Elastic Constants

Their Significance in Residual Stress Measurement and Their Experimental Determination

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27 September 2023

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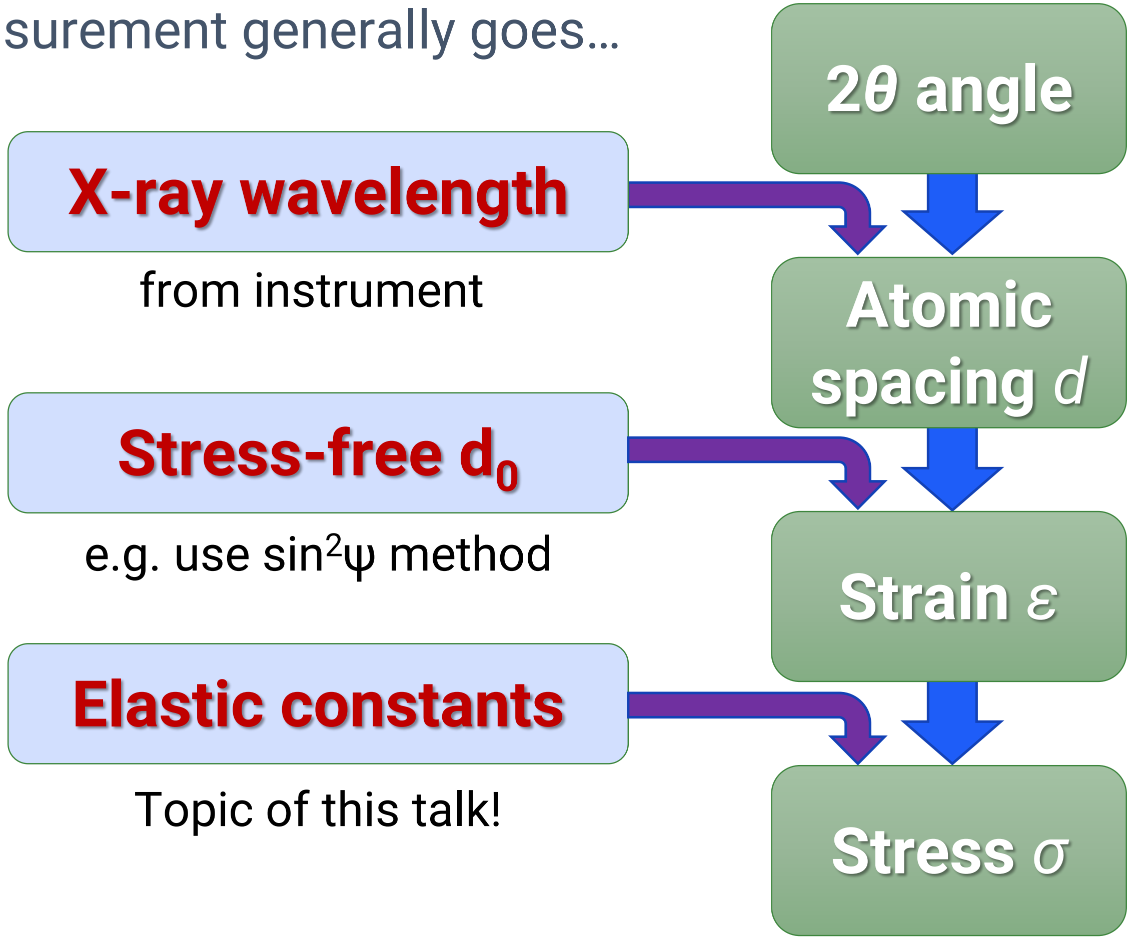
The need for elastic constants

- X-ray stress measurement generally goes…
- …for which we need some information…



2θ angle

Atomic spacing d

Strain ε

Stress σ

X-ray wavelength

from instrument

Stress-free d_0

e.g. use $\sin^2\psi$ method

Elastic constants

Topic of this talk!

