What do we know ?

- 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  $\langle 110 \rangle$  direction
- Relatively good understanding what happen when a single crystal is deformed

# What we struggle with

- How does deformation work in a polycrystalline aggregate



$\beta$  phase IPF colour key

# Deformation heterogeneity

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

# 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

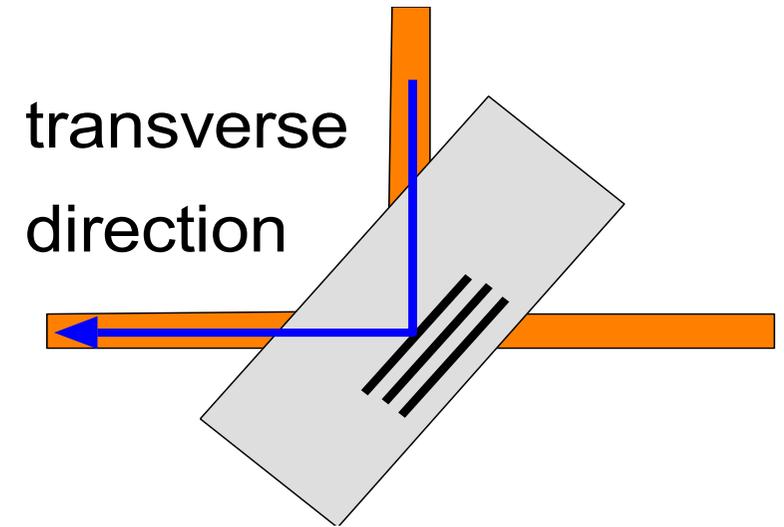
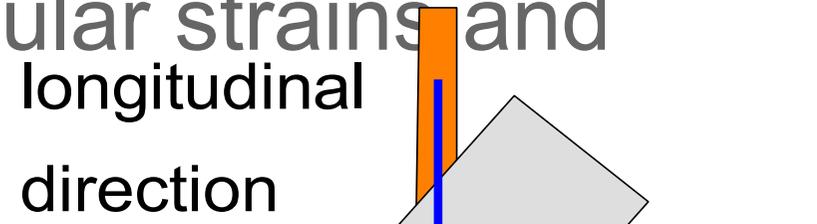
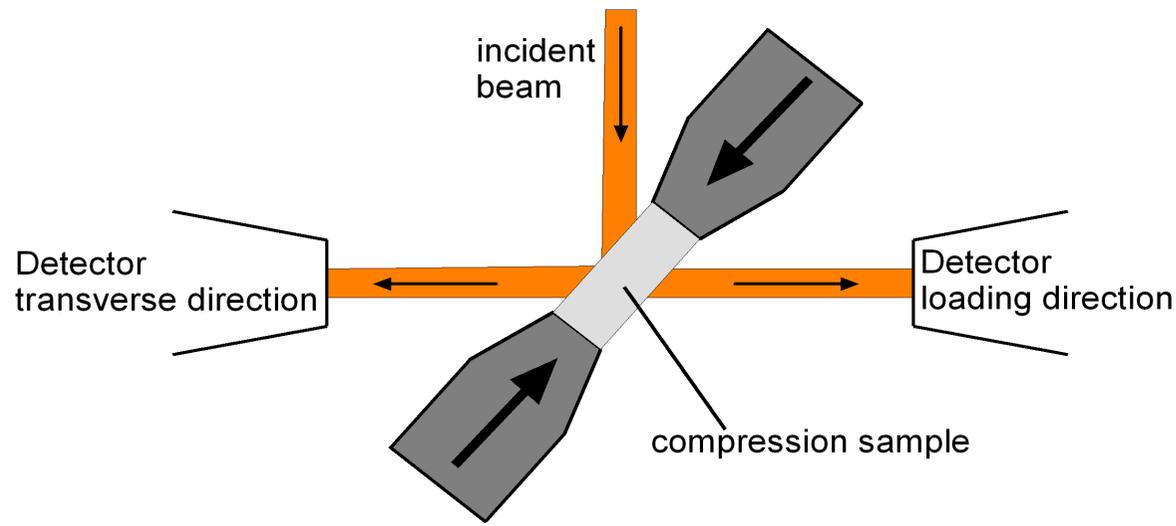
# Why do we care ?

- 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



# Experimental Methodologies

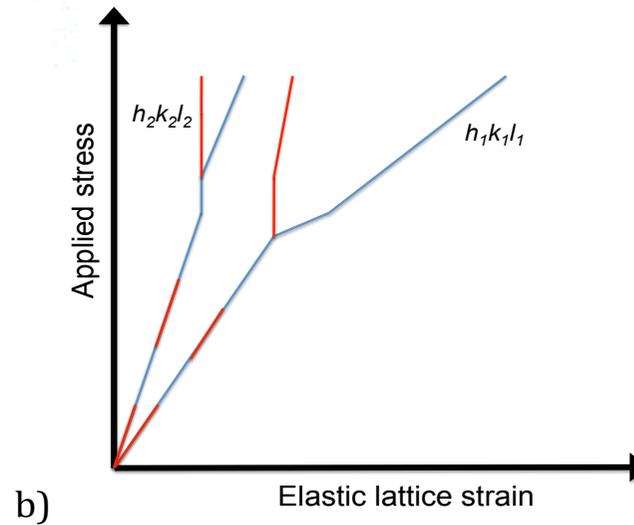
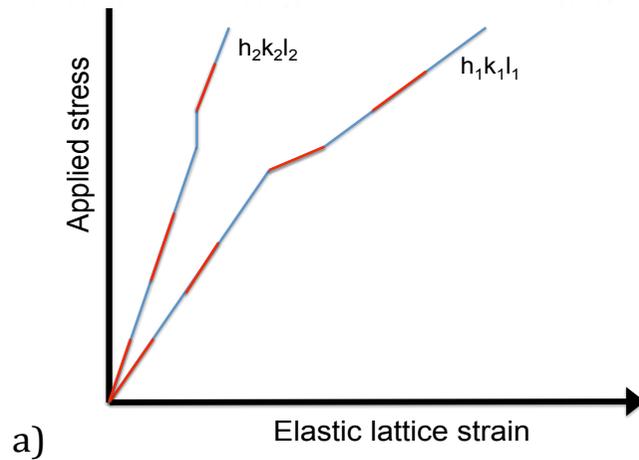
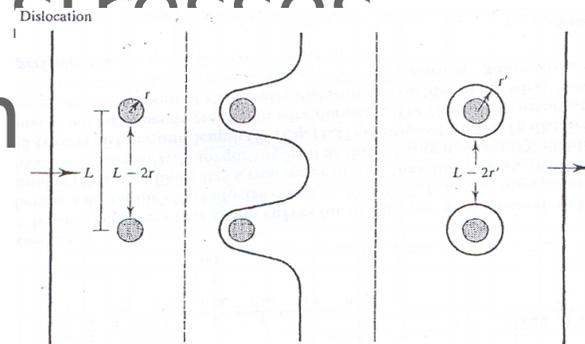
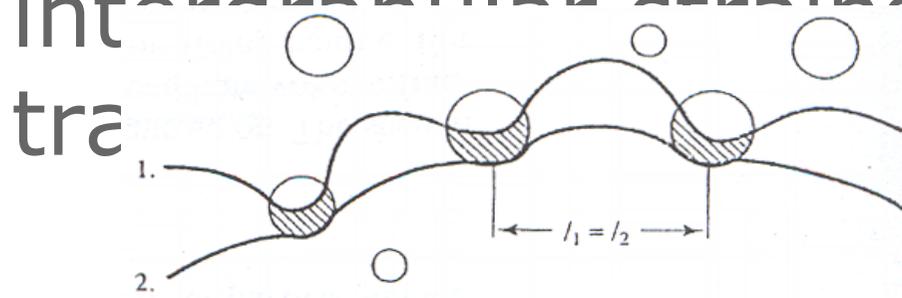
- Use of neutron diffraction and high energy synchrotron x-ray diffraction characterising residual stresses, intergranular strains and phase transformation



