residual stress analysis using XRD (sin²ψ method)

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Coatings - effect of stress

- **Tensile (+) stress**
  - Leads to cracking and crack growth

- **Compressive (-) stress**
  - Good, can close cracks
  - Too high ➔ buckling

---

Compressive and tensile stress

\[
\begin{align*}
d_i < d_0 < d_1 & \quad \text{compressive in film} \\
d_{\parallel} > d_0 > d_{\perp} & \quad \text{tensile in film} \\
\end{align*}
\]

Birkholtz, Thin film analysis by X-ray scattering, p245

- Stress ➔ Changes of d
  - Can get info on strain ➔ Can get info on stress
X-ray diffraction

Bragg’s Law

$$\lambda = 2d \sin \Theta$$

The value of $d$ can be obtained from the peak position (2$\theta$) of the XRD pattern.

The change of $d$ can be obtained from XRD @ many different angles $\rightarrow$ info on strain $\rightarrow$ info on stress
Macro-stress & Micro-stress

- **Macro-stress**: stress is uniform over large distances
- **Micro-stress**: vary from one grain to another on a microscopic scale
- Macro-strain is uniform → peak shift
- Micro-strain is nonuniform → peak broadening

- Diffraction does not measure stresses directly
  - Changes in d-spacing → strains (macro-strain)
  - Changes in line width → micro-strain
  - The lattice planes of the individual grains in the material act as strain gauges

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

Applied stress & Residual stress

- Stress = applied stress + residual stress
- Applied stress: any externally applied load
- Residual stress:
  - stress existing in a solid body in the absence of applied force
    - Typically caused by forming or heating (mechanical working, differential thermal expansion)
    - Especially welding, casting, forging, rolling, machining, cooling, etc.
    - Important in Fatigue Life, Corrosion Resistance, Dimensional Stability, Brittle Fracture, Distortion
    - Can be found in metals, ceramics, biological materials, composites, films - everything
  - can affect material performance
  - can be beneficial or detrimental
    - Residual Surface Stress (e.g. in toughened glass)
    - Stress corrosion cracking
- We can’t measure stress directly, only strains
Residual stress

- tension or compression which exists in the bulk of a material without application of an external load

\[ \sigma_{\text{present}} = \sigma_{\text{applied}} + \sigma_{\text{residual}} \]

\[ \sigma_{\text{applied}} = \frac{F}{A} \]

When \( F = 0 \) (no external force), \( \sigma_{\text{present}} = \sigma_{\text{residual}} \)

\[ \sigma_{\text{present}} \geq \sigma_{\text{fail}} \]
\[ \sigma_{\text{applied}} + \sigma_{\text{residual}} \geq \sigma_{\text{fail}} \] → Unexpected failure

\[ \sigma_{\text{applied}} + \sigma_{\text{residual}} < \sigma_{\text{fail}} \] → Safe design

Residual stress

- When the nuts on the central bar are tightened, the bar is put into tension and the outer frame into compression
- There is no external load but the components are stressed
- During welding the central bar undergoes thermal expansion
- On cooling, this leaves the bar under tension and the outer frame under compression
Residual stress

- Bend a bar so that the outer and inner parts of the bar deform plastically, but the inner portion is only deformed elastically (b).
- If the external stress is released, the inner part of the bar will try to return to its original shape, but the outer part cannot, because it has plastically deformed.
- The bar does not completely return to its original shapes, and there are residual stresses.

Residual stress - no external forces

![Diagram of residual stress](image1)

- Plastically deformed region
- Loaded below elastic limit
- Loaded beyond elastic limit
- Unloaded
Stress in thin films

- **Intrinsic stress**
  - Stress developed during film deposition
  - Misfit strain
  - Microstructural change (e.g. grain growth)
  - Phase transition (due to differences in density)

- **Extrinsic stress**
  - Thermal stress (due to difference of CTE b/w film and substrate)

CTE: coefficient of thermal expansion

How to measure stress?