- Elastic constants allow stress to be found from strain or length measurements
- Function of material being measured
- Unlike d_0 …
  - Cannot be handled implicitly
  - But generally little variation within and between samples

Plane-specific and bulk constants

- X-ray elastic constants can differ considerably from the material's bulk elastic properties
  - Specific to *hkl* plane being measured
  - Diffraction only measures grains with this *hkl* plane suitably oriented
  - Why are the X-ray constants not the same as the ordinary bulk constants?
    - **Crystal anisotropy**: Individual crystallites have different stiffnesses in different *hkl* directions
    - **Microstructure**: The grains that surround a measured grain will affect the stress state there
  - For multi-peak (Rietveld) measurements, bulk elastic properties good enough
    - Individual *hkl* planes may be more or less stiff than the bulk material
    - Average of many *hkl* planes usually close to bulk material

How elastic constants are specified

- Properties of linear isotropic elastic solid defined by two scalar numbers
  - Normally use Young's modulus E and Poisson's ratio υ
  - Sometimes bulk modulus K, shear modulus G, Lame parameter λ

$$K = \frac{E}{3(1-2\nu)} \qquad G = \frac{E}{2(1+\nu)} \qquad \lambda = \frac{E\nu}{(1+\nu)(1-2\nu)}$$

  - For X-ray diffraction, can use S_1 and $\frac{1}{2}S_2$:

$$S_1 = \frac{-\upsilon}{E} \qquad \tfrac{1}{2}S_2 = \frac{(1+\upsilon)}{E}$$

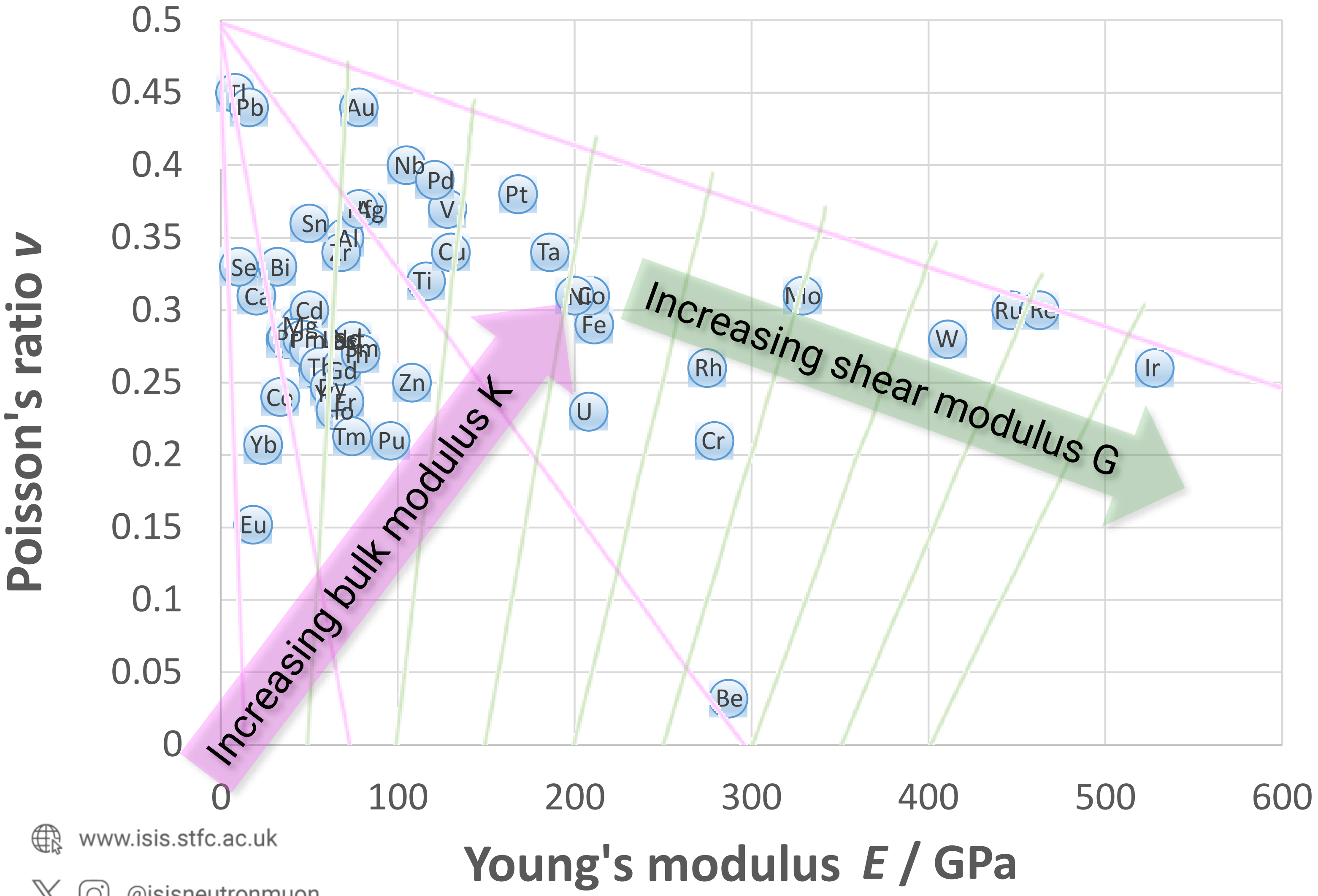
  - S_1 should be negative, but positive value sometimes quoted