# Case Study – Ni base Superalloy

- Use of neutron diffraction and high energy synchrotron x-ray diffraction characterising residual stresses in intermetallics and alloys

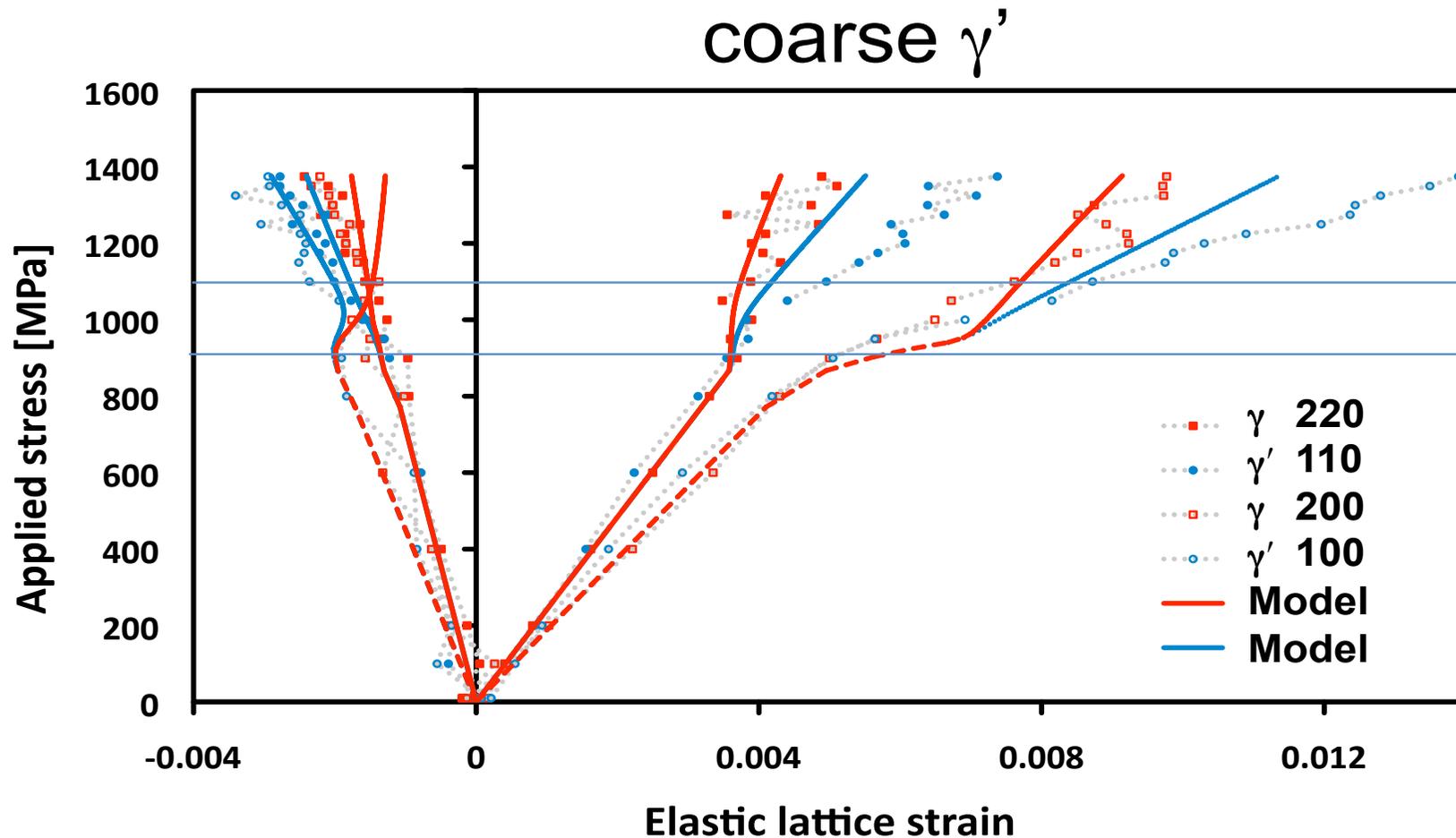
Example – Ni base Superalloy



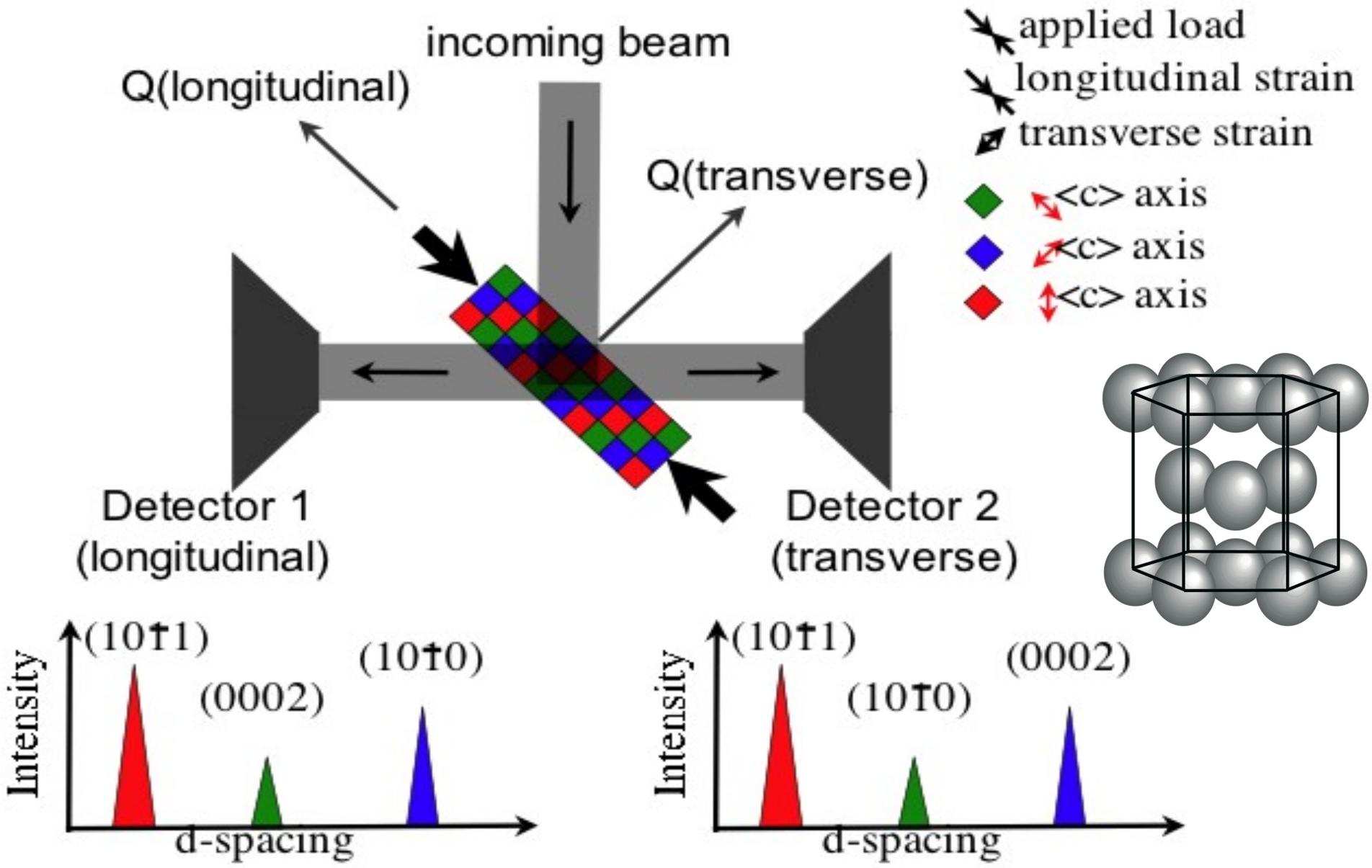
