The University of Manchester

17th Oxford School on Neutron Scattering
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Neutrons in Engineering

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Outline

- Neutron diffraction in engineering
- Stress, strain and residual stress
- Bragg’s Law
- Set-up of Engineering Instrument
- Diffraction methods available
- Residual stress measurement techniques
- Case Studies
- Conclusions on neutrons pros/cons

Introduction

Problem setting

Neutrons in Engineering

Neutron diffraction (ND) in engineering is typically used:

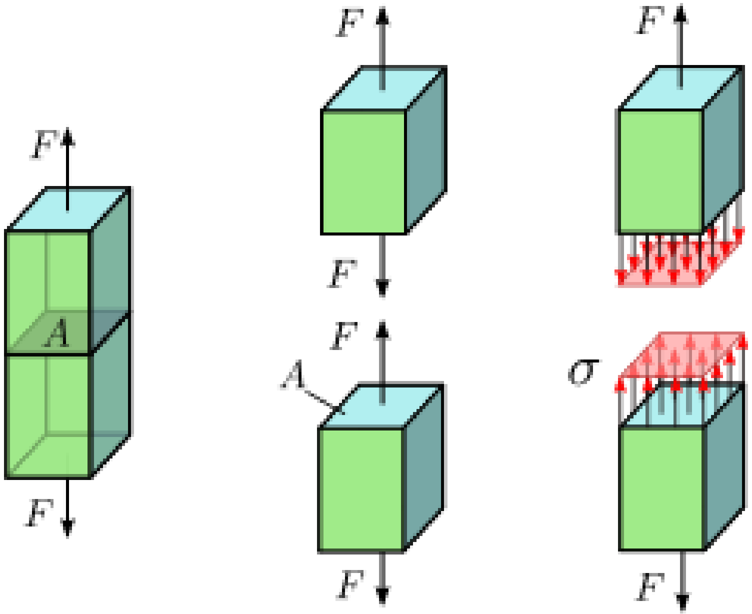
- to measure residual stress (RS),
- alteration/damage of the crystalline due to severe conditions,
- Deformation heterogeneity

But before…back to basic concepts and principles.

Stress, Strain

Basic Engineering Principles

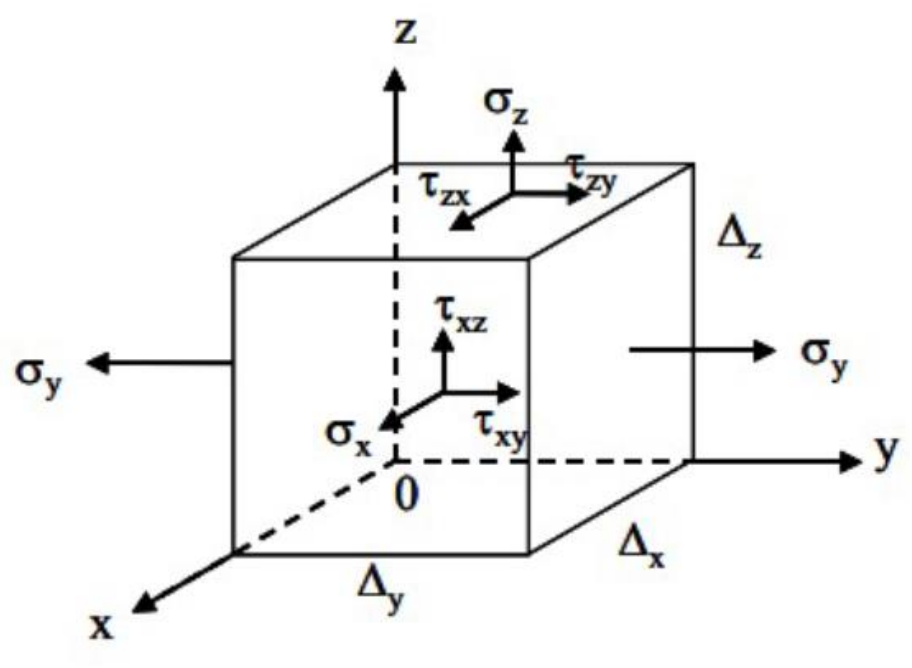
What is Stress?



$$\sigma = \frac{F}{A}$$

https://en.wikipedia.org/wiki/Stress_%28mechanics%29

Stress Types & Components



σ_x / σ_y / σ_z :

- **Normal** stress acting in the x/y/z direction.
- Acts on plane **perpendicular** to the x/y/z direction.

✓ positive values of normal stress → tensile stress

✓ negative values → compressive.

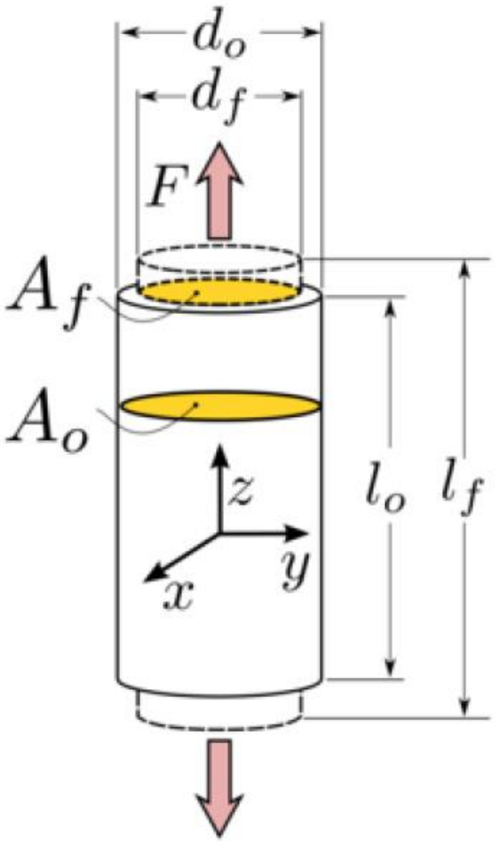
τ_{xy} / τ_{xz} / τ_{yz} :

- **shear** stress
- Acts on plane parallel to the x/y/z planes.

Can we measure Stress?

…. we can measure Strain!

What is Strain?



Engineering strain is captured by:

$$e = \frac{l_f - l_o}{l_o}$$

True strain is captured by its rate of change:

$$d\varepsilon = \frac{dl}{l}$$

$$\varepsilon = \int_{l_o}^{l} \frac{dl}{l} = \ln\left(\frac{l_f - l_o}{l_o} + 1\right)$$

$$\varepsilon = \ln(e + 1)$$

From Strain to Stress

- Hooke's Law
- $\sigma = E\varepsilon$ (simple uniaxial tension/compression)
- 3D equation (tensor form)

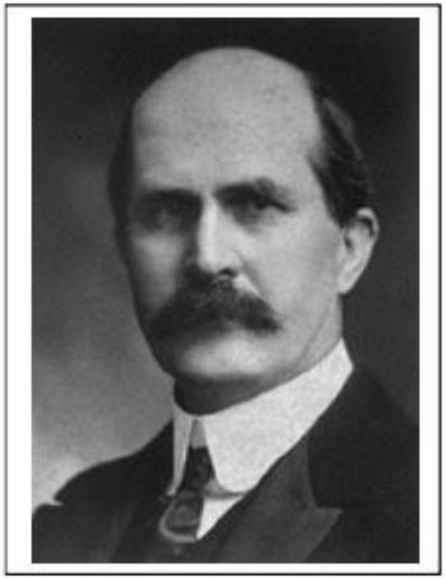
$$\begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{23} \\ \sigma_{13} \\ \sigma_{12} \end{bmatrix} = \frac{E}{(1+\nu)(1-2\nu)} \begin{bmatrix} 1-\nu & \nu & \nu & 0 & 0 & 0 \\ \nu & 1-\nu & \nu & 0 & 0 & 0 \\ \nu & \nu & 1-\nu & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1-2\nu}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1-2\nu}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1-2\nu}{2} \end{bmatrix} \begin{bmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ 2\varepsilon_{23} \\ 2\varepsilon_{13} \\ 2\varepsilon_{12} \end{bmatrix}$$

Assuming isotropic material

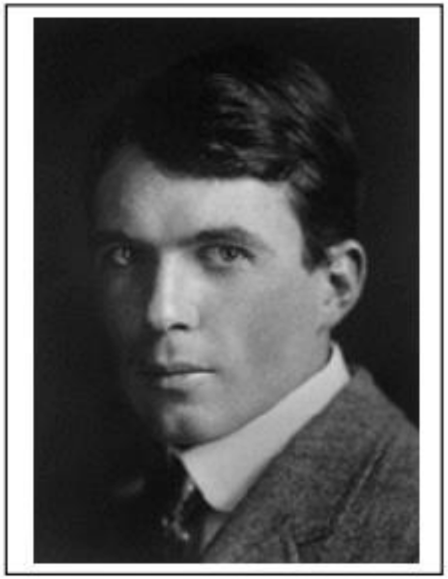
Bragg’s Law!

Diffraction Basic Principles

The Braggs



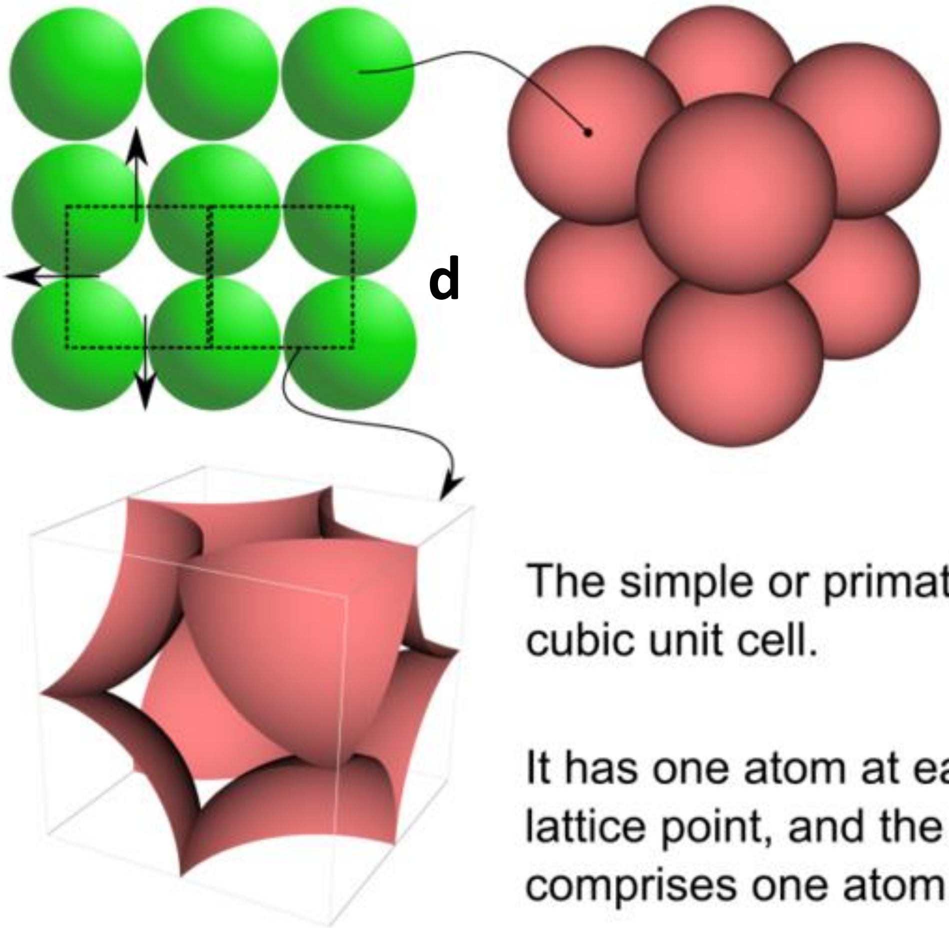
W.H. Bragg
(1862–1942)



W.L. Bragg
(1890–1971)

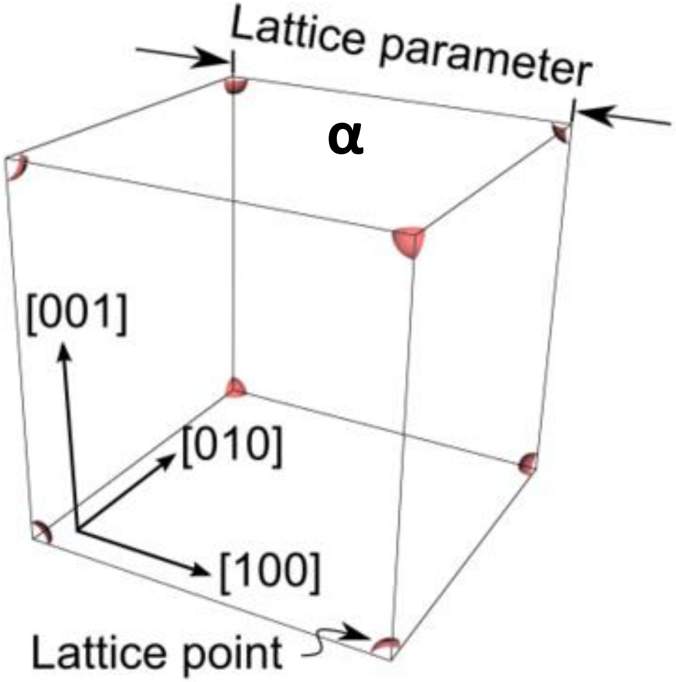
Nobel Prize in Physics (1915)

Unit cell, d spacing, lattice parameter α



The simple or primative cubic unit cell.