How elastic constants are specified

- Two constants are needed to specify linear elastic behaviour in isotropic material
- Several possible choices, including:

Quantities	Symbol	Advantages	Areas of use
Young’s modulus Poisson’s ratio	E ν	Simple description of uniaxial deformation	Mechanical design, materials testing
Bulk modulus Shear modulus	K G	Separates change in volume from change in shape	Geology, solid state physics
Lame constants	λ μ $(=G)$	Convenient stress-strain relation formulas in 3D	Mathematics of elasticity
S_1 and $½S_2$	S_1 $½S_2$	Convenient formulas for diffraction-based measurements	X-ray stress measurement

Elastic properties of the elements



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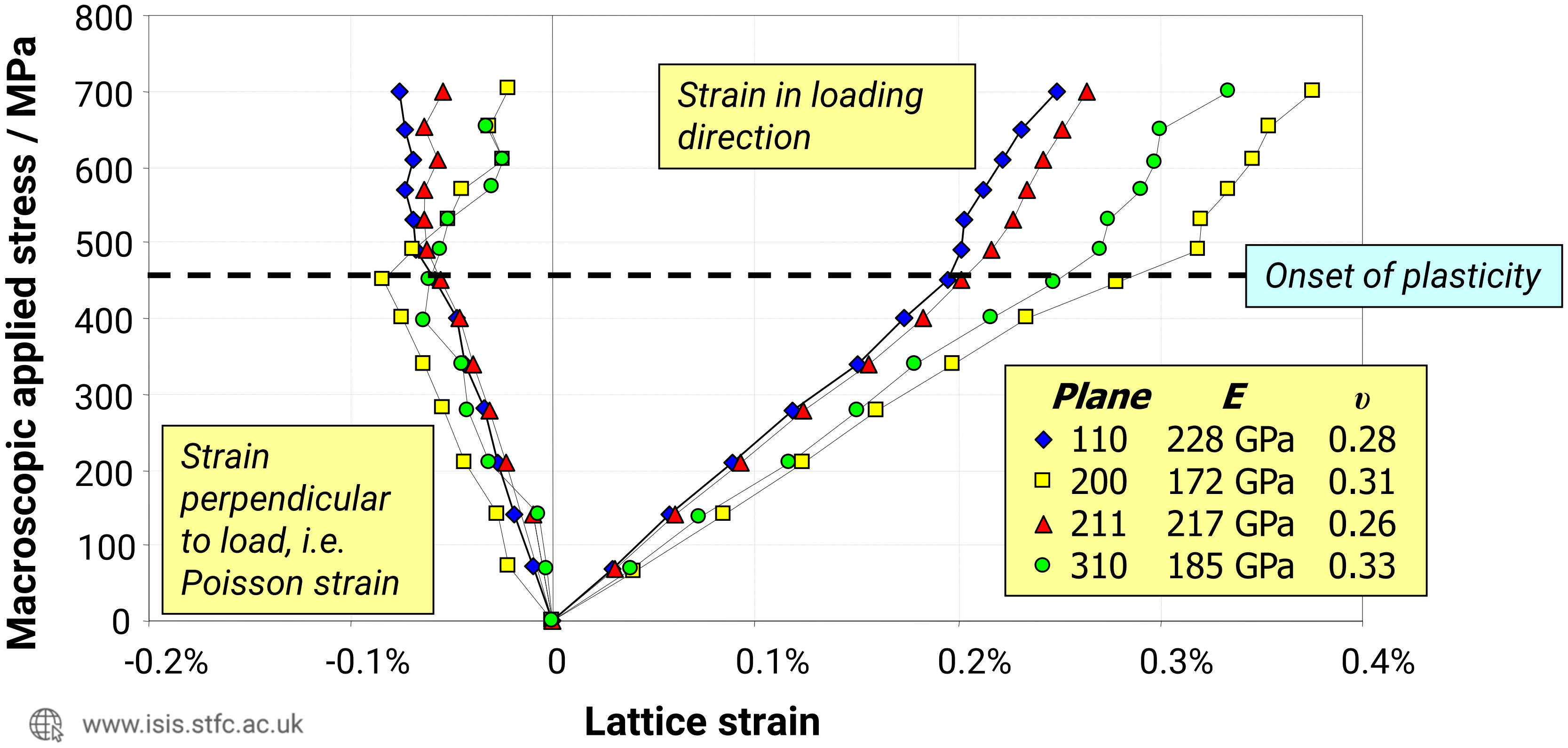
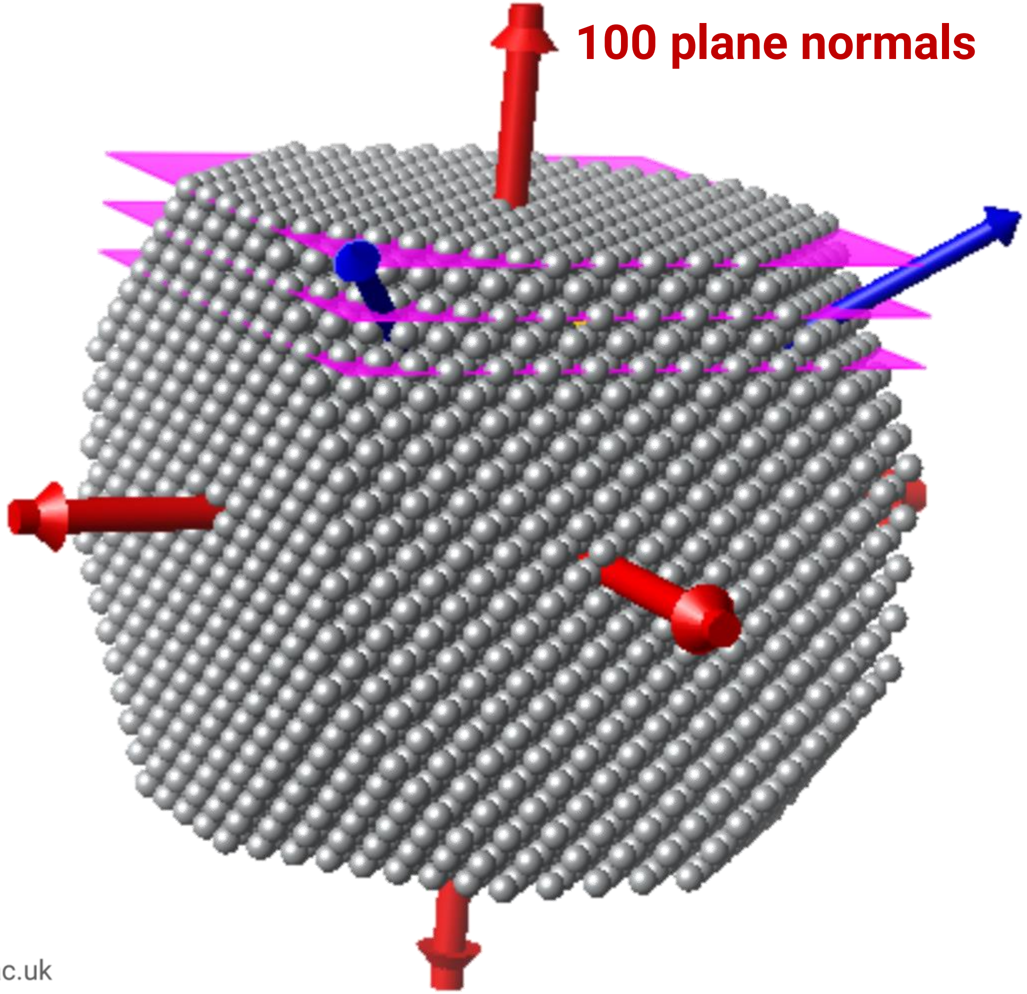
Stress-strain in BCC steel

