1 Notes

1.1 X-Ray Imaging

1.1.1 Multiscale Characterization

Diffraction with X-Rays is very good at looking into things like:

- Batteries
- Layered Things
- Polycrystalline Structures
- Grains
- Dislocations in Materials
- Inside of Molecules

For instance, it is possible to image a sample of cast aluminum alloy and deduce where the void defects are.

This can then be compared to models of stresses and strains!

Example. It's important to be able to characterize the evolution of cracks in wind turbines.

Using X-Ray tomography, this can be directly examined in 3D.

1.1.2 X-Ray Radiology

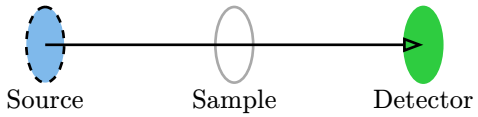
The classical thing about radiography is that depth is difficult

Definition 1.1.1. The "linear attenuation coefficient" is termned as

$$\frac{\mathrm{d}I}{\mathrm{d}x} = -\mu(x)I(x)$$

which solves to:

$$-\ln\left(\frac{I_{\text{det}}}{I_0}\right) = \int_{\text{path}} \mu(x)dx$$



Definition 1.1.2. The "attenuation coefficient"

$$\mu \propto \sum_i \frac{Z_i^4 \rho_i}{E^3}$$

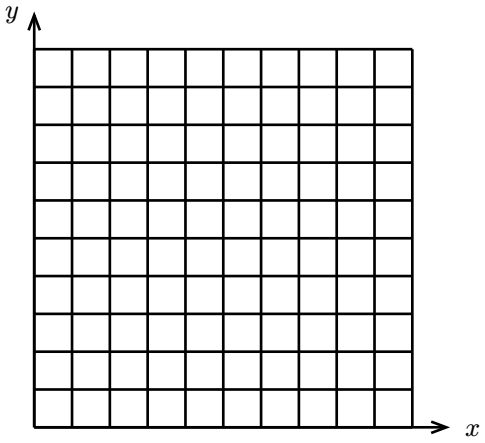
1.1.3 Radiography Setup

The principle is to sweep, then record angular deviations.

TODO: More detail

1.1.4 Algebraic Reconstruction

Consider a 2D slice of a voxel grid:



$$\mathbf{Mf} = \mathbf{p}$$

...

1.1.5 Filtered Backprojection

In most commercial instruments, a Fourier Transform-based approach is used.

1. A sample is recorded as $P_\theta(t)$.
2. This is "projected" to (t,θ) chart is recorded.
3. The fourier transform of the (t,θ) is computed, producing a (ω,θ) diagram.
4. This is reconstructed back to a (u,v) fourier space.

1.1.6 Discrete Tomography

TODO: ??

1.1.7 Synchrotrons

You build a large circle, and accelerate electrons to near the speed of light with large electromagnets.

They become pulsed, naturally.

When they travel sufficiently fast, the bending of the electrons cause the emission of very powerful, very parallel X-Rays.

1.1.7.1 Brilliance

How many useful X-Rays are there?

$$\text{brilliance} = \frac{\text{photons}}{\text{mrad}^2 \cdot \text{mm}^2 \cdot 0.1\% \cdot \text{sec}}$$

These days, modern synchrotrons can reach a brilliance of 10^{21}.

What can be done with more x-rays?

Speed Hard things can be imaged faster - even to the point of real-time.

Materials Very dense things can be imaged faster.

Example. **Speed**: They were able to make a 3D movie of a fly, where it barely manages to flap its wings between frames.

Aka. they can see inside of the fly, including colors of ex. the muscles, the moving organs, etc. .

Example. **Resolution**. They can image down to 5 nm now!

Electrons are still, with their theoretical resolution of 5 Å.

1.1.8 Phase Contrast Tomography

Consider the incoming wave. Not only the "shadow" aka. absorption can be used; the phase, too, is available.

As it turns out.