- Only strain can be measured

\[ \varepsilon = \frac{1 - l_0}{l_0} = \frac{\Delta l}{l_0} \]

- Stress is calculated

\[ \sigma = C^* \cdot \varepsilon \]

stiffness
Residual Stress Measurement

- Mechanical methods
  - Hole-drilling technique
  - Deep hole
  - Sectioning
  - Contour
  - Excision, Splitting, Curvature, Layer removal, Slitting, etc.
- Diffraction methods
  - X-ray diffraction
  - Synchrotron X-ray diffraction
  - Neutron diffraction
- Magnetic Barkhausen noise method
- Ultrasonic method
- Thermoelastic, Photoelastic (birefringent), Indentation

Non-destructive methods have an advantage
measurements can be repeated at will and further data can be collected
RS measurement techniques

<table>
<thead>
<tr>
<th>Technique</th>
<th>Advantage</th>
<th>Disadvantage</th>
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</thead>
<tbody>
<tr>
<td>X-ray diffraction</td>
<td>Versatile, Widely available, Portable, Wide range of materials, Macro and Micro RS</td>
<td>Lab-based systems, Small components, surface stress measurement</td>
</tr>
<tr>
<td>Synchrotron XRD</td>
<td>Improved penetration &amp; resolution of X-rays, Depth profiling, Fast, Macro and micro RS</td>
<td>Special facility needed, Lab-based systems</td>
</tr>
<tr>
<td>Neutron Diffraction</td>
<td>Optimal penetration &amp; resolution, 3D maps, Macro and Micro RS</td>
<td>Special facility needed, Lab-based system</td>
</tr>
<tr>
<td>Hole Drilling</td>
<td>Fast, Easy use, Widely available, Hand-held, Wide range of materials, Deep hole drilling for thick section components</td>
<td>Destructive, Interpretation of data, Limited strain sensitivity and resolution</td>
</tr>
<tr>
<td>Sectioning</td>
<td>Wide range of material, Economy and speed Hand-held</td>
<td>Destructive, Interpretation of data, Limited strain resolution</td>
</tr>
<tr>
<td>Contour</td>
<td>High-resolution maps of the stress normal to the cut surface, Hand-held, Wide range of material, Larger components</td>
<td>Destructive, Interpretation of data, Impossible to make successive slices close together</td>
</tr>
<tr>
<td>Barkhausen Noise</td>
<td>Very fast, Hand-held, Sensitive to microstructure effects especially in welds</td>
<td>Only ferromagnetic materials, Need to divide the microstructure signal from that due to stress</td>
</tr>
<tr>
<td>Ultrasonic</td>
<td>Widely available, Very fast, Low cost, Hand-held</td>
<td>Limited resolution, Bulk measurements over whole volume</td>
</tr>
<tr>
<td>Raman/Fluorescence</td>
<td>High resolution, Portable systems</td>
<td>Surface measurements, Interpretation, Calibration, Limited range of materials</td>
</tr>
</tbody>
</table>
Why use diffraction?

- Diffraction methods offer a nondestructive method for evaluating stress and residual stress in a material
  - Understanding residual stress is important as it is not just the external stress that determines when a material will fail
- Alternative methods are destructive
- Diffraction can be used to examine stresses in multiphase materials and how they are partitioned between phases
  - Useful in composites to understand e.g. how a fiber reinforcement is performing
- Modern X-ray methods allow measurements on a micron length scale → stress distributions can be mapped out

Stress measurement by diffraction

- Diffraction techniques do not measure stresses in materials directly
  - Changes in d-spacing → strains
  - Changes in line width → microstrain
  - The lattice planes of the individual grains in the material act as strain gauges

- To get an estimate of the stress in a part of the diffraction, measurement must be calibrated or a calculation must be performed
RS Measurement > cutting vs. diffraction, diffraction vs. strain gauge

- Compliance/cutting methods
  - Cutting or drilling changes the restraint and the object deforms
  - The stresses can only be calculated in one direction

- Diffraction methods
  - The distance between atoms in crystalline materials can be measured by diffraction (X-ray, neutron)
  - All stress directions can be measured

- Diffraction methods
  - Measured lattice strains are “absolute quantities” relative to a zero-strain data
  - Allows RS as well as applied stress to be measured

- Strain gauge
  - Can only measure the strain difference between the initial condition when the gauge was attached and some subsequent condition

RS Measurement > XRD

- Advantages
  - Non-destructive; Widely available; Macro and micro stresses can be measured;
  - Laboratory or "on-site" measurements; Bi-axial residual stress measurements;
  - Small gauge volume → great for measuring surface stress gradients;
  - High magnitude residual stresses are measured accurately;
  - Complex shapes can be measured providing rotation of the measuring head is not restricted;
  - Very quick and easy to apply the process, and therefore cheap