Blue: elastic strain response of  $\gamma'$   
 Red: elastic strain response of  $\gamma$

# Case Study – Ni base Superalloy

- Use of neutron diffraction and high energy synchrotron x-ray diffraction

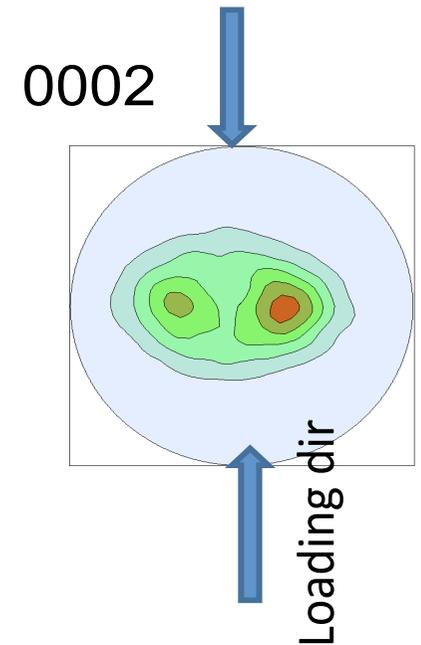
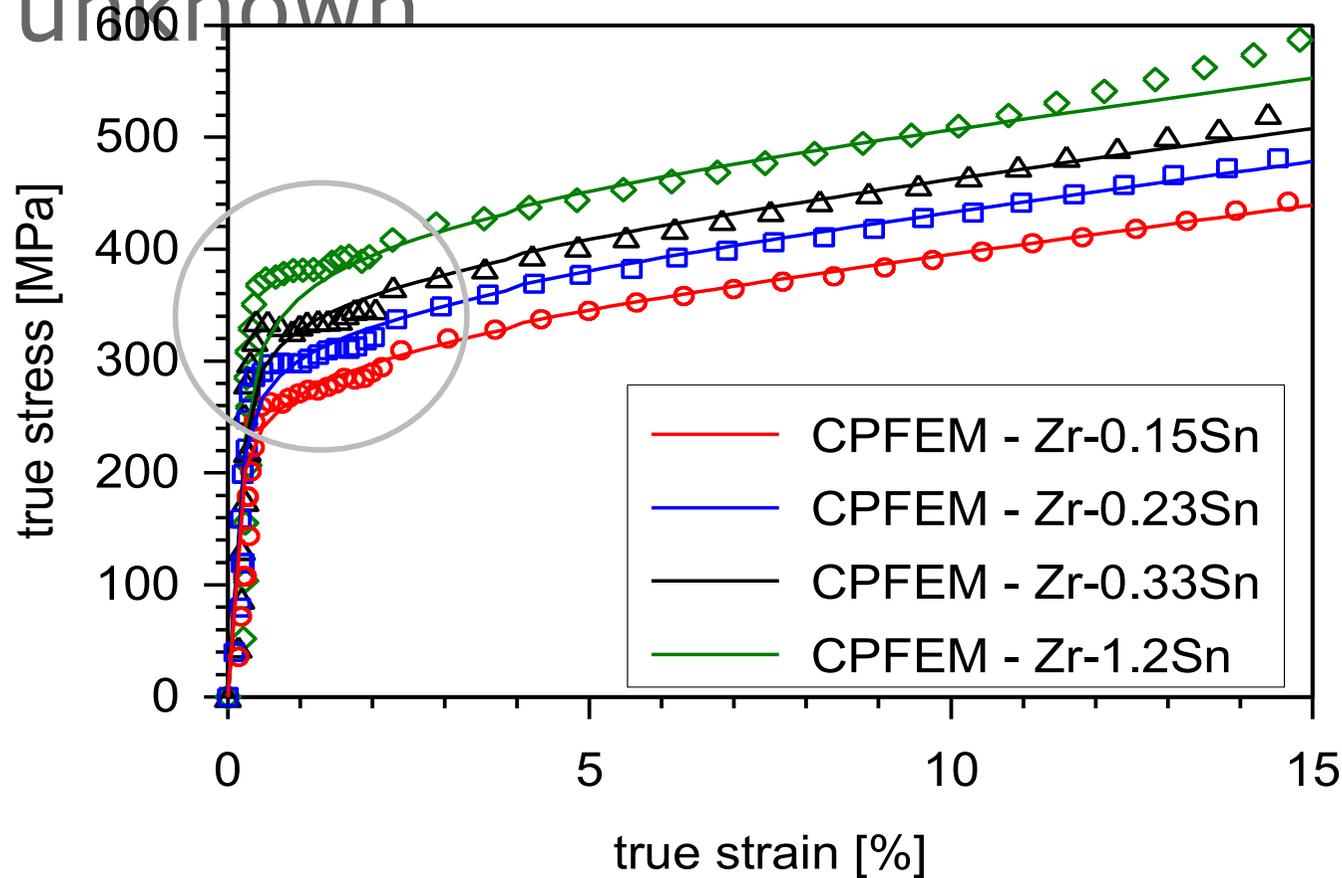