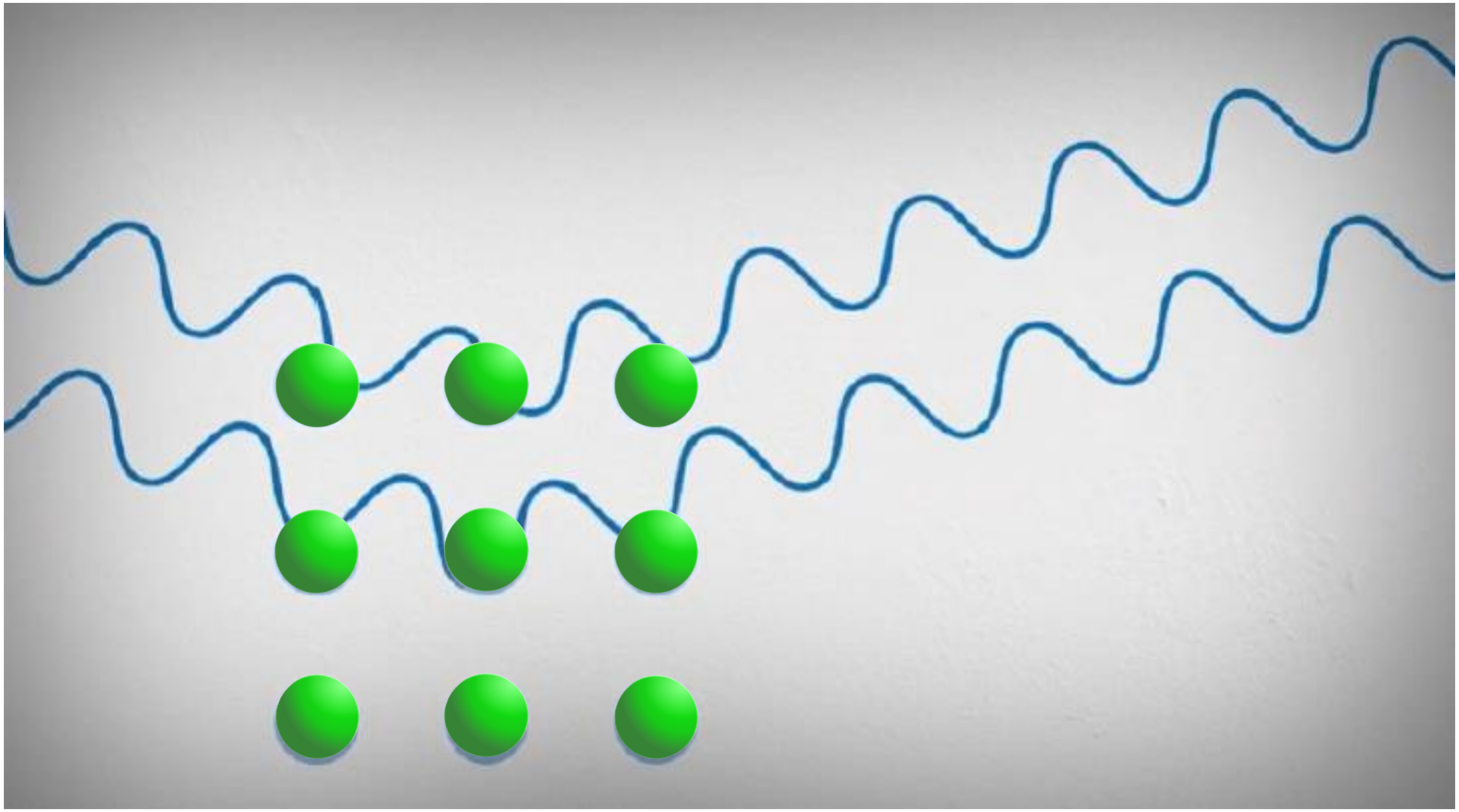
It has one atom at each lattice point, and the cell comprises one atom.



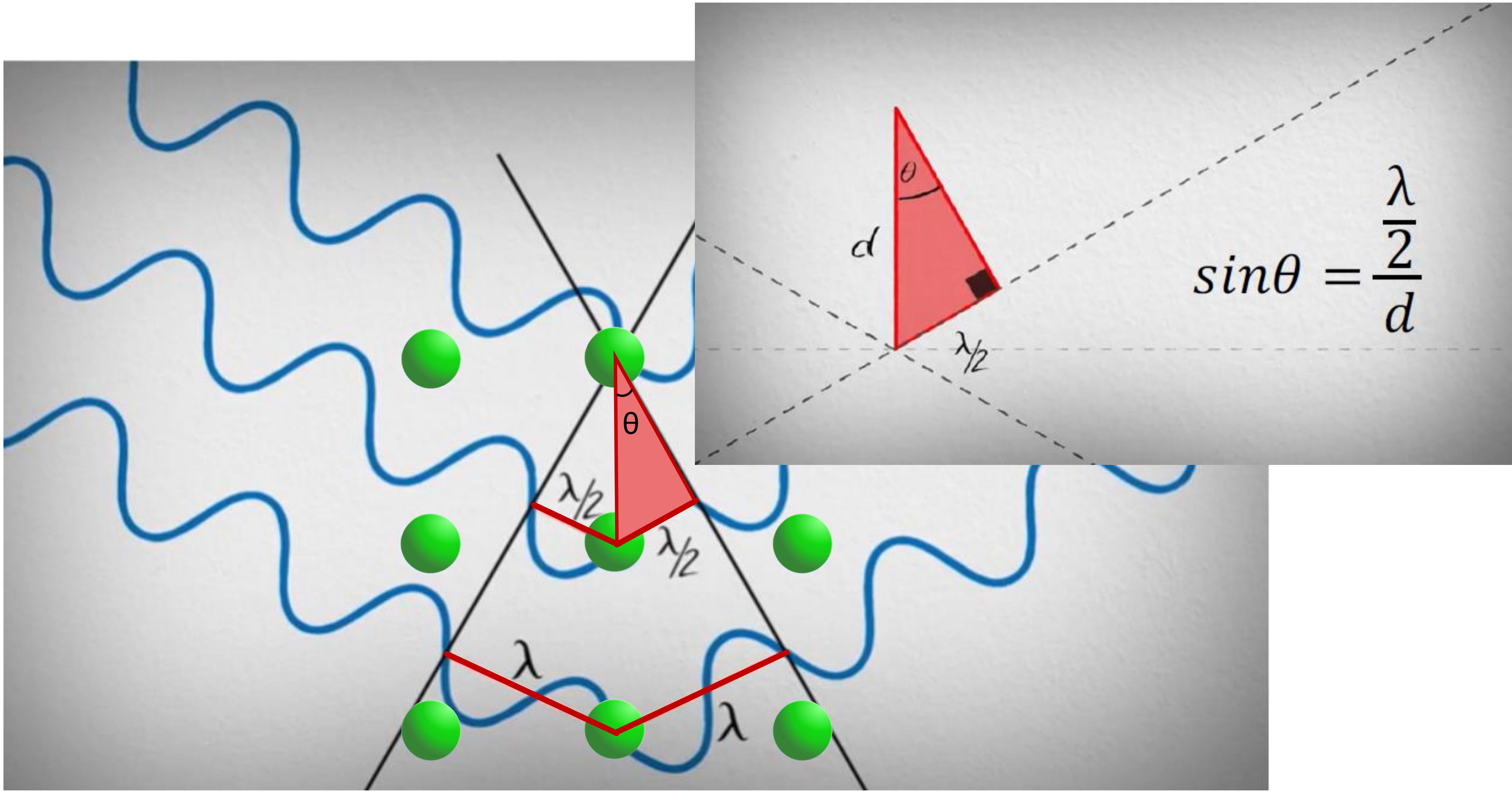
The unit cell is the smallest *repeating unit* in a crystal structure.

(2020, M.J. Roy) Materials 1, Teaching material, The University of Manchester

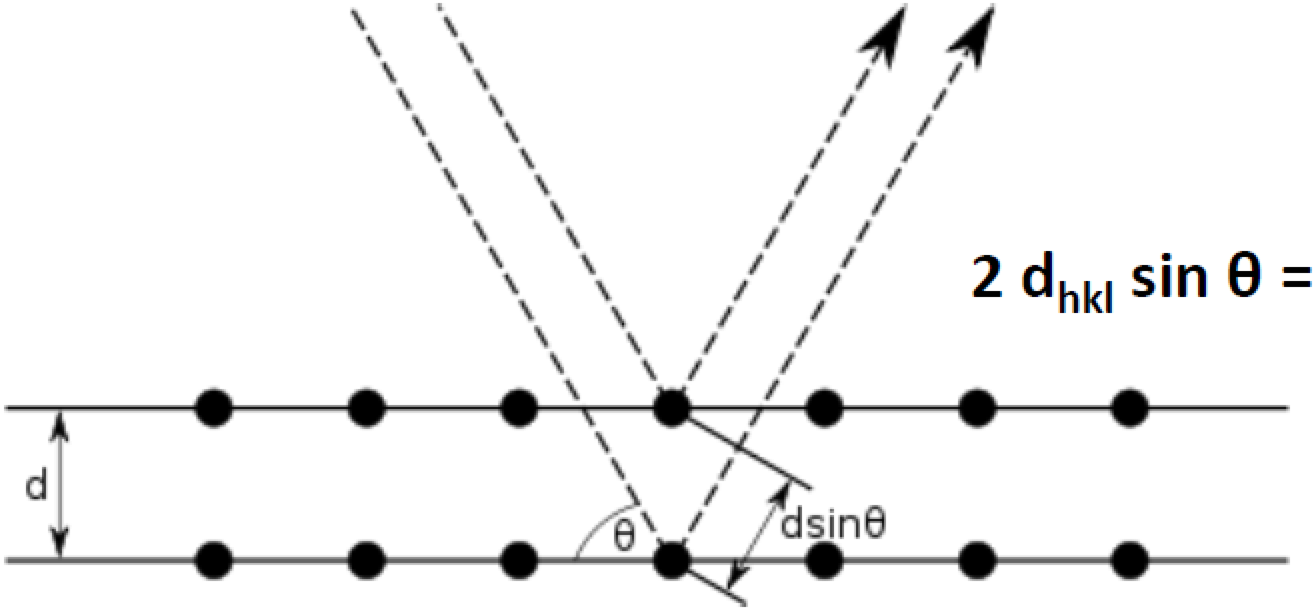
Bragg’s Law



Bragg's Law



Bragg's Law



$2\, d_{hkl} \sin\theta = n\,\lambda$

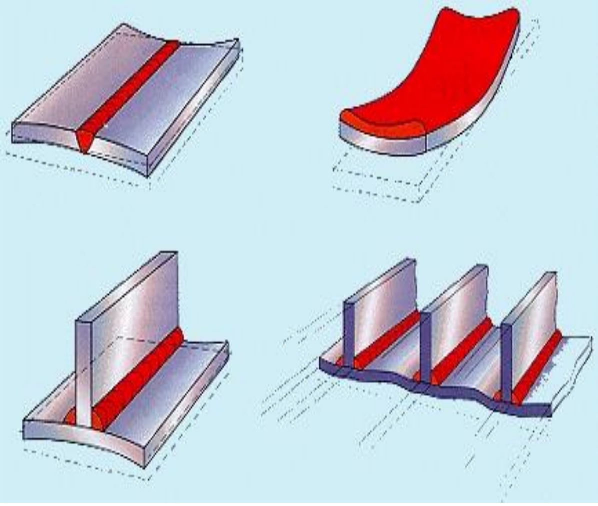
λ : the wavelength of the incident radiation (fixed in most diffractometers)
d_{hkl} : the distance between the (hkl) planes (geometric function of the size and shape of the unit cell)
θ : the incident angle (the angle between the planes and the incident beam)
n : the diffraction order (integer)

Residual Stress

Definition

What is Residual Stress?

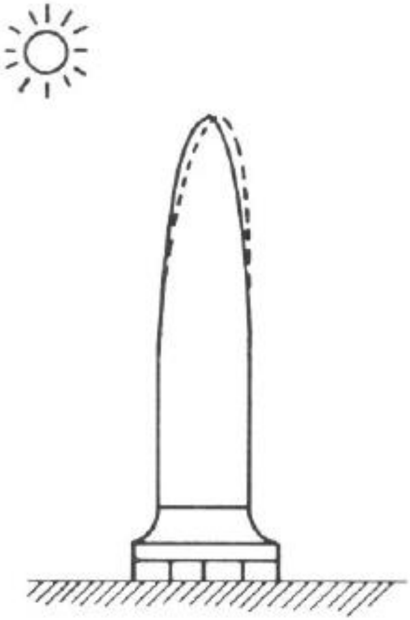
Residual stresses: Stresses that **remain** in a solid material after the original cause of the stresses has been removed.