- Disadvantages
  - Measurement depths of only 10-20μm as standard,
    - when coupled with electro-polishing, surface removal depths of up to 1-1.5mm are achievable;
  - Only applicable to polycrystalline materials;
  - Accuracy seriously affected by grain size and texture;
  - A good component surface finish is essential, so may need delicate preparation.

www.veqter.co.uk/residual-stress-measurement/x-ray-diffraction
Conventional XRD

- Penetration depth ~ 10s of um
  - Surface stress measurement
  - Irradiated volume can be considered to be in a state of plane stress (biaxial stress)
  - Simple stress-strain equation, no need for precise determination of stress-free lattice plane dimension

Synchrotron XRD

- Penetration depth ~ 100s of mm
  - Irradiated volume cannot be considered to be in a state of plane stress.
  - Full 3-Dim stress condition must be considered.
  - Need to have precise value of stress-free lattice plane dimension (major source of error)

Neutrons vs. X-rays

- Absorption is not such a big issue for neutrons.
- You can make measurements inside components.

<table>
<thead>
<tr>
<th></th>
<th>neutron</th>
<th>X-ray</th>
</tr>
</thead>
<tbody>
<tr>
<td>Z</td>
<td>( \mu_l(\text{cm}^{-1}) )</td>
<td>( t_{50%} (\text{mm}) )</td>
</tr>
<tr>
<td>Al</td>
<td>0.10</td>
<td>69.3</td>
</tr>
<tr>
<td>Ti</td>
<td>0.45</td>
<td>15.4</td>
</tr>
<tr>
<td>Fe</td>
<td>1.12</td>
<td>6.19</td>
</tr>
<tr>
<td>Ni</td>
<td>1.86</td>
<td>3.73</td>
</tr>
<tr>
<td>W</td>
<td>1.05</td>
<td>6.60</td>
</tr>
</tbody>
</table>
RS Measurement > X-ray & Neutron diffraction

- **X-ray** strain measurement provides information on the surface of a material.
  - Surface information is important as failure often starts at the surface.
  - Info from the inside can be obtained.

  - Removing the surface layer can destroy the specimen, and the relaxation can change the residual stress.

- **Neutron** diffraction can be used to make measurements inside a part.

---

How to measure stress using XRD?

- Diffraction does not measure stress or strain → gives the changes in d-spacing (change in peak position)

- d-spacing → strain → stress;
  - need to understand assumptions

\[
\varepsilon = \frac{l - l_0}{l_0} = \frac{\Delta l}{l_0}
\]

\[
\sigma = E \cdot \varepsilon
\]

- Accurate/precise (A/P) stress ← A/P strain ← A/P peak position ← excellent alignment of diffractometer

- Instrument alignment/calibration is VERY important
Stress-strain

\[ \sigma = E \cdot \varepsilon \]

\[ \varepsilon_{ij} = \frac{1 + \nu}{E} \sigma_{ij} - \delta_{ij} \frac{\nu}{E} \sigma_{kk} \]

**Tensor properties of stress & strain**

\[
\begin{bmatrix}
\sigma_{11} & \sigma_{21} & \sigma_{31} \\
\sigma_{21} & \sigma_{22} & \sigma_{23} \\
\sigma_{31} & \sigma_{32} & \sigma_{33}
\end{bmatrix}
\]

Nye, page 82

**Poisson ratio** \( \nu \)

\[ \varepsilon = \frac{\sigma}{E} \]

\[ \varepsilon = -\nu \frac{\sigma}{E} \]

---

**Uniaxial stress on a bar specimen**

- **Uniaxial stress:**
  - Parallel: \( \varepsilon = \frac{\sigma}{E} \)
  - Transverse: \( \varepsilon = -\nu \frac{\sigma}{E} \)

- \( E = \) Young's modulus \( \nu = \) Poisson's ratio

- \( E_{\text{steel}} = 200 \text{ Gpa} \quad \nu_{\text{steel}} = 0.28 \)
  - Let \( \sigma_{11} = 200 \text{ MPa} \):
  - \( \varepsilon_{\text{parallel}} = 0.001 = (\Delta d/d)_{\text{parallel}} \)
  - \( \varepsilon_{\text{transverse}} = -0.00028 = (\Delta d/d)_{\text{transverse}} \)

- \( \lambda = 2d \sin \theta \rightarrow \Delta \theta = -(\Delta d/d) \tan \theta \)

- At \( \theta = 45^\circ \):
  - \( (\Delta \theta)_{\text{parallel}} = -0.115^\circ \)
  - \( (\Delta \theta)_{\text{transverse}} = +0.0321^\circ \)

Krawitz
Strain as a function of direction

- When the d-spacing of a reflection is measured, only grains with the planes oriented in a given direction contribute to diffraction.