# Case Study – hcp metal

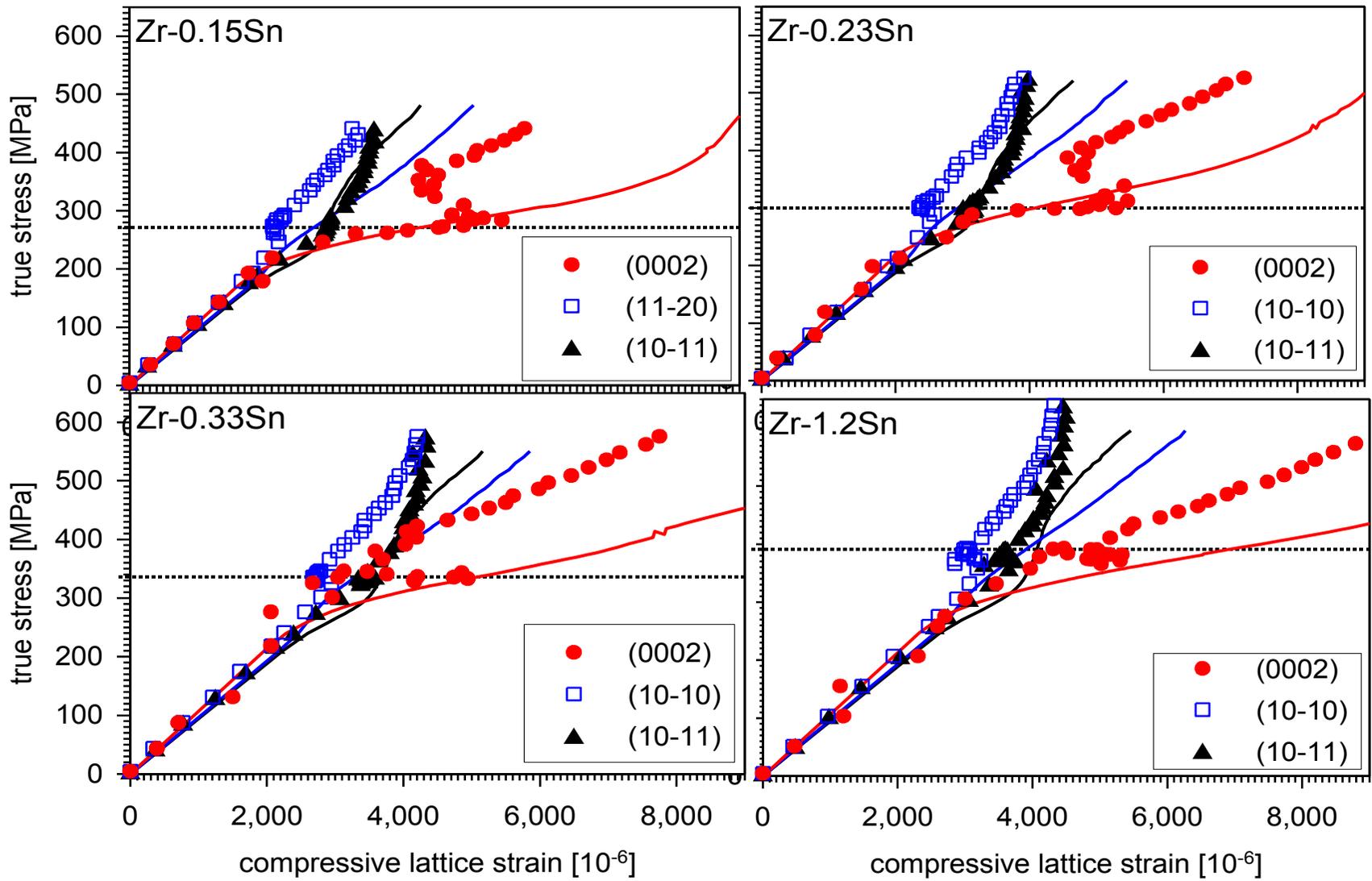


# Effect of Sn on twinning in Zr alloys

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

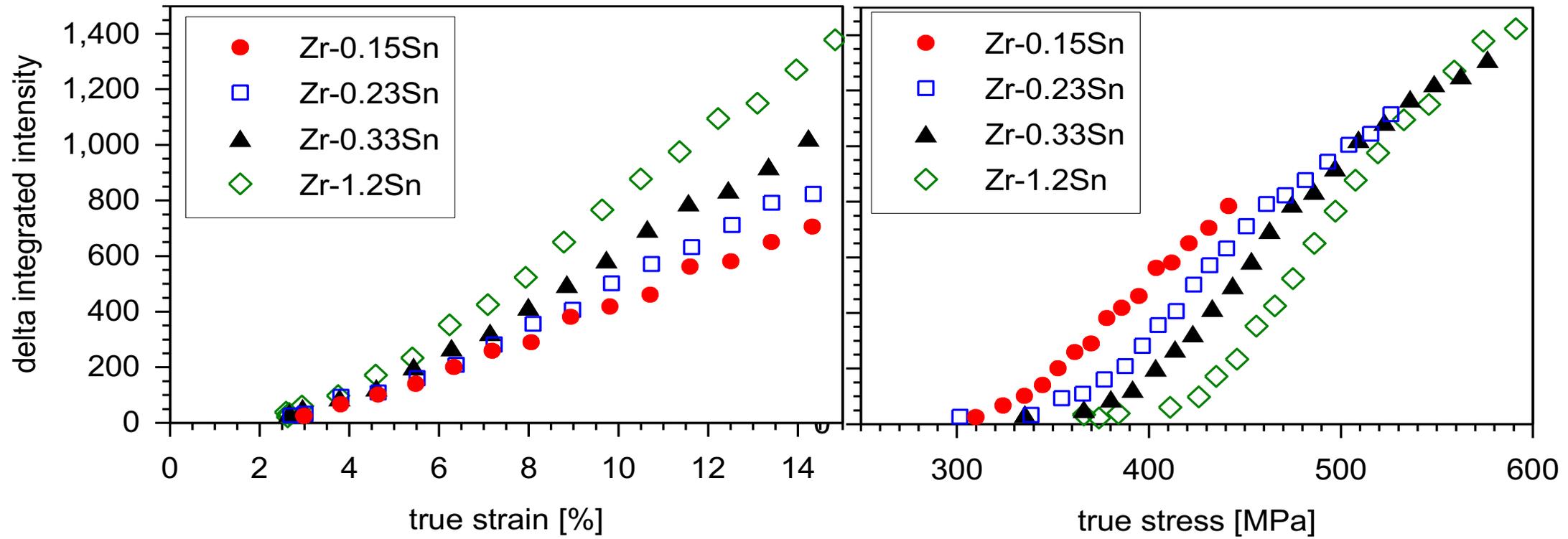


# Role of Sn on intergranular strain development



Lattice strain recorded in the loading direction