- Four peaks measured during uniaxial loading
  - From MR Daymond and HG Priesmeyer, Elastoplastic deformation of ferritic steel and cementite studied by neutron diffraction and self-consistent modelling, Acta Mater. **50**(6), p1613-1626 (2002)



Plane	***E***	ν
◆ 110	228 GPa	0.28
□ 200	172 GPa	0.31
▲ 211	217 GPa	0.26
● 310	185 GPa	0.33

Single crystals are anisotropic



100 plane normals

111 plane normals

Single crystal elastic constants

- Single crystal elastic constants of selected fcc metals.

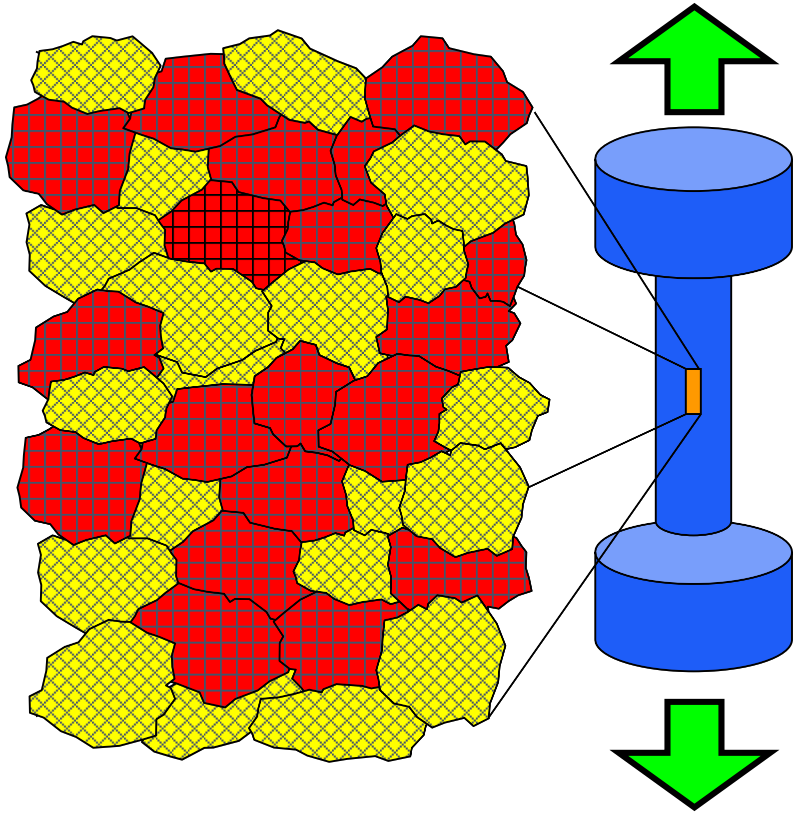
E{hkl} MPa	Al	Cu	Ni	Y-Fe
E{111}	76.1	191.1	260.9	300.0
E{200}	63.7	66.7	120.5	93.5
E{220}	72.6	130.3	202.0	193.2
E{311}	69.0	96.2	161.4	138.3
E{420}	69.1	97.0	162.4	139.6
E{331}	73.6	143.6	216.2	215.5
$(2(S_{11}\text{-}S_{12}))/S_{44}$	1.22	3.20	2.37	3.80

- Single crystal elastic constants of selected bcc metals.