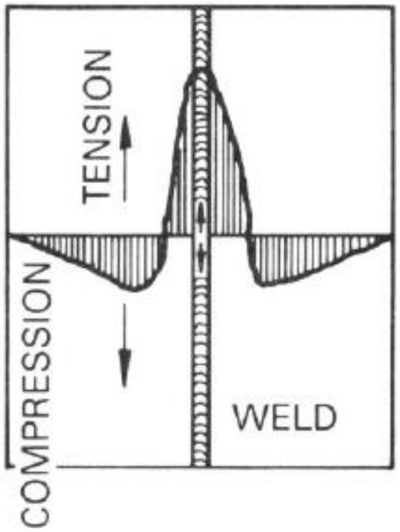
Occur through various mechanisms:

- Plastic deformations
- Temperature gradients (thermal cycle)
- Structural changes (phase transformations)

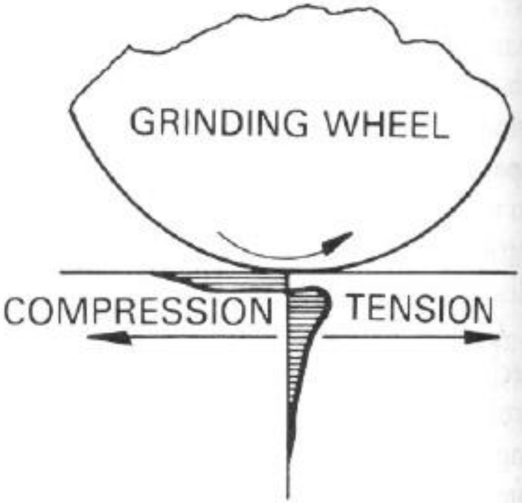
Examples of Residual Stress



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



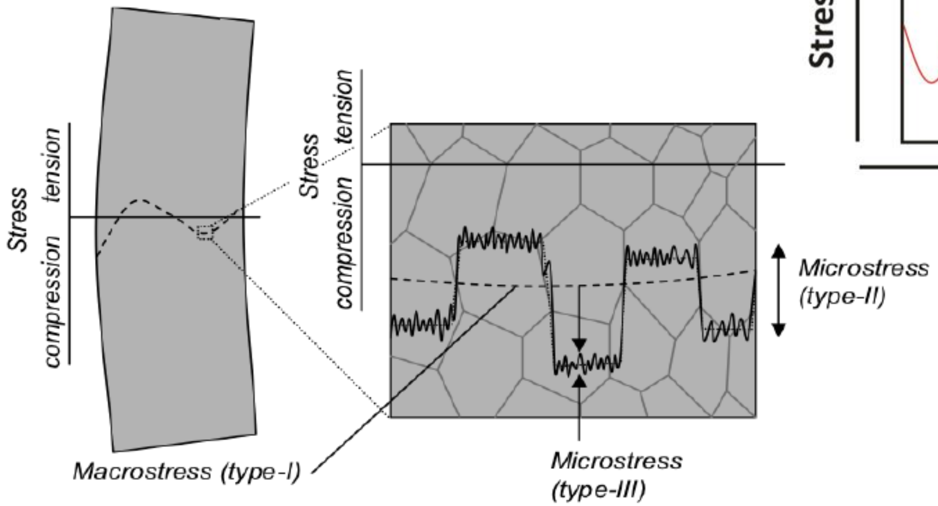
(B) Residual Stresses Due to Welding



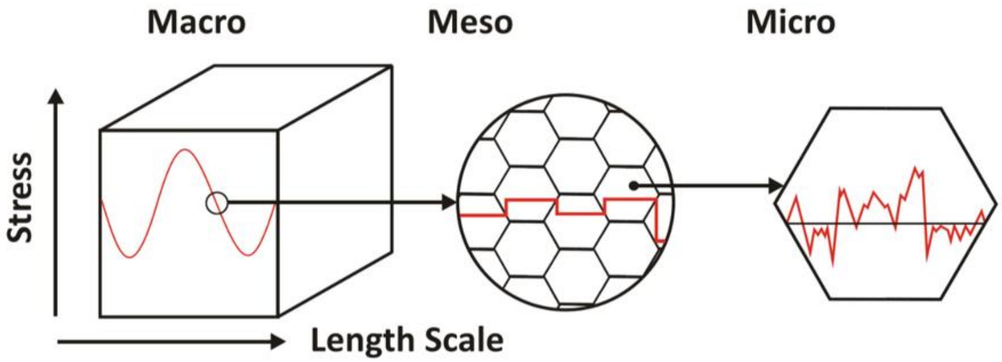
(C) Residual Stresses Due to Grinding

Residual Stress Types

- TYPE I (long range over multiple grains, macrostresses)
- TYPE II (intergranular, vary between grains, microstresses)
- TYPE III (atomic level)



Bent Bar



Internal stresses
Caused by a misfit

Why care about Residual Stress?

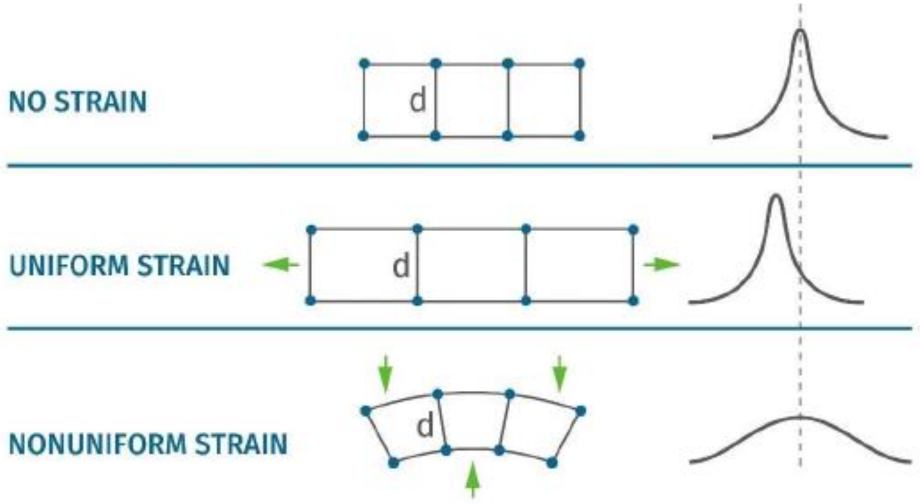
- Play a significant role in affecting the long-term structural performance.
- Can contribute to the driving force for crack growth.
- Can activate degradation mechanisms such a creep and stress-corrosion cracking, even in the absence of operating stresses.
- Cause deformation *(distortion, dimensional accuracy).*

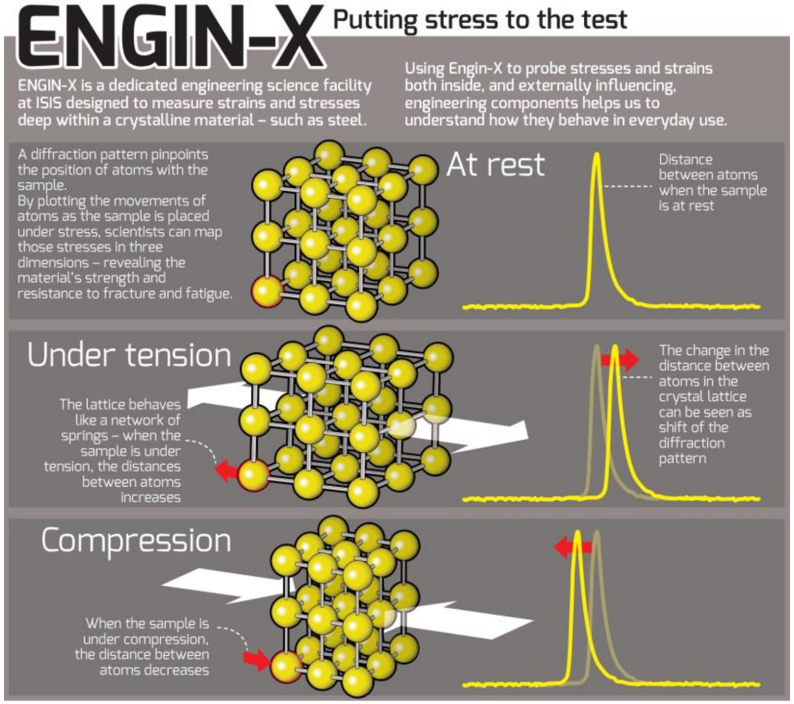
Diffraction for Measuring Residual Stress

Overview

Effect of elastic strain on diffraction signal

- When measuring residual stress, we actually measure residual STRAIN!! *(stress is strain energy density)*
- Diffraction measures elastic lattice strain as **peak shifts**
- Uses the poly-crystalline lattice planes as internal strain gauges




ENGIN-X Putting stress to the test

ENGIN-X is a dedicated engineering science facility at ISIS designed to measure strains and stresses deep within a crystalline material – such as steel.

Using Engin-X to probe stresses and strains both inside, and externally influencing, engineering components helps us to understand how they behave in everyday use.

A diffraction pattern pinpoints the position of atoms with the sample.
By plotting the movements of atoms as the sample is placed under stress, scientists can map those stresses in three dimensions – revealing the material's strength and resistance to fracture and fatigue.

At rest

Distance between atoms when the sample is at rest

Under tension

The lattice behaves like a network of springs – when the sample is under tension, the distances between atoms increases

The change in the distance between atoms in the crystal lattice can be seen as shift of the diffraction pattern

Compression

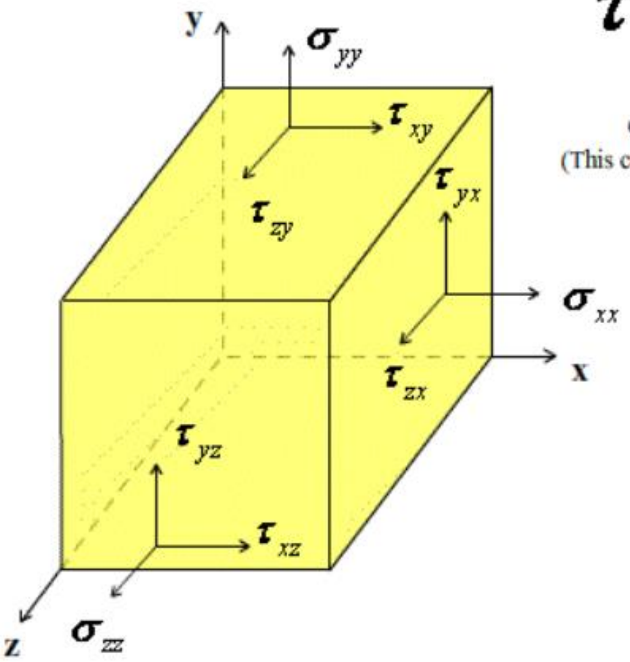
When the sample is under compression, the distance between atoms decreases

Data Analysis Workflow

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

Data Analysis Workflow

- 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!)

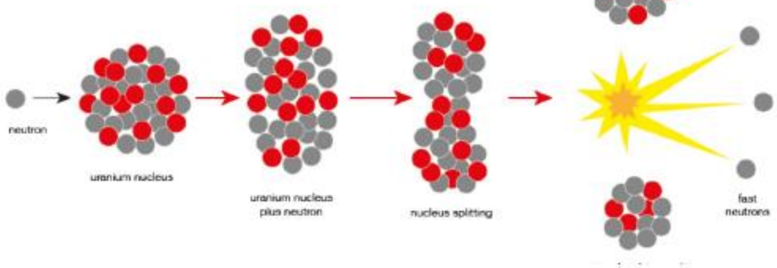
Types of neutron sources

Overview, set-up, typical examples

Neutron Sources

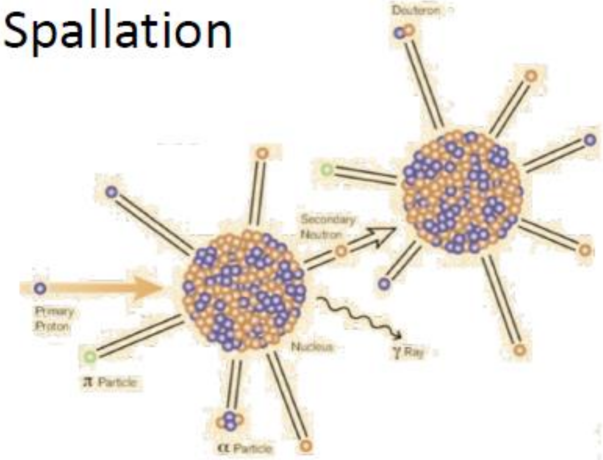
- **Reactor-based (steady state/continuous)**
  - Slow neutron capture of 235 U
  - Constant wavelength/Single Peak
  - Fission source

Fission



- **Short-pulse spallation (pulsed)**
  - Nuclei bombarded with high energy particles
  - Accelerator Sources
  - Time-of-flight (ToF) / Full Spectra / Riet