- If we change the orientation of the specimen and re-measure the d-spacing, we are looking at a different population of grains and we get a different d-spacing due to different stress levels.

Orientation dependence of d-spacing

- Length of vector; d-spacing
- Direction of vector; plane-normal direction

\[ N_s; \text{normal to specimen surface} \]
\[ N_p; \text{normal to diffraction plane} \]
Elastic constants

- The elastic constants \( \mathbf{E} \) in \( \mathbf{\sigma} = \mathbf{E} : \mathbf{\varepsilon} \) used in the stress calculation should be obtained from diffraction measurements on reference materials or by using values mechanically measured in different directions on single crystal specimens.
  - Individual crystallites are not elastically isotropic.
  - Young’s modulus and Poisson’s ratio for the (111) reflection will not in general be the same as those e.g. for the (110) reflection.

\[
\varepsilon_{ij} = \frac{1 + \nu}{E} \sigma_{ij} - \delta_{ij} \frac{\nu}{E} \sigma_{kk}
\]

- \( E \) can also change when the stress state changes

Stress free reference

- Strain is obtained from a diffraction measurement using \( \varepsilon = (d_{\psi \phi} - d_0)/d_0 \)
  - \( d_{\psi \phi} \): measured d-spacing in some direction \( \psi \phi \)
  - \( d_0 \): d-spacing for the stress free material
    - It is very difficult to get \( d_0 \) directly \( \Leftarrow \) to prepare a stress free piece of material with exactly the same composition is very difficult.
    - Using a similar piece of material may not be good enough as we are trying to measure very small changes in d-spacing.
  - We can sometimes avoid the need to measure \( d_0 \) by making diffraction measurements at several angles \( \psi \).
Optics & sample preparation

- Using a divergent beam is not desirable. The instrument needs constant realignment.
- **Parallel beam** optics are the way to go. sample displacement and focusing are not issues.

Sample preparation

- Smooth clean surface
- The polishing of the surface can change the stresses that you wish to measure!

Stress as a function of depth

- To measure residual stress as a function of depth using X-rays, you may need to carefully remove some of the surface.
- The stress relief that occurs will have to be accounted for.

Residual stress in ground steel close to the surface
Sample preparation

- Sample preparation
  - Smooth clean surface
  - However, if you try to polish the surface, you will change the stresses that you wish to measure !!!!

- Portable instrument
  - In case one needs to measure surface residual stress in large components, it is possible to buy small mobile diffractometers that can be moved to the specimen and mounted on the specimen surface.

Practical problems

- Stress measurement uses positions of powder diffraction lines (d-spacing).

- If the sample contains very large grains, you do not really have powder lines, just single crystal spots. It can be very difficult to accurately estimate the position of a powder line under these conditions.

- Texture can lead to very low intensity for some sample orientations.

- Highly textured bodies may not be elastically isotropic \( \Rightarrow \) some of the assumptions (isotropic, biaxial stress) that go into the basic theory for converting the strain measurements to stress tensor components in \( \sin^2 \psi \) method, fail.
Residual stress

Deformation of a rod induced by external force

deformation $\rightarrow$ strain $\rightarrow$ displacement in the body relative to a reference length

Deformation of simple cubic induced by external force

deformation $\rightarrow$ strain $\rightarrow$ displacement relative to inter-atomic length

Deformation of simple cubic induced by residual stress

Residual stress can be calculated from displacement

Displacement of atoms $\rightarrow$ change of lattice parameter

Residual stress measurement

$$\varepsilon_{\text{total}} = \frac{L - L_0}{L_0}$$

$$\varepsilon_{\text{grain}} = \frac{l - l_0}{l_0}$$

Assumption: isotropic materials
Stress measurement by XRD

- **Film subjected to biaxial tension**

  ![Diagram of film under biaxial tension](image)

  - The elastic strain $\perp$ to the plane of the film
    \[ \varepsilon_{zz} = \frac{d_{hkl} - d_0}{d_0} \]

  - The intensity of the diffracted beam is very small
    - small interaction volume
  - How to align the sample??