E{hkl} MPa	Stainless steel	V	Mo	Cr
E{110}	210.5	141.3	305.3	268.5
E{200}	125.0	80.5	357.1	333.3
E{211}	210.5	141.3	305.3	268.5
E{220}	210.5	141.3	305.3	268.5
E{310}	146.4	102.3	336.6	306.7
E{222}	272.7	176.5	291.3	252.1
$(2(S_{11}\text{-}S_{12}))/S_{44}$	2.51	2.13	0.79	0.71

Origin of plane-specificity

- 'Uniform' stress is unevenly distributed among grains
  - Grain stiffness is function of *hkl* direction
  - More load carried by grains that are stiff in the loading direction
  - *hkl* spacing normal to loading direction is thus affected



Sources of elastic constants

- Theoretical models
  - Mathematical relation to single crystal constants
  - Finite element simulation of microstructure
- Published data
  - Compiled tables for common *hkl* planes and alloys
  - Intergranular stress studies
- Measure your own
  - For unusual materials, textured materials, thin films
  - Synchrotron or neutron transmission
  - Laboratory $\sin^2$psi on tensile or bending rig

Sources of elastic constants: Theoretical models

- Single crystal constants often already known
- Polycrystal straining models give plane specific constants
  - Voigt model: all grains have same strain
  - Reuss model: all grains have same stress
  - Hill model: average of Voigt and Reuss behaviour
    - Voigt and Reuss are upper and lower bounds
    - Average of these easy way to get plane-specific data
  - Kröner model: grain behaves like single crystal surrounded by isotropic material
    - Calculated using finite element model

Effective elastic constants from the Kröner model

- Effective elastic constants of selected polycrystalline FCC metals obtained using the Kröner model.

E{hkl} MPa	Al	Cu	Ni	Y-Fe
E{111}	73.4	159.0	224.6	247.9
E{200}	67.6	101.1	160.0	149.1
E{220}	71.9	139.1	203.9	212.7
E{311}	70.2	122.0	185.0	183.5
E{420}	70.3	122.5	185.6	184.4
E{331}	72.3	144.3	209.5	221.8

v{hkl} MPa	Al	Cu	Ni	Y-Fe
v{111}	0.34	0.31	0.30	0.24
v{200}	0.35	0.38	0.36	0.34
v{220}	0.34	0.33	0.33	0.28
v{311}	0.35	0.35	0.33	0.31
v{420}	0.35	0.35	0.33	0.31
v{331}	0.34	0.32	0.31	0.27

Sources of elastic constants: Published data

- Textbooks on diffraction
  - e.g. Cullity's Elements of X-ray Diffraction
    - Table 16-1, p460-461: Ferritic, austenitic, nickel, aluminium, copper alloys, for preferred *hkl* planes
- Published in-situ loading experiments
  - Normally for intergranular stress / plasticity studies
    - For references, look at D Dye, HJ Stone & RC Reed, Intergranular and Interphase Microstress, Current opinion in solid state & materials science 5 (1): 31-37 (2001)
  - Digitise data and do linear fit on the elastic region
    - Engauge digitiser (free) & any spreadsheet
  - These are also useful for choosing an *hkl* plane