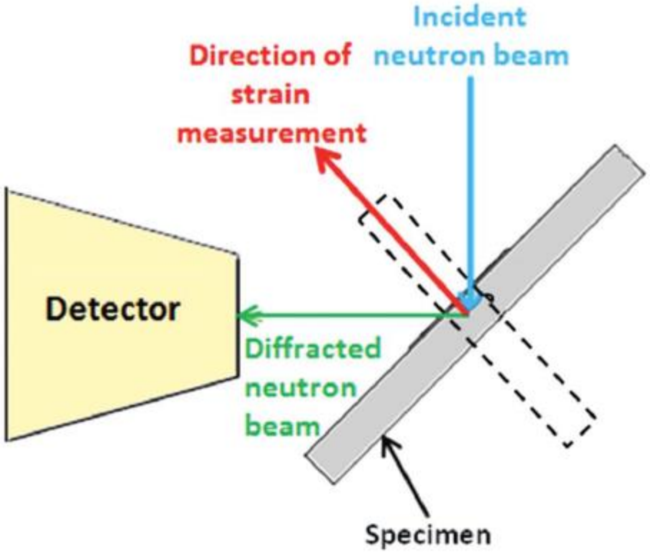
Spallation



Monochromatic vs ToF

Monochromatic (CW)

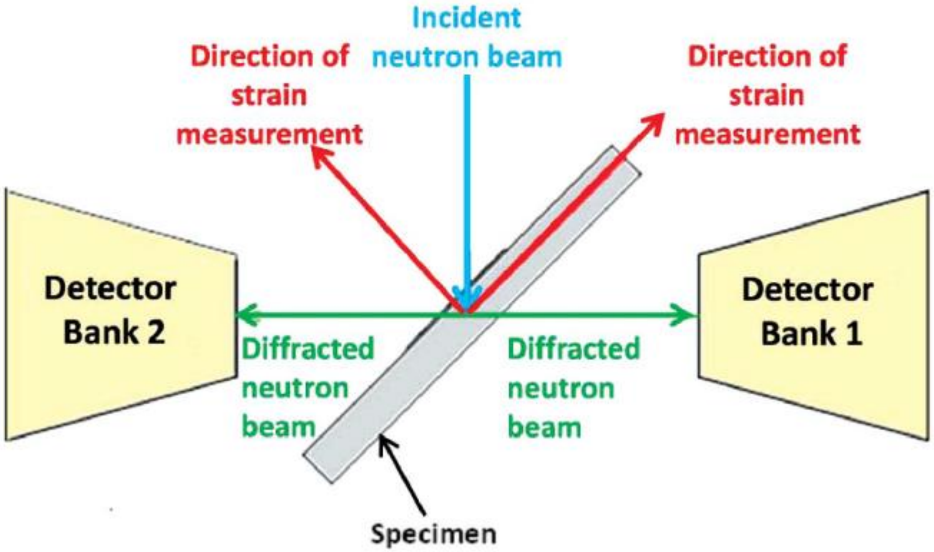
- Fix wavelength and scan detector angle
- Multiple 2θ required to cover Q(d) spacing range
- Q(d) spacing limit 4π/λ (2π/d)
- Instrumental count rate factors: Source power, monochromator reflectivity, detector coverage and efficiency, etc



Diffraction
angle
90°

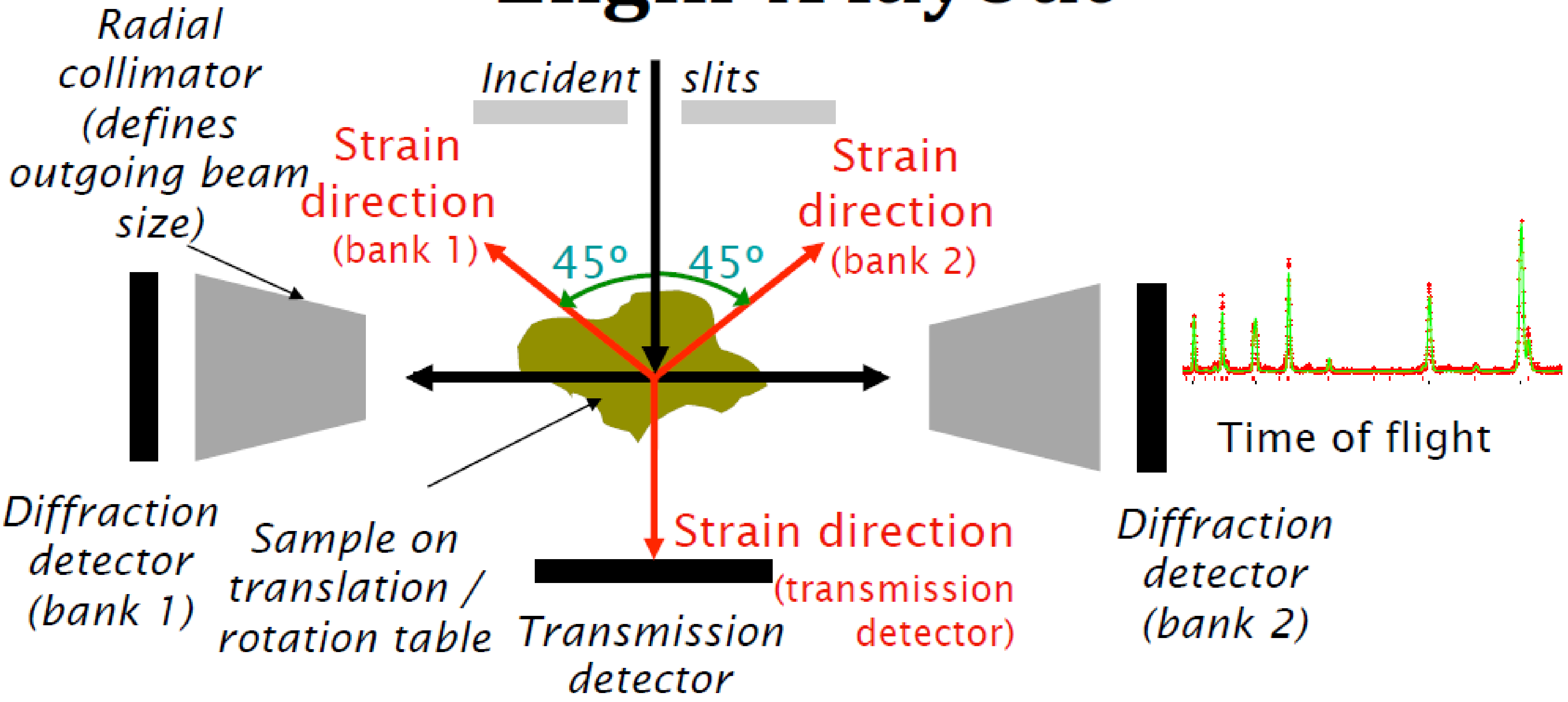
Time of Flight (ToF)

- Fix detector angle and scan wavelength
- Single 2θ covers range of Q(d) space
- Q(d range) determined by λmax, λmin and θ
- Instrumental count rate factors: Source power, moderator performance, beam transport efficiency, detector coverage and efficiency, etc



Set-up of Engineering Instrument: Spallation/ToF

Engin-X layout



Radial collimator (defines outgoing beam size)

Incident slits

Strain direction (bank 1)

45°

45°

Strain direction (bank 2)

Time of flight

Diffraction detector (bank 1)

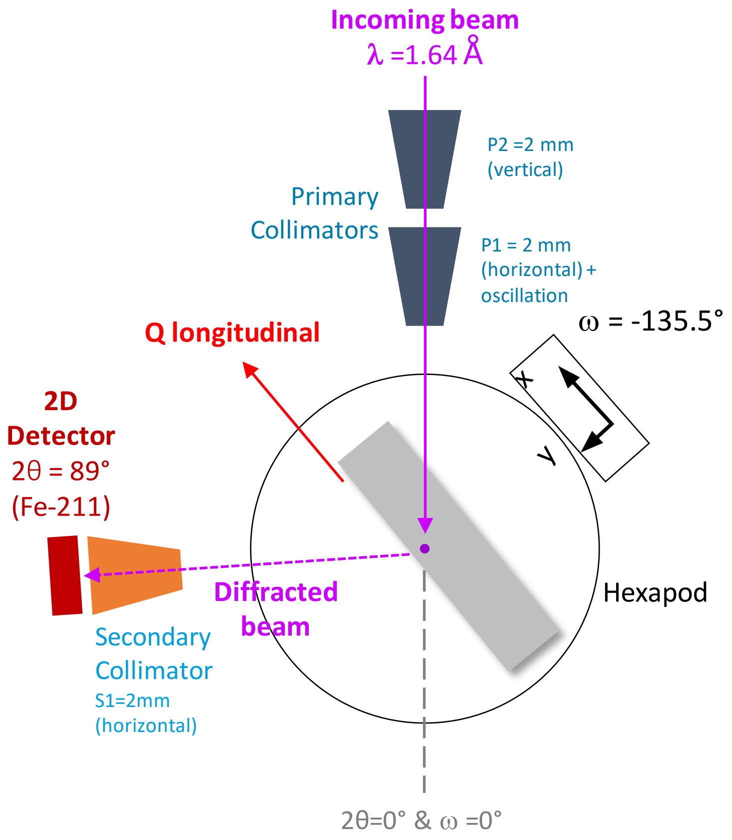
Sample on translation / rotation table

Strain direction (transmission detector)

Transmission detector

Diffraction detector (bank 2)

Set-up of Engineering Instrument: Reactor-based



Incoming beam

λ =1.64 Å

Primary Collimators

P2 =2 mm (vertical)

P1 = 2 mm (horizontal) + oscillation

ω = -135.5°

Q longitudinal

2D Detector

2θ = 89° (Fe-211)

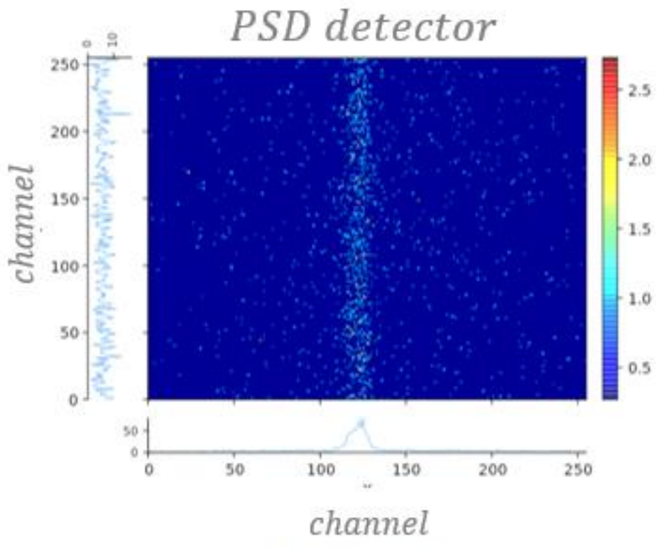
Diffracted beam

Secondary Collimator

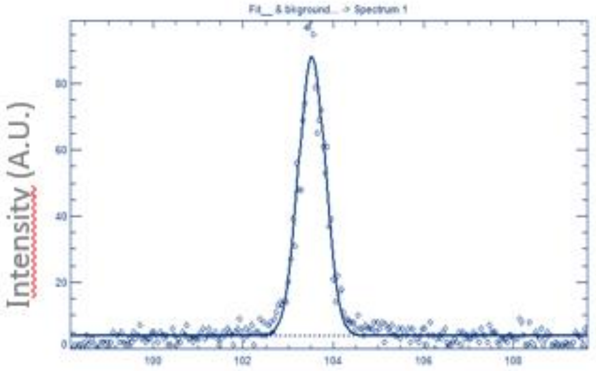
S1=2mm (horizontal)

Hexapod

2θ=0° & ω =0°



PSD detector



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NEUTRONS FOR SOCIETY

Research Reactors

- http://neutronsources.org/

Europe (25)