- **The intensity of the diffracted beam is very small**
  - small interaction volume
- **How to align the sample??**

---

Stress measurement by XRD

- **high intensity of diffracted beam**
- **simple sample alignment**

![Diagram of stress measurement](image)

Strain is proportional to inclination angles with respect to sample normal
Stress measurement by XRD

Assumption: isotropic materials, biaxial stress

Unstressed sample

Stressed sample

In stressed sample, diffraction angle changes with the offset angle

Residual stress measurement: determine the variations in lattice parameter as a function of the offset angle

\[ \lambda = 2d \sin \theta \]

\[ \varepsilon_{s11} \] can be determined by \[ \varepsilon_{L33} \] values at different \( \psi \)'s

\[ S_3 \]

\[ x\text{-ray} \]

\[ L_3 \]

Measured data

direction cosine matrix

\[ \varepsilon_{s11} \]
Symbol

superscript : reference frame
L : Laboratory reference frame
S : Specimen reference frame

d : interplanar spacing

strain

ε

σ

Laboratory reference frame

33

Normal strain that is // to L3 direction

subscript : component of tensor

σ_{ii} : normal stress

σ_{ij} : shear stress (i ≠ j)

L_1 = L_x, L_2 = L_y, L_3 = L_z

Stress measurement by XRD

\[ d_{\psi} = d_0 \frac{1 + \nu}{E} \sigma \sin^2 \psi + d_0 (1 - \frac{2\nu}{E}) \]
Angles

- **2-theta (2θ)** - The Bragg angle, the angle between the incident (transmitted) and diffracted X-ray beams
- **Omega (ω)** - The angle b/w the incident X-ray beam and the sample surface. Both ω and 2θ lie in the same plane
- **Phi (φ)** - The angle of rotation of the sample about its surface normal
- **Chi (χ)** - Chi rotates in the plane normal to that containing ω and 2θ. This angle is also sometimes (confusingly) referred as ψ
- **Psi (ψ)** - Angle through which the sample is rotated, in the \( \sin^2 \psi \) method. We start at \( \psi = 0 \), where ω is half of 2θ and add (or subtract) successive ψ offsets. For example, 10, 20, 30 and 40°.
States of stress

- possible states
  - 3 unequal principal stresses \((\sigma_1, \sigma_2, \sigma_3)\) \(\rightarrow\) Triaxial state of stress
  - 2 out of 3 principal stresses are equal (say \(\sigma_1, \sigma_2 = \sigma_3\)) \(\rightarrow\) Cylindrical state of stress
  - All 3 are equal (say \(\sigma_1 = \sigma_2 = \sigma_3\)) \(\rightarrow\) Hydrostatic/spherical state of stress
  - 1 of 3 is zero (say \(\sigma_1, \sigma_2, \sigma_3 = 0\)) \(\rightarrow\) Biaxial/2D state of stress
  - 2 of 3 is zero (say \(\sigma_1, \sigma_2 = \sigma_3 = 0\)) \(\rightarrow\) Uniaxial state of stress

By convention, the diffracting planes are normal to \(L_3\)

- \(L_i\) laboratory coordinate system
- \(S_i\) sample coordinate system

Reference frame

- \(S\): specimen reference frame
- \(L\): laboratory reference frame
- If \(\phi = \psi = 0\), \(L = S\)

\[ \varepsilon_{33}^L = \varepsilon_{\psi\phi} \]
Translation L→S

- Direction cosine matrix: transformation from the L frame to S frame

\[
\mathbf{a}_{ij}^{LS} = \begin{pmatrix}
\cos\psi \cos\phi & \sin\psi \cos\phi & -\sin\phi \\
-\sin\psi & \cos\phi & 0 \\
\cos\psi \sin\phi & \sin\psi \sin\phi & \cos\phi
\end{pmatrix}
\]

\[
\sum_{i,j} a_{ij}^{LS} a_{ij}^{LS} \varepsilon_{ij}^{S} = \sum_{i,j} a_{ij}^{LS} a_{ij}^{LS} \varepsilon_{ij}^{S}
\]