# Critical stress and strain for twinning



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

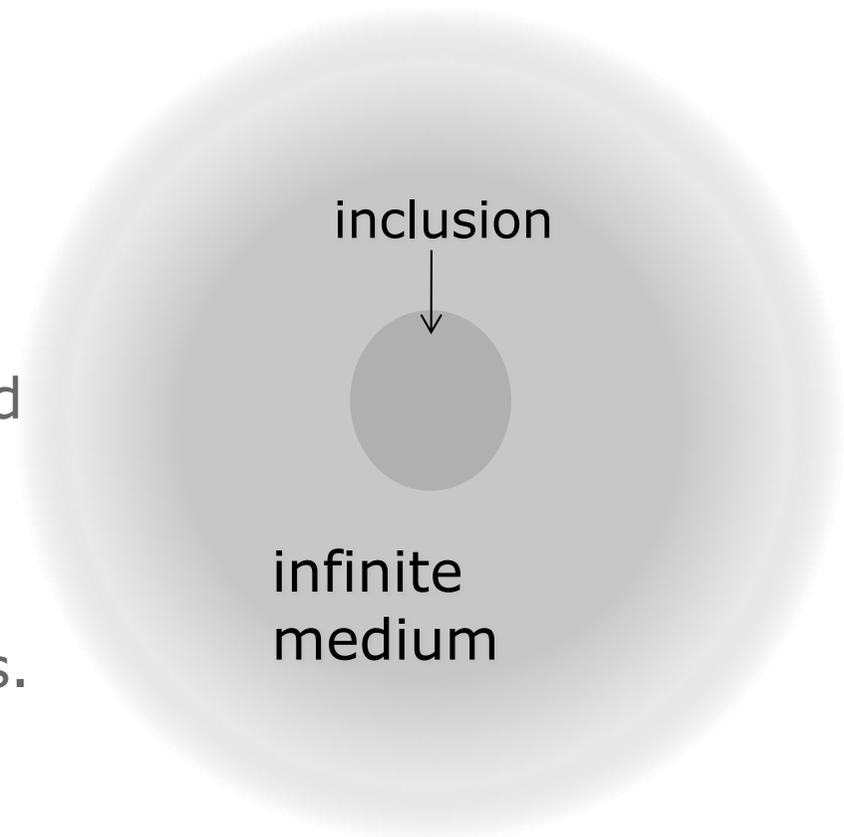
(0002) Integrated intensity recorded in loading direction vs. stress

# 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 ?

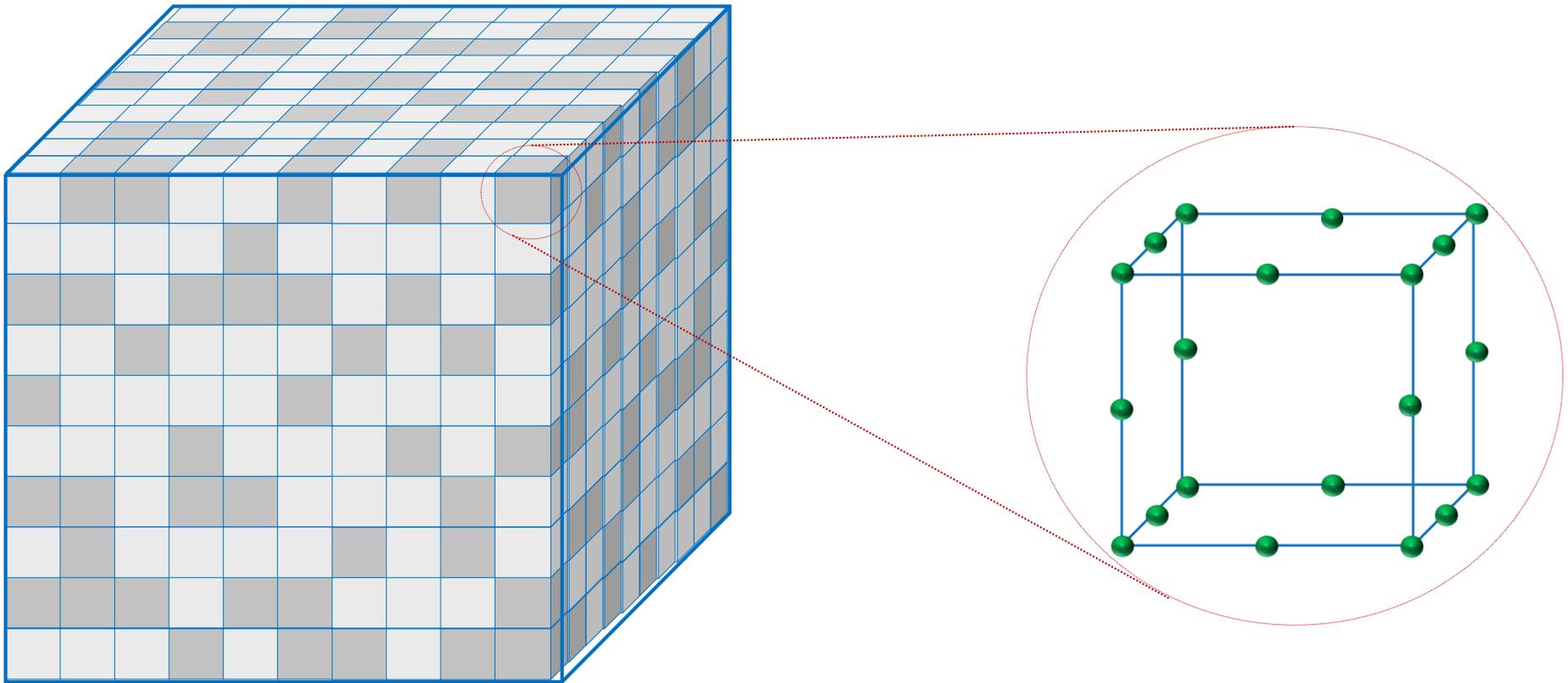
# EPSC Modelling

- 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.