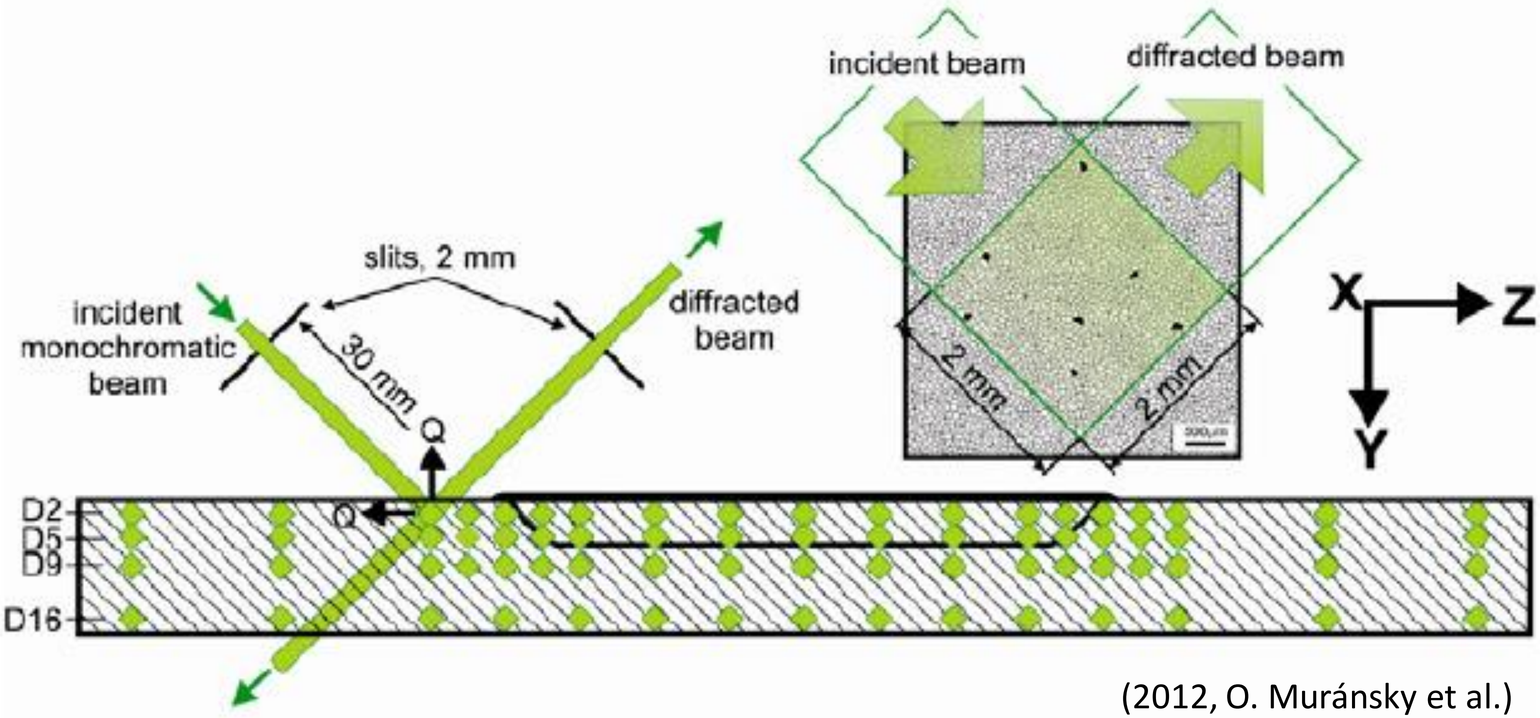
Americas (9)

Asia-Oceania (12)

Africa (1)

The gauge-volume

ND set-up & gauge volume



(2012, O. Muránsky et al.)

doi:10.1016/j.ijsolstr.2011.07.006

The schematic drawing of the neutron diffraction geometry, the positions of measuring points on the D plane (along the weld centerline, see Fig. 2(a)), and the gauge volume depicting a random number of grains satisfying the diffraction condition (black grains

General Overview: Diffracting Gauge Volume

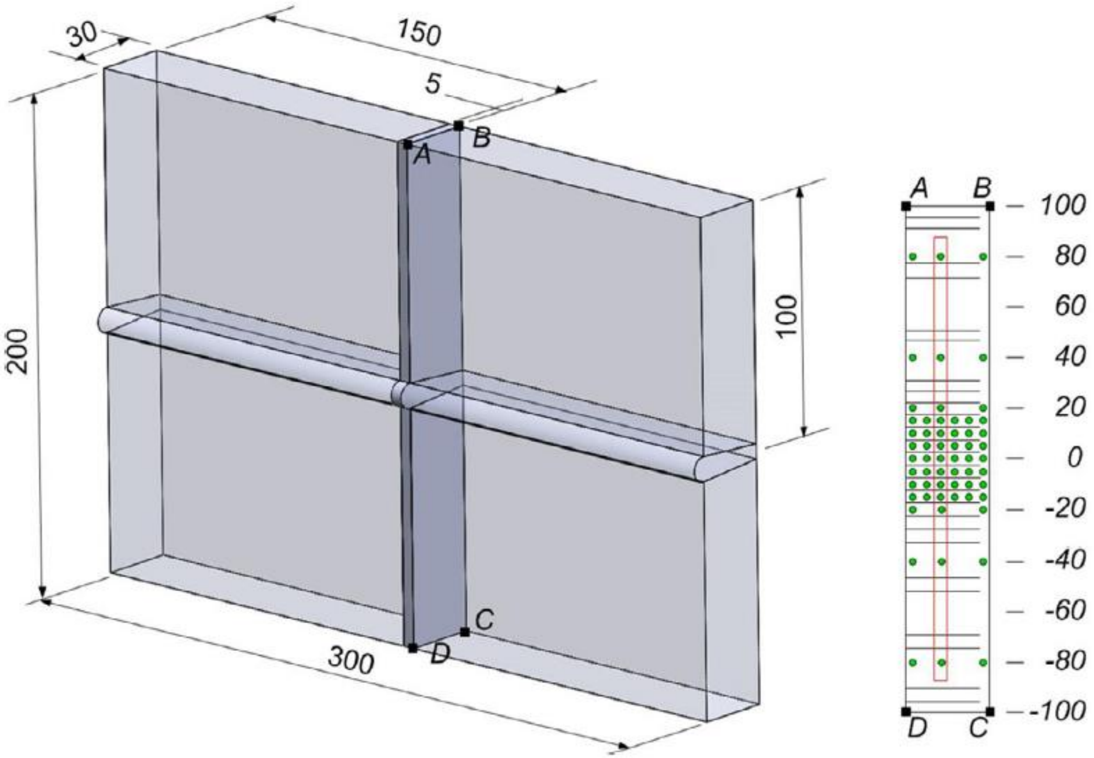
Volume element of the material in which the recorded scattering takes place

- 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

The d0 specimen

d0 samples

- **Comb**
- Pins
- Slice



d0 samples

- Comb
- **Pins**
- Slice

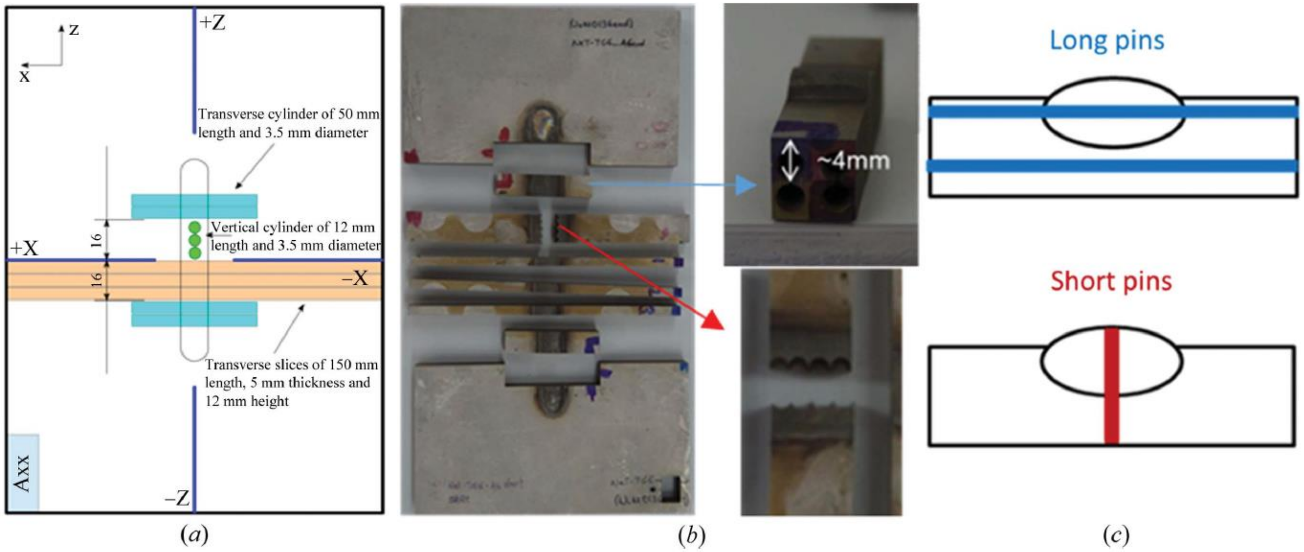
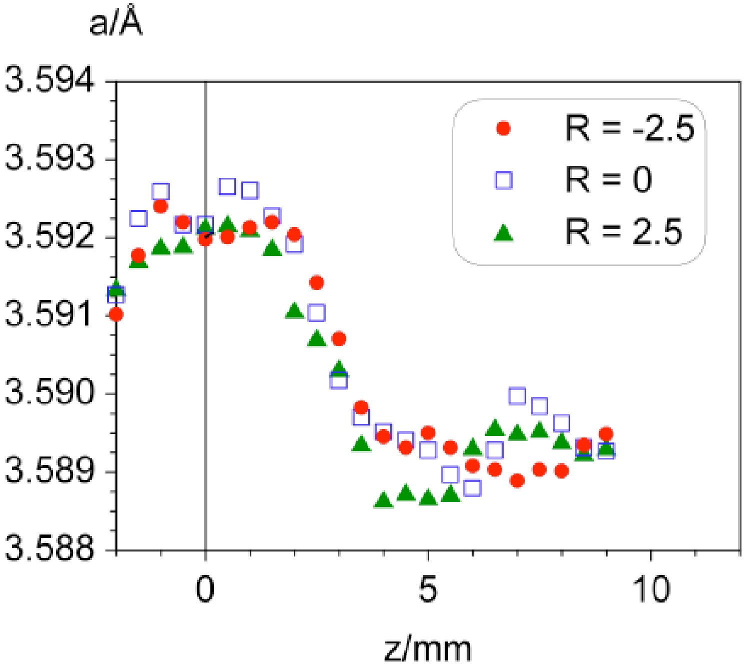


Figure 4
(*a*) The cutting plan for extraction of reference specimens from the A6, TG6 specimen (Ohms *et al.*, 2015). (*b*) The A6 specimen after extraction of the stress-free pins and slices. (*c*) The exact locations of the extracted pins used as stress-free reference samples.

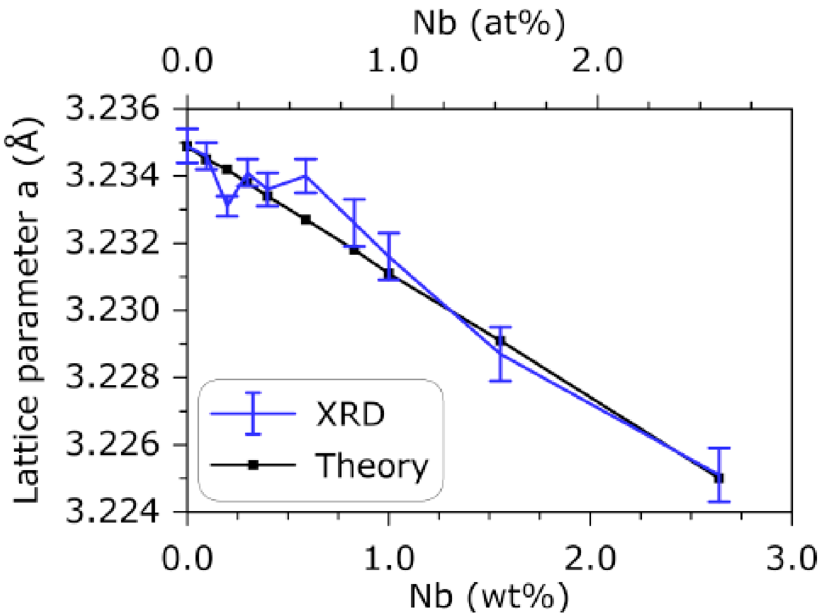
d0 variation

Accurate strain analysis relies on accurate determination of d_0

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



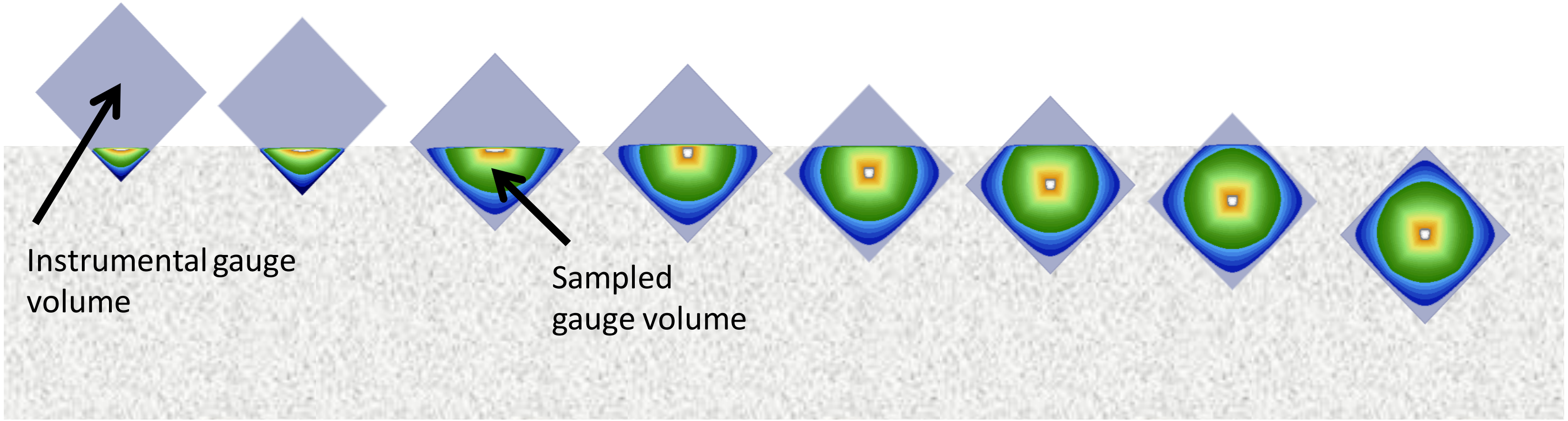
Example of d_0 variation across a tubular Nickel weld