\[
\varepsilon_{33}^L = a_{3k} a_{3l} \varepsilon_{kl}
\]

\[
\varepsilon_{33}^L = \varepsilon_{11}^S \cos^2\phi \sin^2\psi + \varepsilon_{12}^S 2 \cos\phi \sin\phi \sin^2\psi + \varepsilon_{13}^S \cos\phi \sin 2\psi
\]

\[
+ \varepsilon_{22}^S \sin^2\phi \sin^2\psi + \varepsilon_{23}^S \sin\phi \sin 2\psi + \varepsilon_{33}^S \cos^2\psi
\]
Translation \( L \rightarrow S \)

\[
\varepsilon^L_{33} = \varepsilon^S_{11} \cos^2 \phi \sin^2 \psi + \varepsilon^S_{12} \sin 2\phi \sin^2 \psi + \varepsilon^S_{13} \cos \phi \sin 2\psi
+ \varepsilon^S_{22} \sin^2 \phi \sin^2 \psi + \varepsilon^S_{23} \sin \phi \sin 2\psi + \varepsilon^S_{33} \cos^2 \psi
\]  

(1)

Strains measured in \( L \) frame (diffraction plane) \( \rightarrow \) strains in the \( S \) frame (sample)

---

Residual stress measurement

\[ \varepsilon_{\text{total}} = \varepsilon_{\text{grain}} \]

Assumption: isotropic materials biaxial stress
Strain and Stress

Strain

\[ \varepsilon = \frac{l - l_0}{l_0} = \frac{\Delta l}{l_0} \]

\[ \varepsilon_1 = \frac{d_1 - d_0}{d_0} \]

\[ \varepsilon_2 = \frac{d_2 - d_0}{d_0} \]

\[ \varepsilon_3 = \frac{d_3 - d_0}{d_0} \]

Relationship between Stress and Strain

\[ \varepsilon_{ij} = \frac{1 + \nu}{E} \sigma_{ij} - \delta_{ij} \frac{\nu}{E} \sigma_{kk} \]

\[ \sigma_{kk} = \sigma_{11} + \sigma_{22} + \sigma_{33} \]

\( \delta_{ij} \) : Kroenecker’s delta

\[ \delta_{ij} = 1 \quad (i = j) \]

\[ \delta_{ij} = 0 \quad (i \neq j) \]

Normal strain

Shear strain

Hooke’s Law

\[ \varepsilon_{ij} = \frac{1 + \nu}{E} \sigma_{ij} - \delta_{ij} \frac{\nu}{E} \sigma_{kk} \]

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

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

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

\[ \varepsilon_{23} = \frac{1 + \nu}{E} \sigma_{23} \]

\[ \varepsilon_{31} = \frac{1 + \nu}{E} \sigma_{31} \]

\[ \varepsilon_{12} = \frac{1 + \nu}{E} \sigma_{12} \]

\[ \varepsilon_{33}^L = \varepsilon_{33}^S \cos^2 \phi \sin^2 \psi + \varepsilon_{12}^S \sin 2\phi \sin^2 \psi + \varepsilon_{31}^S \cos \phi \sin 2\psi \]

\[ + \varepsilon_{22}^S \sin^2 \phi \sin^2 \psi + \varepsilon_{23}^S \sin \phi \sin 2\psi + \varepsilon_{33}^S \cos^2 \psi \]

(1)

(2)
\[ \epsilon_{33}^{L} = \frac{1 + \nu}{E} \left( \sigma_{11}^s \cos^2 \phi + \sigma_{12}^s \sin 2\phi + \sigma_{22}^s \sin^2 \phi - \sigma_{33}^s \right) \sin^2 \psi + \frac{1 + \nu}{E} \sigma_{33}^s \]

\[ \epsilon_{33}^{L} = \frac{1 + \nu}{E} \left( \sigma_{11}^s \cos^2 \phi + \sigma_{12}^s \sin 2\phi + \sigma_{22}^s \sin^2 \phi - \sigma_{33}^s \right) \sin^2 \psi + \frac{1 + \nu}{E} \sigma_{33}^s \]

\[ \epsilon_{33} = \frac{1 + \nu}{E} \sigma_{11}^s \sin^2 \psi - \frac{V}{E} \left( \sigma_{11}^s + \sigma_{22}^s \right) \]