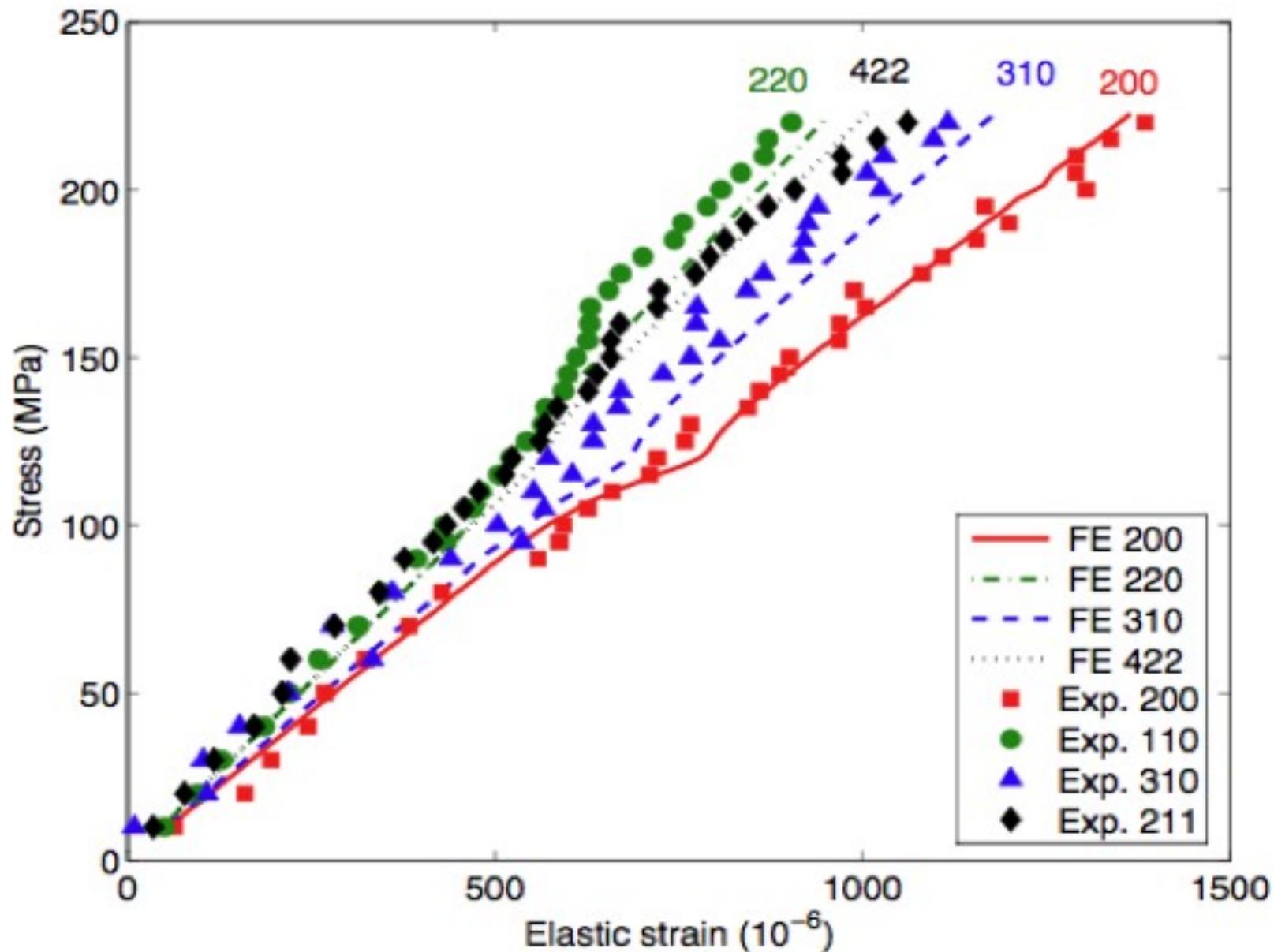


# CPFEM

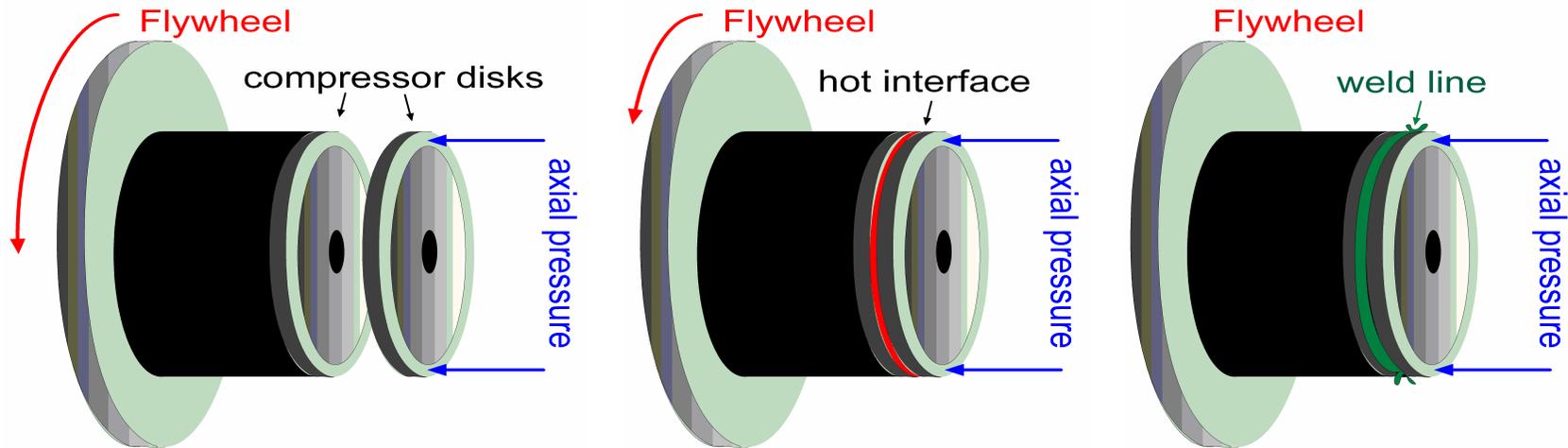
- CPFEM is more computer intensive than EPSC modelling, however, it enables the simulation of specified grain structures.