The Vegard Law
Example: Nb in Zr

Near surface

Near surface measurements



Instrumental gauge volume

Sampled gauge volume

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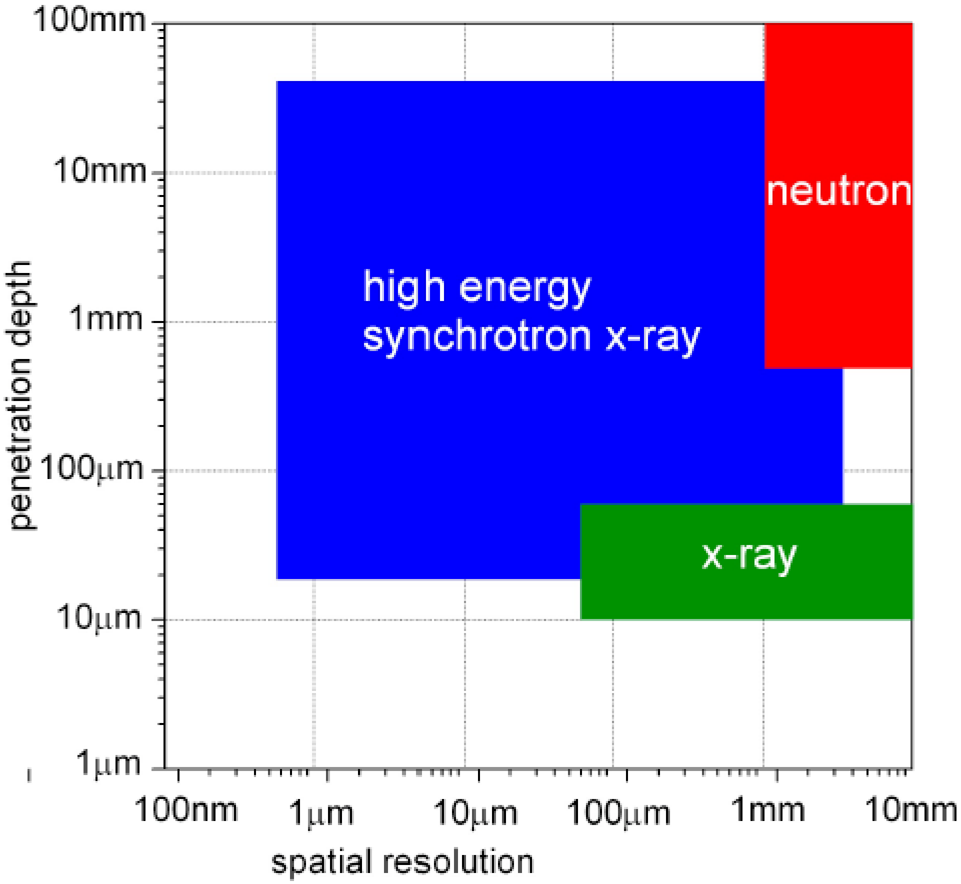
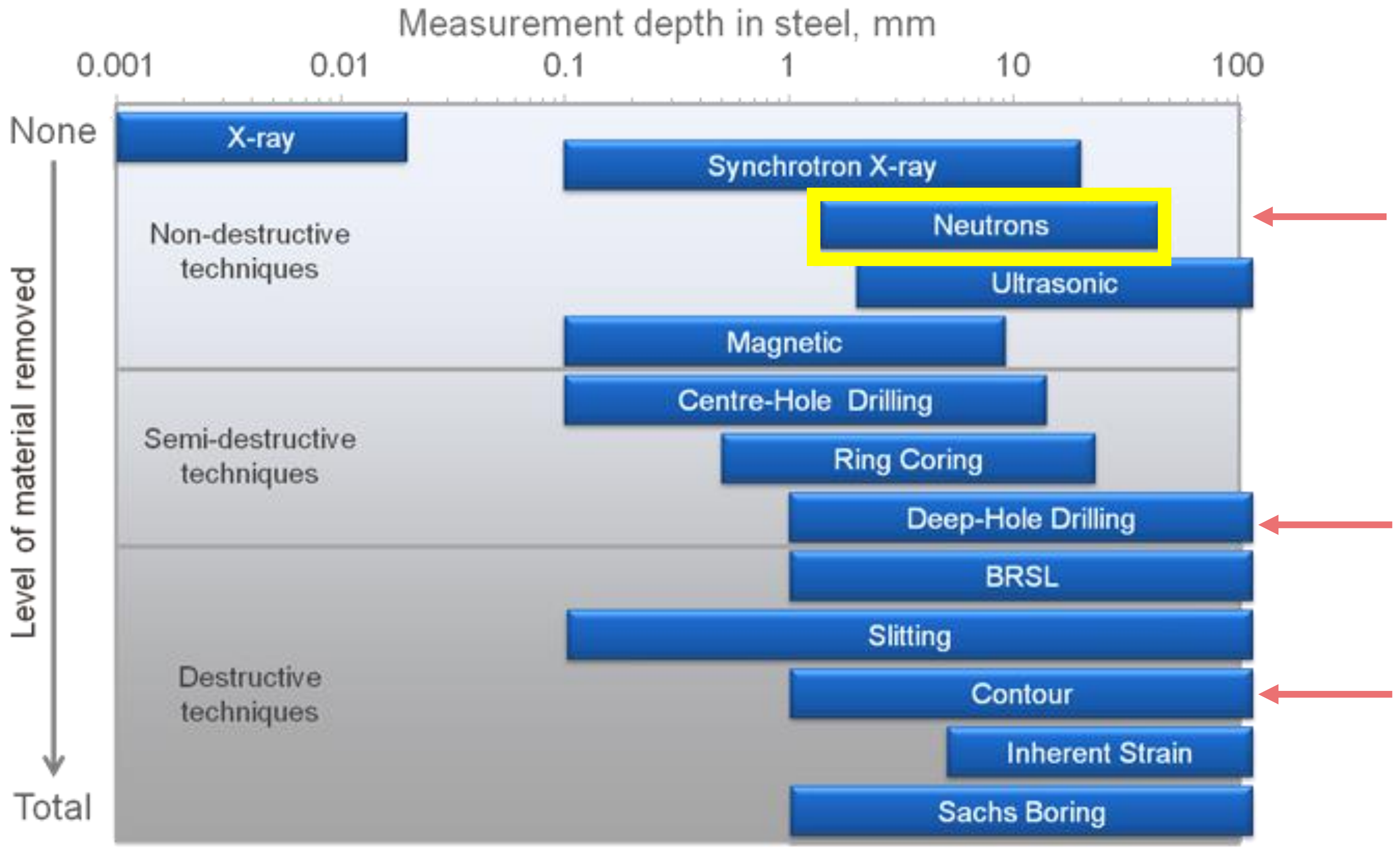
Neutrons vs Other measurement techniques

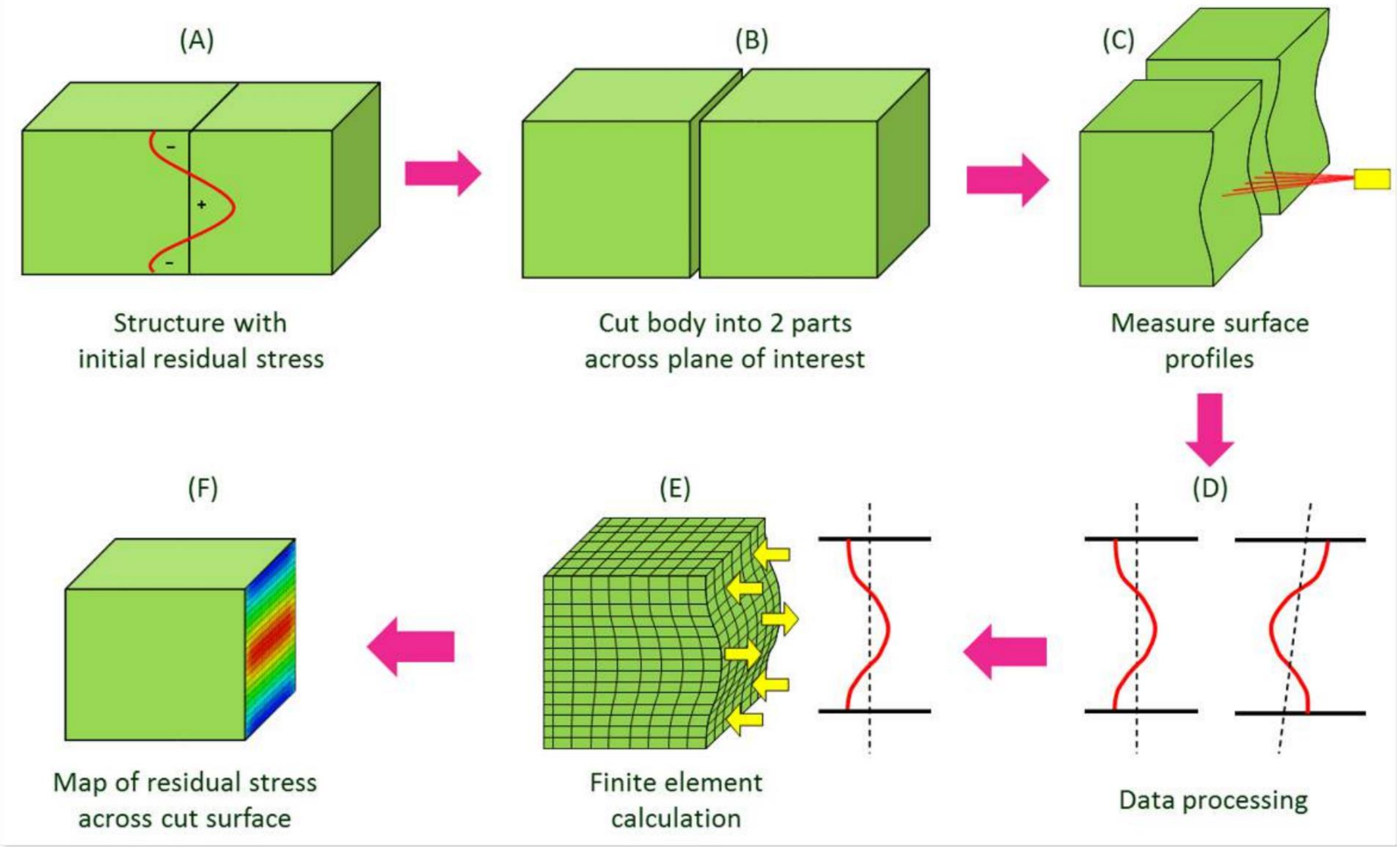
ND vs other diffraction methods



ND vs Other Residual stress measurement techniques



The Contour Method



Structure with initial residual stress

Cut body into 2 parts across plane of interest

Measure surface profiles

Data processing

Finite element calculation

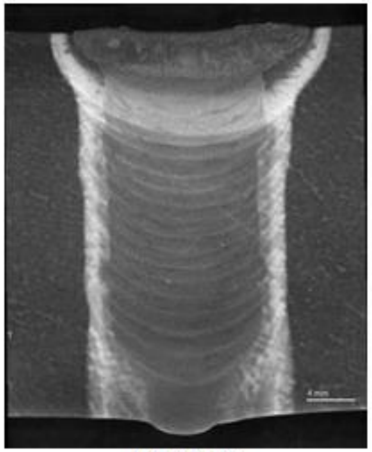
Map of residual stress across cut surface

Case Studies

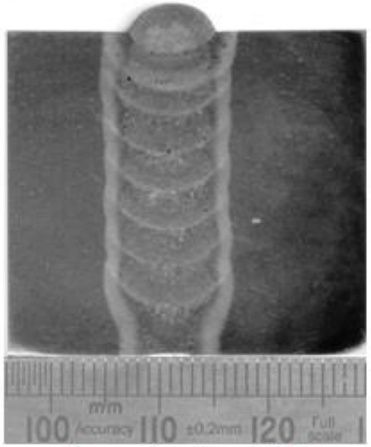
Challenges, considerations and implications

Case study: Cross process comparison – NNUMAN welds

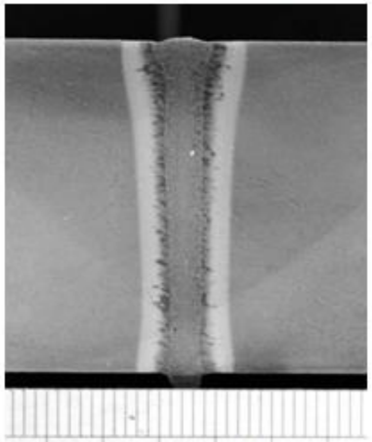
NG-SAW
(18 passes, 2 passes per layer)



NG-GTAW
(25 passes, one weaved pass per layer)