\[ \epsilon_{33} = \frac{1 + \nu}{E} \sigma_{11}^s \sin^2 \psi - \frac{2V}{E} \sigma_{11}^s \]

\[ \psi \epsilon \propto \sin^2 \psi \quad \text{Linear relationship} \]

\[ \psi \epsilon \rightarrow \Delta \]

\[ \epsilon_{33}^{L} = \frac{1 + \nu}{E} \sigma_{11}^s \sin^2 \psi - \frac{2V}{E} \sigma_{11}^s \]

\[ \frac{d_{11} - d_0}{d_0} = \frac{1 + \nu}{E} \sigma_{11}^s \sin^2 \psi - \frac{2V}{E} \sigma_{11}^s \]

\[ d_{11} = d_0 \frac{1 + \nu}{E} \sigma_{11}^s \sin^2 \psi + d_0 \left(1 - \frac{2V}{E} \sigma_{11}^s \right) \]

\[ d_{11} = d_0 \frac{1 + \nu}{E} \sigma \sin^2 \psi + d_0 \left(1 - \frac{2V}{E} \sigma \right) \]

\[ \psi \epsilon \propto \sin^2 \psi \quad d_{11} \propto \sin^2 \psi \]
\[
\varepsilon_{L33} = \frac{1 + \nu}{E} \sigma_{S11}^s \sin^2 \psi - \frac{2\nu}{E} \sigma_{S11}^s \quad (3)
\]

\[
\varepsilon_{\psi} \propto \sin^2 \psi \quad \text{Linear relationship}
\]

\[
\frac{1 + \nu}{E} \sigma_{S11}^s \quad \text{positive: tensile stress}
\]

\[
\frac{1 + \nu}{E} \sigma_{S11}^s \quad \text{negative: compressive stress}
\]

\[
d_\psi = d_0 \frac{1 + \nu}{E} \sigma \sin^2 \psi + d_0 (1 - \frac{2\nu}{E} \sigma) \quad (4)
\]

\[
\text{Slope}
\]

\[
\text{Intensity}
\]

\[
\text{different } \psi \text{ values}
\]

\[
\text{d(Å)}
\]

\[
\sin^2 \psi
\]

\[
\psi \text{ values}
\]

\[
2\theta
\]

\[
\text{d(Å)}
\]

\[
\sin^2 \psi
\]

\[
\text{Slope}
\]
Step by step

X-ray diffraction $\lambda, \theta, 2\theta$

Bragg’s law

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

Interplanar spacing $d$

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

Strain in the diffraction direction $\varepsilon^L, \varepsilon_{\psi\phi}$

Direction cosine matrix

$\mathbf{a}^{\text{LS}}_{ij} = \begin{pmatrix}
\cos \psi \cos \phi & \sin \psi \cos \phi & -\sin \phi \\
-\sin \psi & \cos \phi & 0 \\
\cos \psi \sin \phi & \sin \psi \sin \phi & \cos \phi
\end{pmatrix}$

Hooke’s law

$\varepsilon_{ij} = \frac{1 + \nu}{E} \sigma_{ij} - \delta_{ij} \frac{\nu}{E} \sigma_{kk}$

Stress of specimen $\sigma^S$

Strain of specimen $\varepsilon^S$

$d_0$: stress-free $d$

sin$^2\psi$ method

Fig. 3 - A $d(311)$ versus sin$^2\psi$ plot for a shot peened 5056-O aluminum alloy having a surface stress of -148 MPa (-21.5 ksi).

Fig. 6 Comparison of $d(21.3)$ versus sin$^2\psi$ data taken 0.176 mm (0.0069 in.) below the surface for a ground Ti-6Al-4V sample using two diffraction peak location methods.
Appearance of $\sin^2\psi$ plots

Biaxial or uniaxial stress gives linear $\sin^2\psi$ plots

Triaxial stress (all principle components of stress tensor are none zero) does not give a straight line $\Rightarrow$ psi-splitting

Oscillatory - significant levels of texture are present (inhomogeneous stress/strain state within the materials) $\Rightarrow$ the material is no longer elastically isotropic

Residual stress measurement using XRD

- Understanding of the assumptions

- Is the sample homogeneous or heterogeneous?
- Texture?
- The relationship between the beam size & grain size?
  Sampling statistics?
- What components of the stress tensors are considered to be zero?
references

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