# Plasticity Modelling (CPFEM)

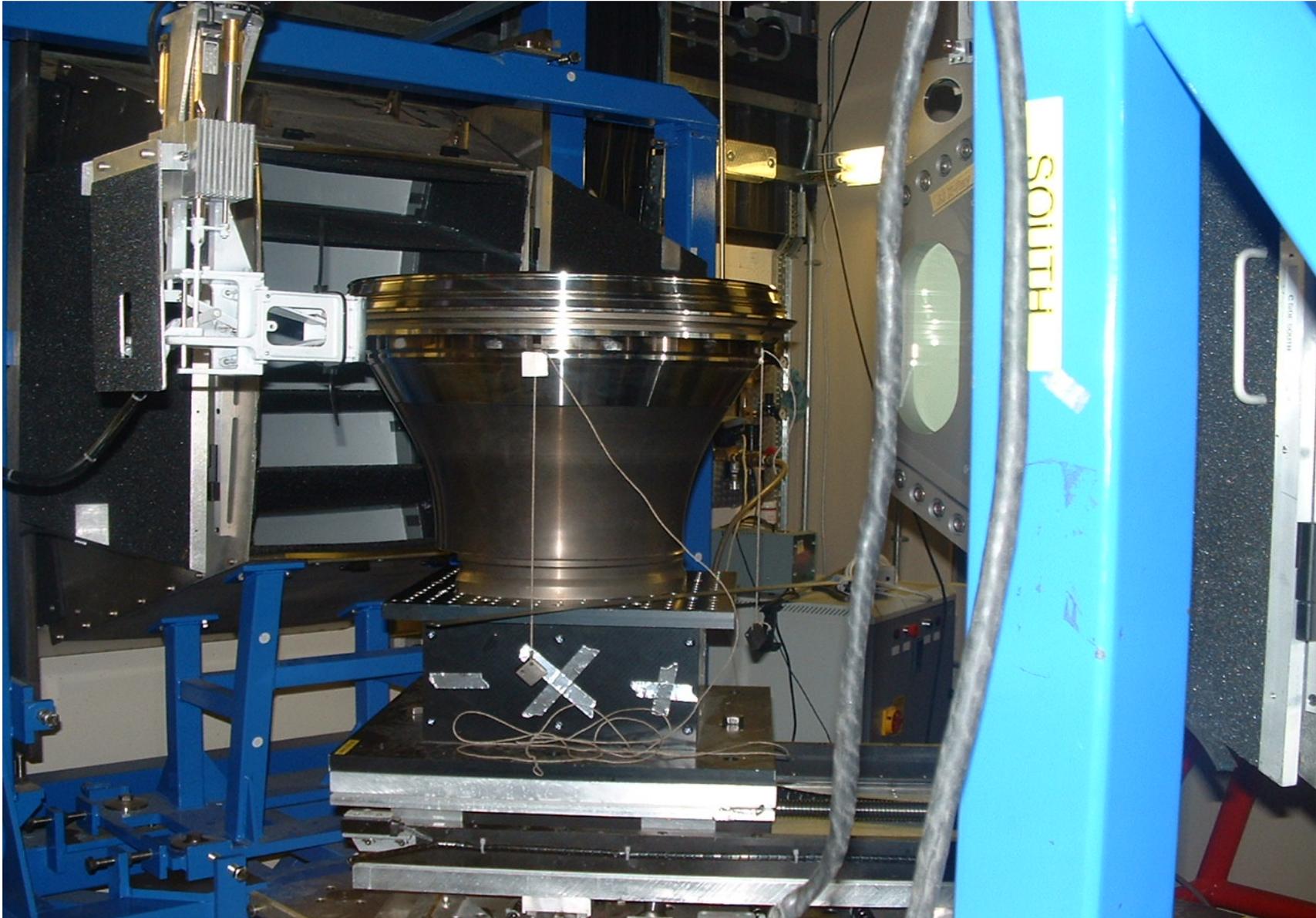


# Case Study: Inertia Friction Welding



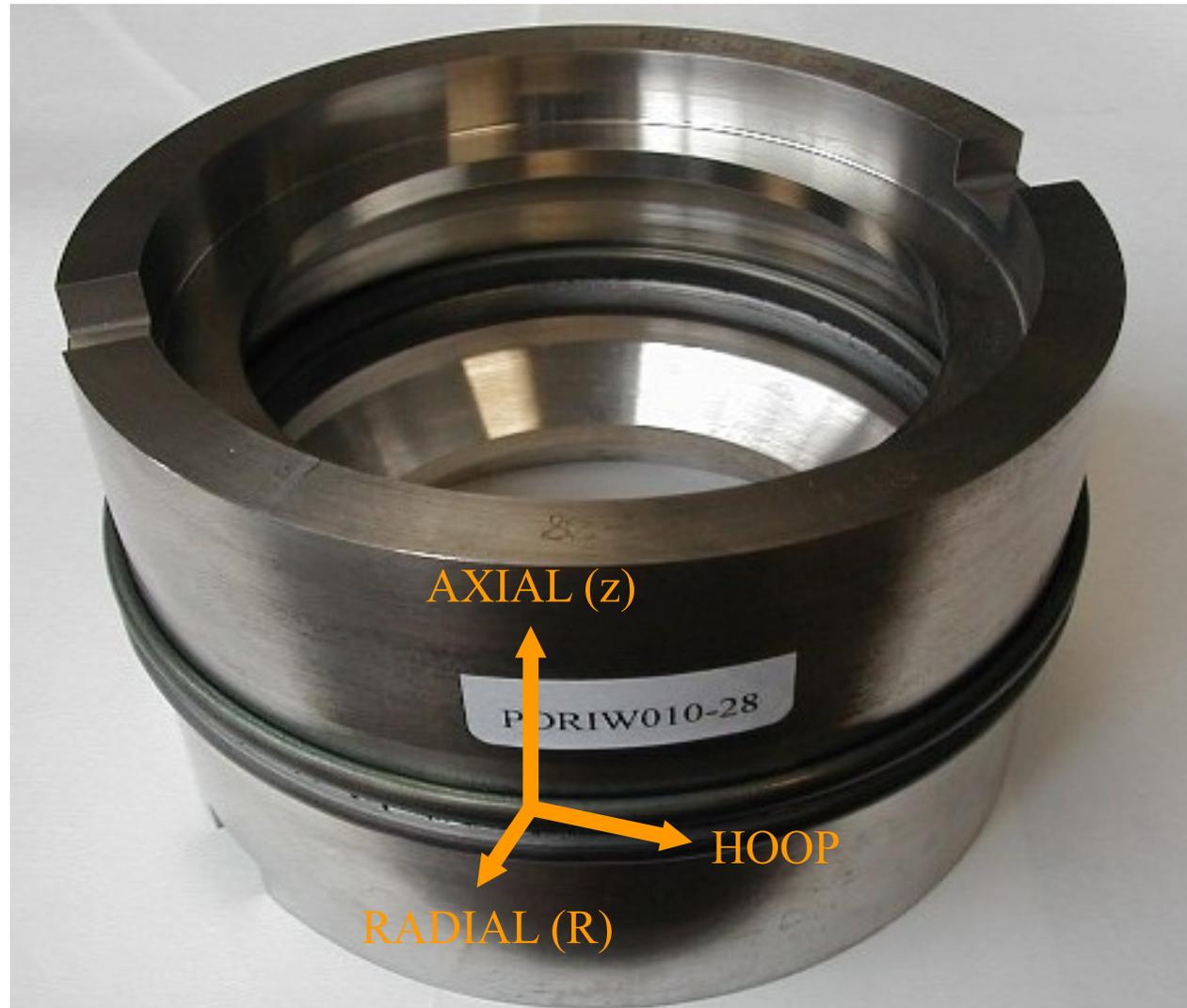
Solid state joining of compressor, turbine discs and shafts