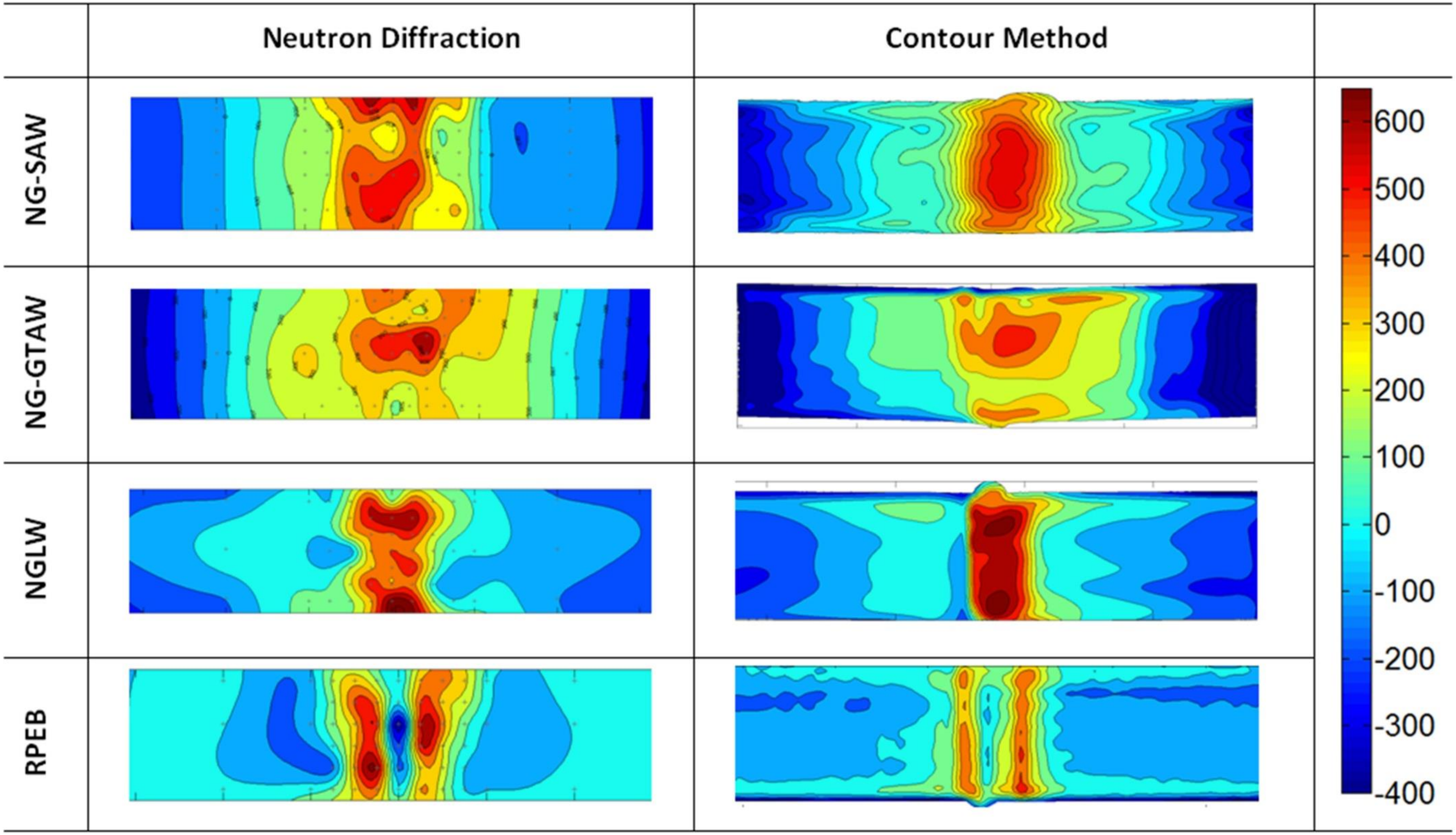
Narrow-Gap Laser Weld
(autogenous root pass, 8 filling passes)



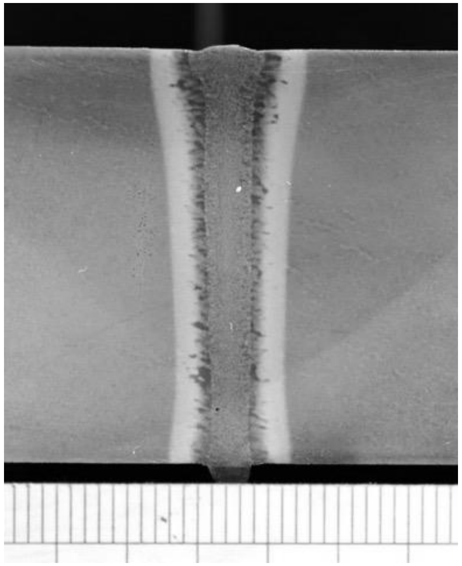
RPEB weld
(single autogenous pass)

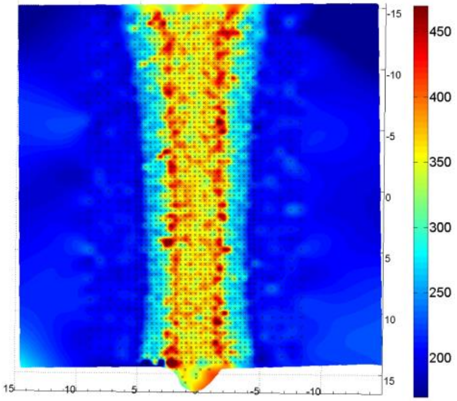
(2018, J. Balakrishnan et al.)
doi:10.1016/j.ijpvp.2018.03.004

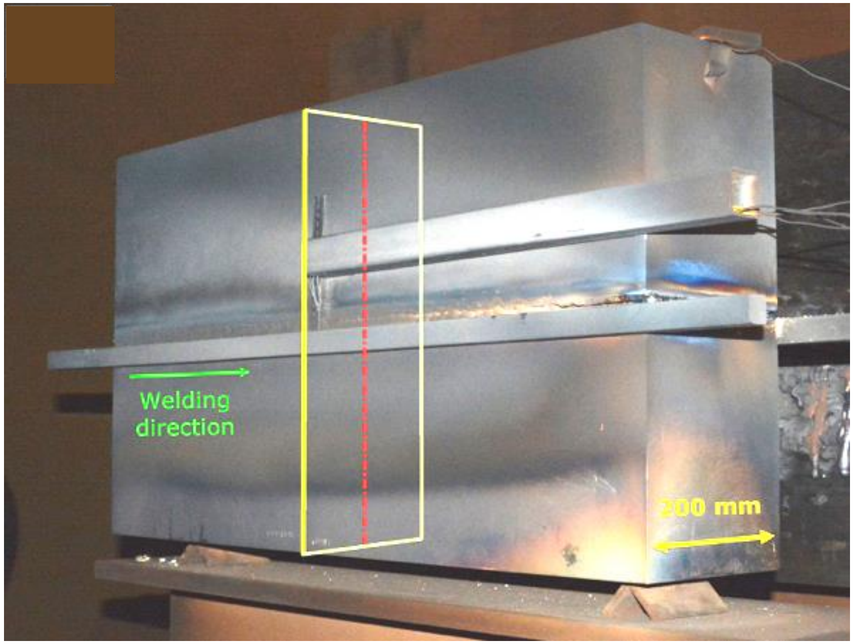
ND *vs* CM

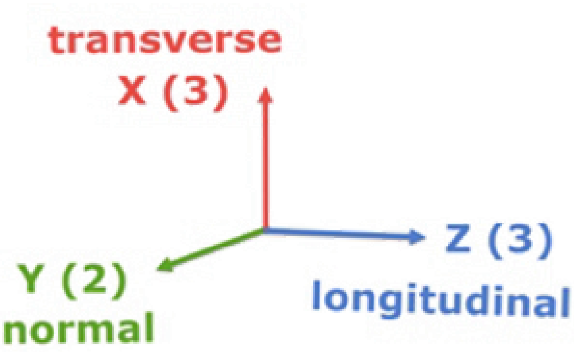

Neutron Diffraction
Contour Method
NG-SAW
NG-GTAW
NGLW
RPEB
600
500
400
300
200
100
0
-100
-200
-300
-400

Case study: EB welds









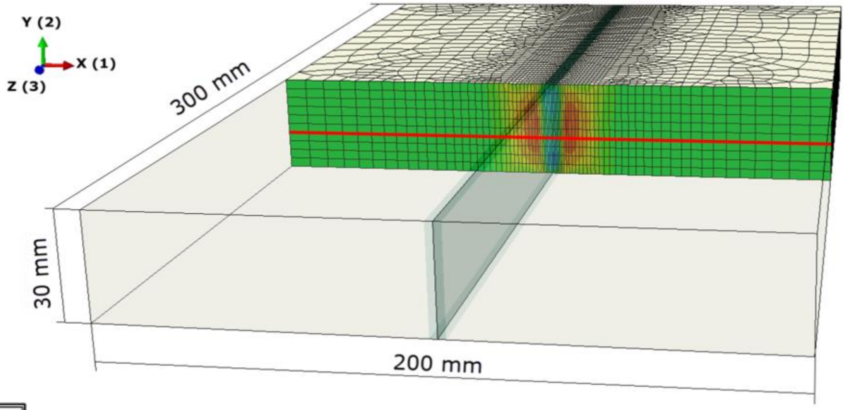
transverse
X (3)