Sources of elastic constants: Experimental measurement

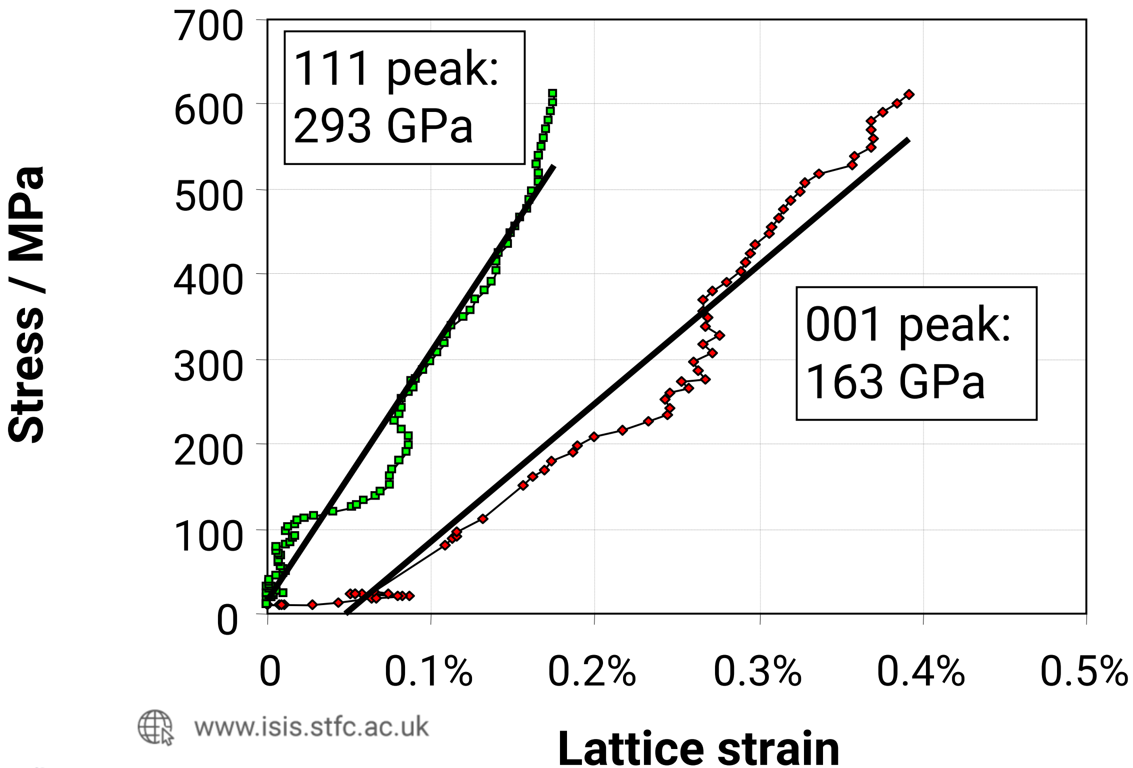
- Sample is measured during incremental loading
  - Relation between individual *hkl* peak and applied bulk stress
  - Linear until plasticity onset
  - Measure in loading direction and perpendicular to it
- Choice of loading rig
  - Laboratory X-ray: 4-point bend
  - Synchrotron X-ray or neutron: Uniaxial tensile test

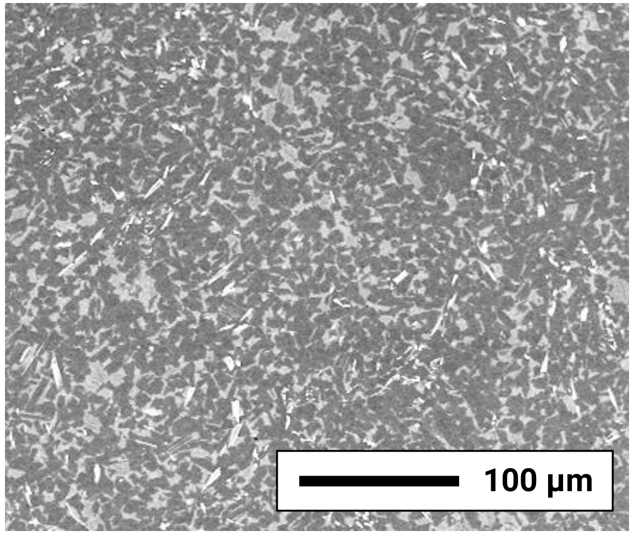
Stresstech 4-point bend system, see www.stresstech.fi for details

In-situ loading for synchrotron measurements

Experimental measurement of elastic constants

- Titanium aluminide (TiAl) with duplex microstructure
  - Synchrotron in-situ loading measured with area detector
  - Nonlinearity due to grain size issues





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