# Case Study: Inertia Friction Welding



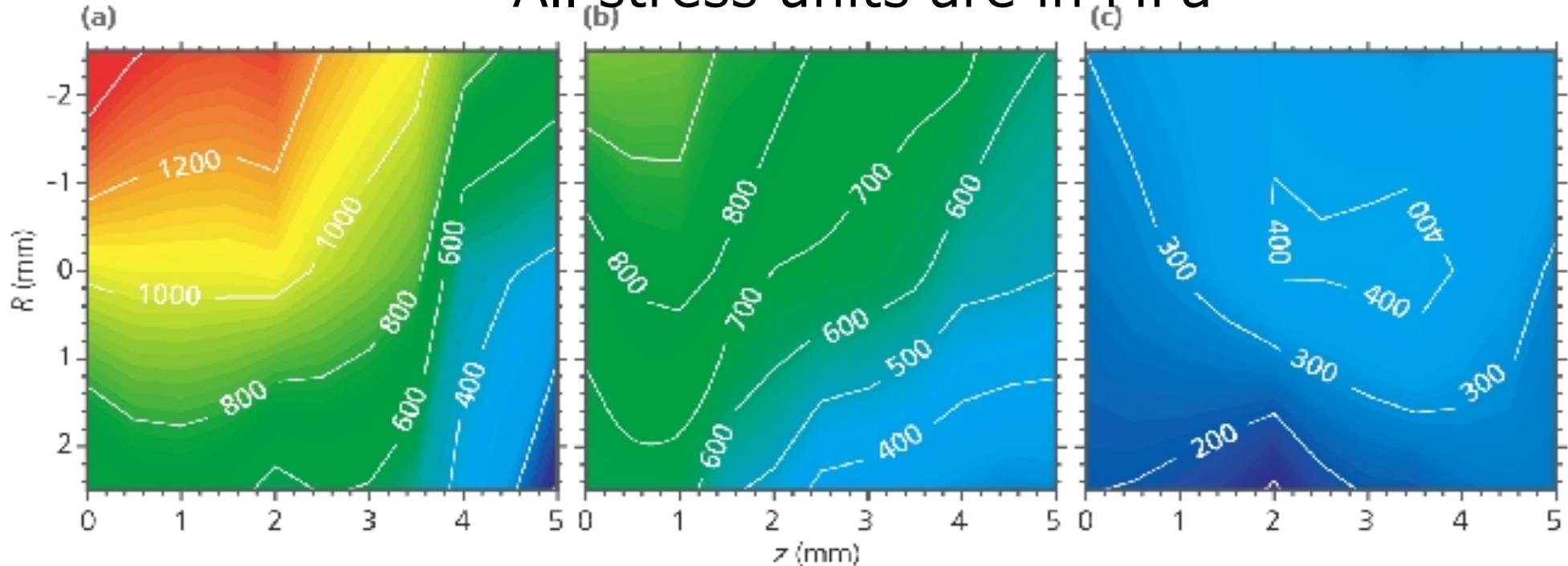
# How would you measure such a sample ?

143mm diameter test inertia friction welds



# Hoop stresses in IFW' d nickel-base superalloy

All stress units are in MPa



As-welded

Conventional

Modified

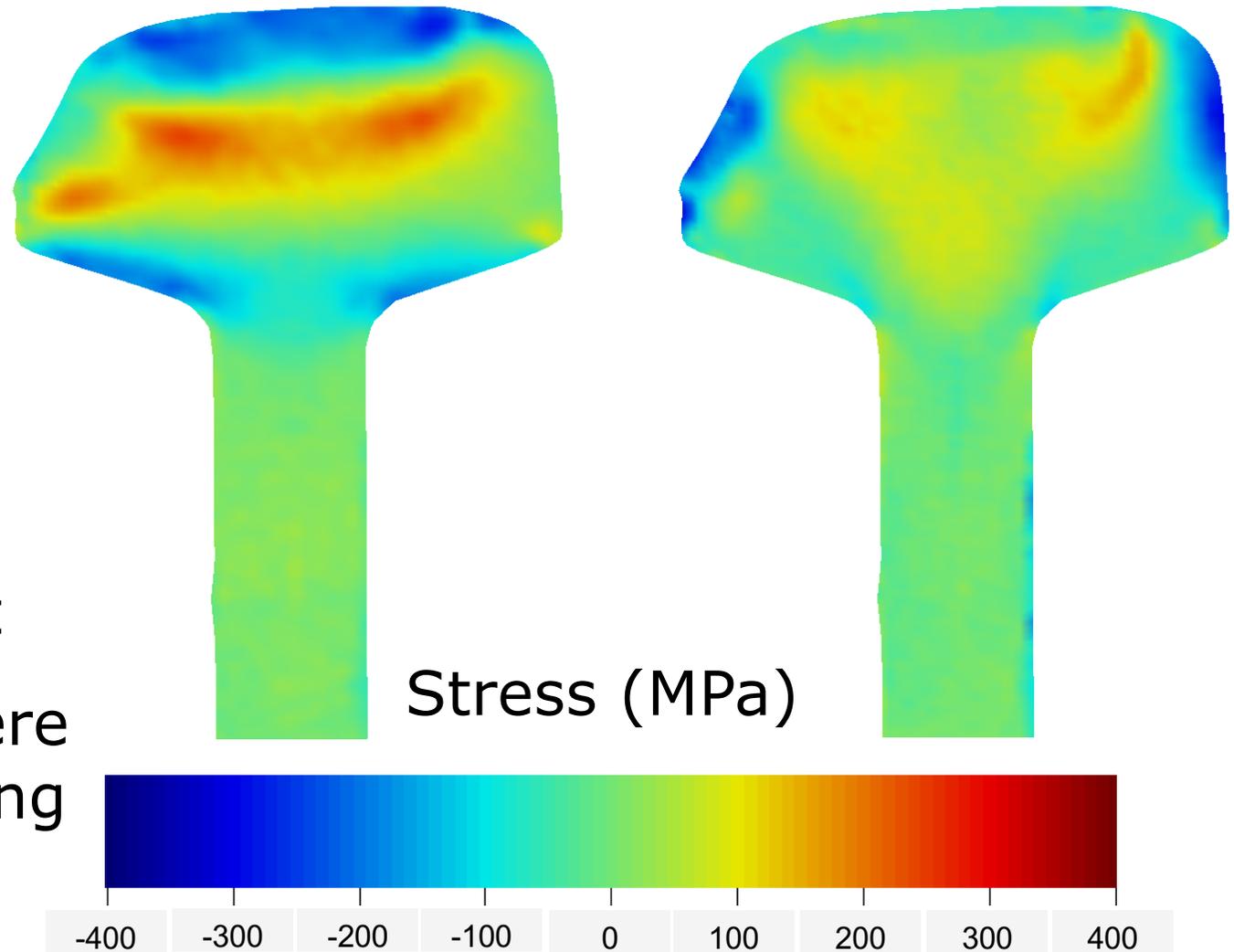
PWHT

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



# 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