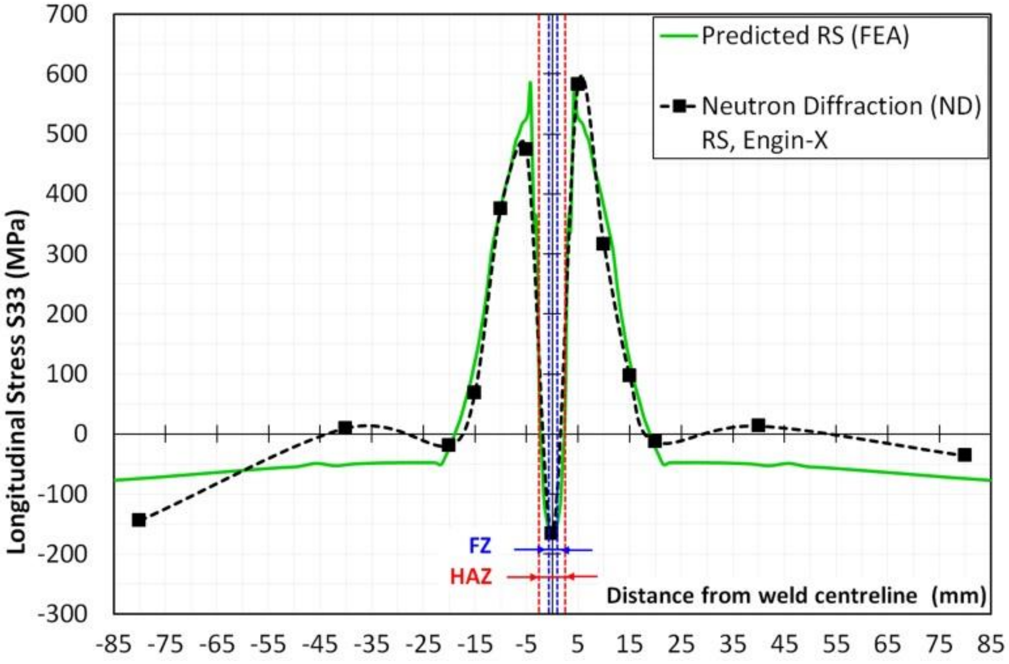
Y (2)
normal

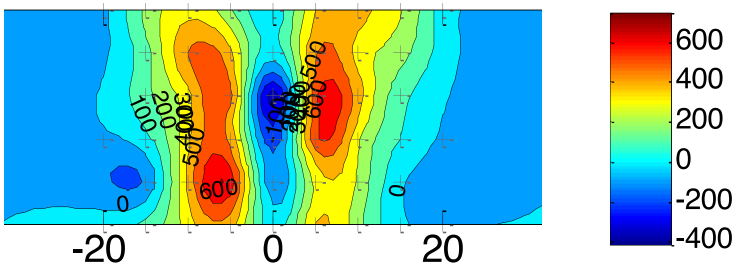
Z (3)
longitudinal

Case study: EB welds

- Challenge: short characteristic length of residual stress distribution

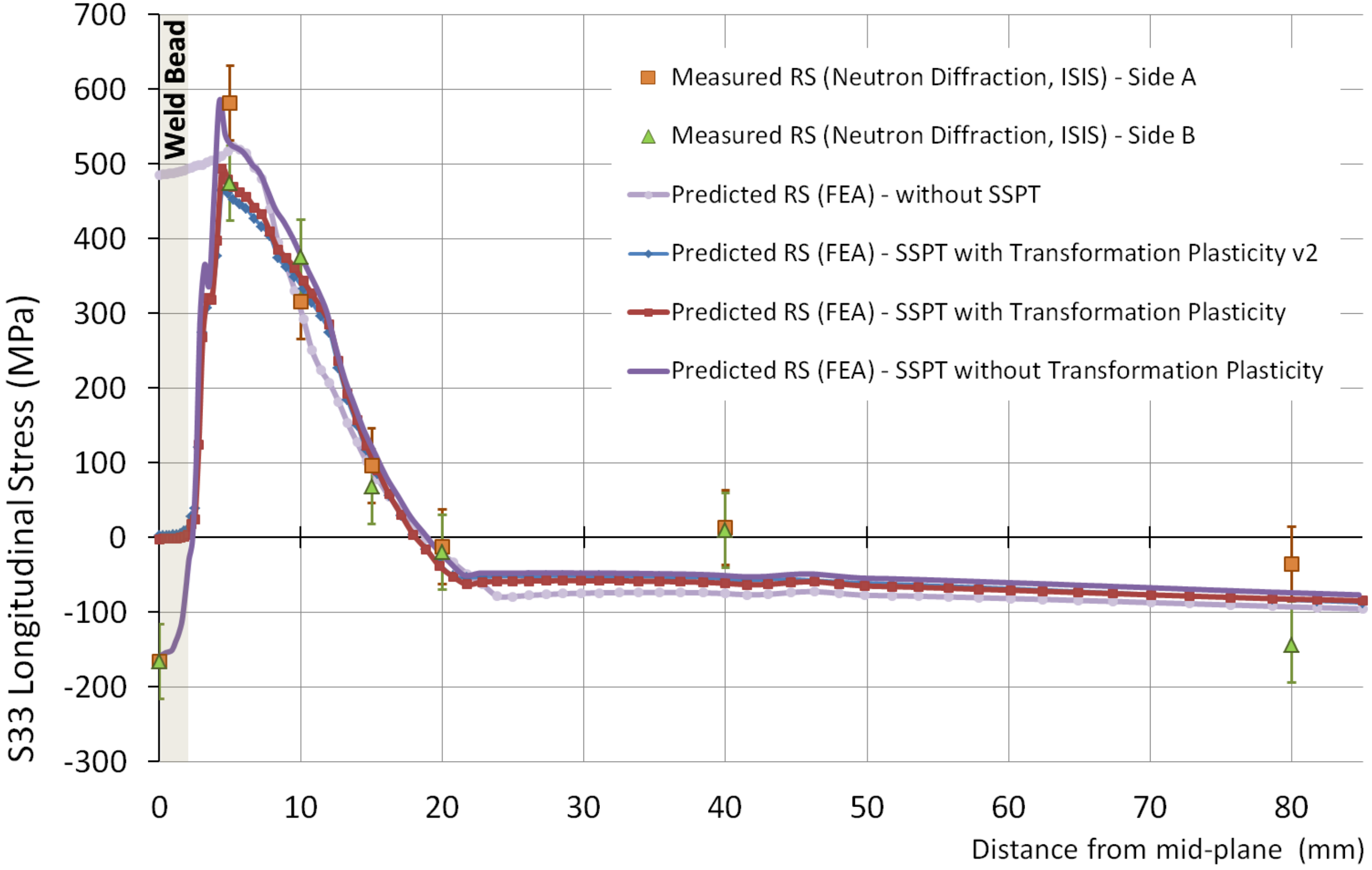






Case study: EB welds

- ND vs FE weld modelling predictions



Case study: the NeT network

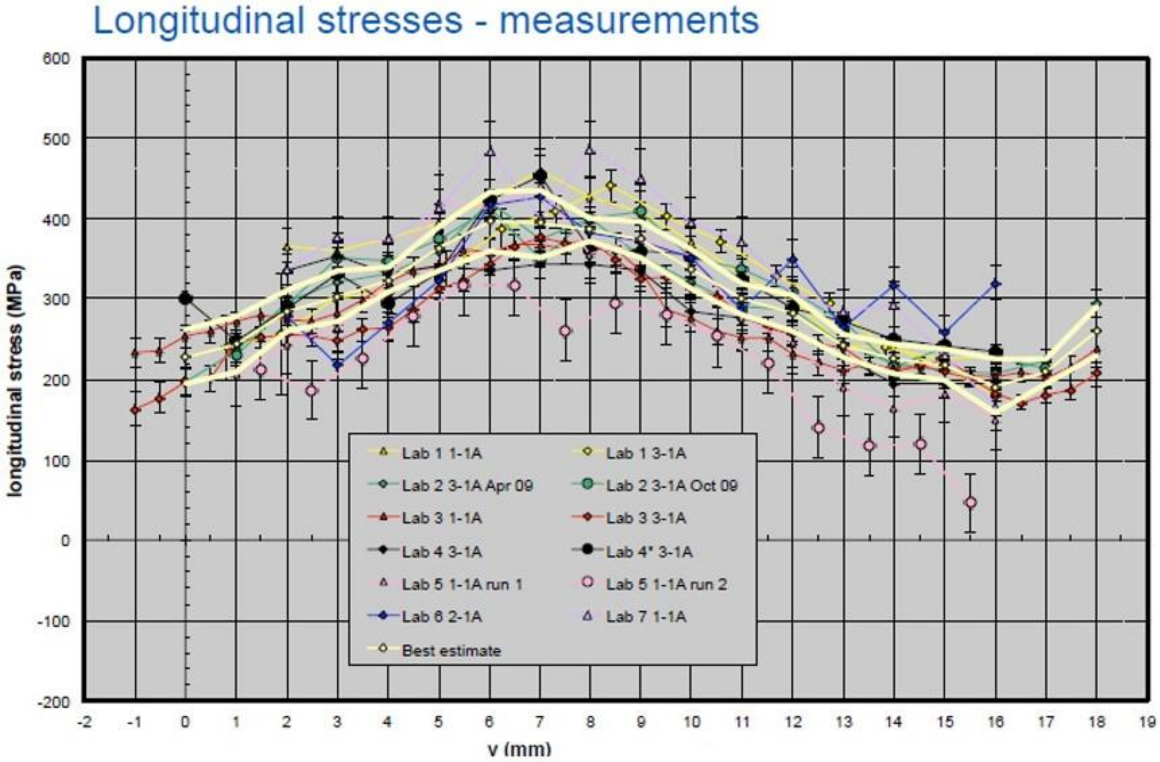
NeT

Network on Neutron Techniques Standarization
for Structural Integrity

- Mission of the Network: to develop experimental and numerical techniques and standards for the reliable characterization of residual stresses in structural welds.
- https://www.net-network.eu
- ISO Draft International Standard 21432:2018

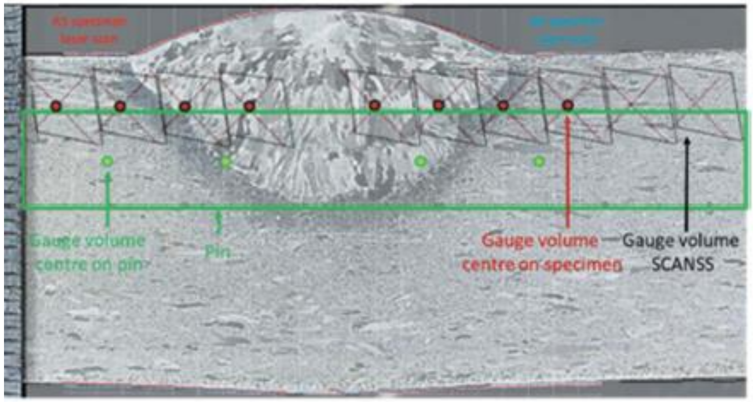
Case study: NeT-TG4

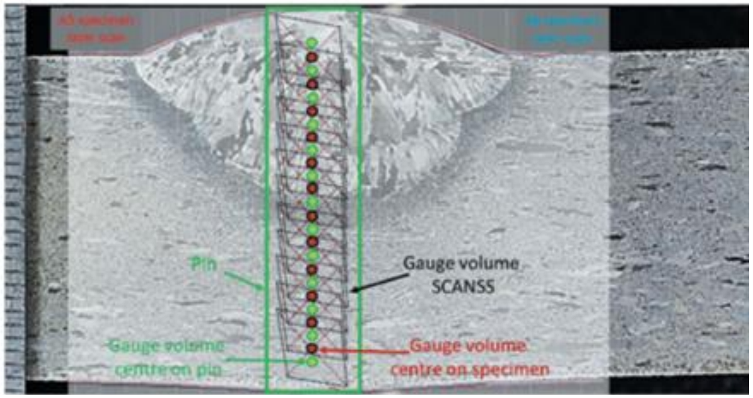
- Repeatability and standardization

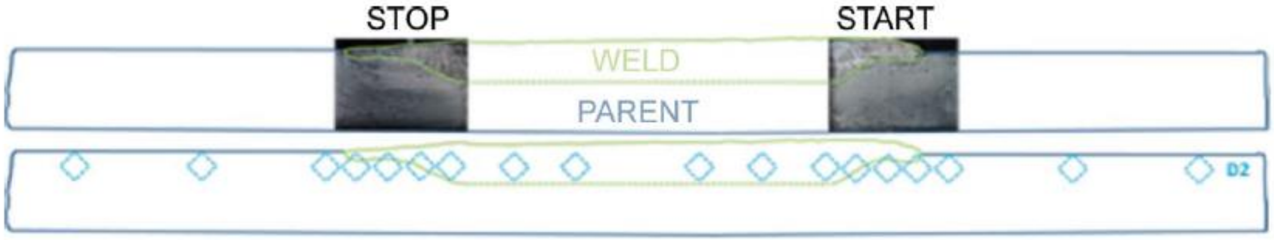


Case study: NeT-TG6

- Dissimilar metals
  - Alloy 600 parent plate
  - Alloy 82 filler wire
- Implication
  - **Interfaces**: how to properly process the data? *[Considering that the gauge volume includes both]*
  - **Misalignments** get critical



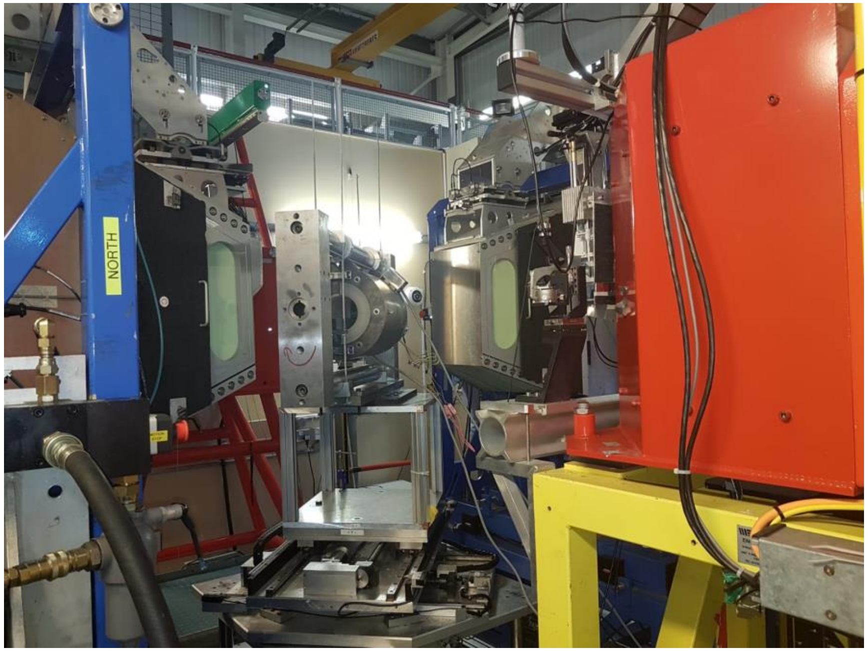




(2020, V. Akrivos et al.)
doi:10.1107/S1600576720009140

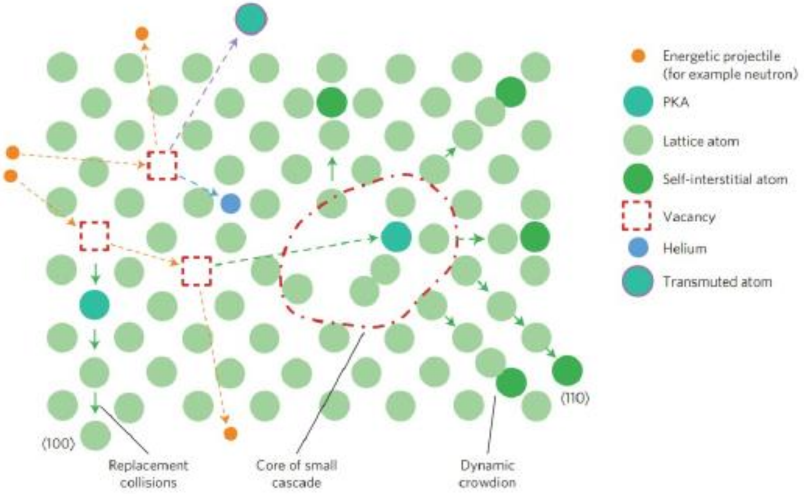
Case study: in-situ PWHT

- In-situ post-weld heat treatment
- Considerations: count time vs evolution of phenomenon



Case study: Irradiation damage

- Lattice defects introduced by irradiation
  - dislocations
  - crystallographic changes
  - changes to secondary phases in the material (amorphisation, dissolution, change in type of particles)



- All these changes can be assessed by diffraction techniques!

Concluding remarks

Neutrons:

- Non-destructive, full stress analysis
- Good penetration depth due to neutrality
- Big bulky sample with low stress gradients
- Variety of materials can be measured (Steels, aluminium, nickel, copper zinc or related)

Not-so good (handle with care): near surface or thin materials, texture (titanium, boron cadmium), high-spatial resolution/steep gradients, high instrumental resolution

Any questions?

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