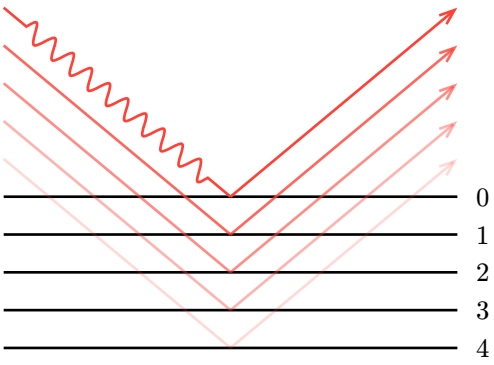
Example. Smallest detectable hole at 25 keV is:
Absorption 20 µm
Phase 0.05 µm

1.1.9 Diffraction Contrast Tomography

Finally, when studying crystals, the diffraction can also be measured to reconstruct the internal structure.

1.2 X-Ray Diffraction Analysis

Once again, "Bragg's Law" is the key!



1.2.1 Diffractometer Orders

A single-crystal will only show one family of peaks.

TODO: Diagram

These peaks correspond to hitting one of the crystallographic directions equivalent to parallel planes.

TODO: Use Bragg's law to predict where the peaks "should" occur, based on direct analysis of a crystallographic lattice

For polycrystals, the peaks will be normally distributed.

1.2.2 Symmetrical X-Ray Path

Consider the case of diffraction from lattice planes parallel to the surface ($\psi = 0$).

Definition 1.2.1 (Information Depth of Symmetric X-Ray Paths). Let

> · μ be the linear absorption coefficient

The "information depth" τ is the depth from which 63% of the diffracted intensity aka. information comes from:

$$\tau = \frac{\sin\theta\cos\psi}{2\mu} = \frac{\int_0^\infty 2e^{-\mu x}dx}{\int_0^\infty e^{-\mu x}dx}$$

Sometimes referred to as "penetration depth", or "absorption weighted average values".

This measure has a strong dependence on the scattering angle 2θ, and otherwise has a high penetration depth.

1.2.3 Asymmetrical X-Ray Path

By using grazing incidence angles, one gets considerably shallower information depths.

Definition 1.2.2 (Information Depth of Asymmetric X-Ray Paths). Let

> · μ be the linear absorption coefficient

Then, the "information depth" τ is the depth from which 63% of the diffracted intensity aka. information comes from:

$$\tau = \frac{1}{\mu}\left(\frac{1}{\sin\gamma} + \frac{1}{\sin(2\theta - \gamma)}\right)$$

In short, the parallel planes are much closer, and the entire thing is much less dependent on the scattering angle 2θ.

1.2.4 Exercise: Measuring Tungsten in a Symmetric-Beam Diffractometer

A sample consisting of tungsten is measured in a diffractometer, which is using a symmetrical beam geometry.

The script is setup like this:

```
import math
import sympy.physics.units as spu
import sympy as sp

diff_angle_deg = sp.Interval(20, 150)
wl_cu = 0.154 * spu.nm
wl_cr = 0.229 * spu.nm
mass_absorp_cu = 171 * spu.cm**2 / spu.g
mass_absorp_cr = 456 * spu.cm**2 / spu.g
density_tungsten = 19.25 * spu.g / spu.cm**3

information_depth = lambda theta, mass_absorp,
rho: sp.sin(theta) / (2*mass_absorp * rho)
```

1.2.5 Applications of XRD for Materials Science

Qualitative and Quantitative Phase Analysis Interpreting 2θ and integrated intensity.

Line Profile Analysis The crystallite size and microstrains.

Residual Stress Analysis Lattice strains and macrostresses, interpreting 2θ as a function of ψ and φ.

Quantitative Crystallographic Texture Interpreting integrated intensity as a function of ψ and φ.

1.2.6 Interpreting the Diffractogram

Look at the peaks on the diffractogram.

- The width and shape of the peak tells us something about the microstrains and crystallite size.
- The position tells us something about the macrostrain and phase.
- The peak intensity tells us something about the phase and the crystallographic texture.

1.3 Role of Mechanical Stress on Lattice Strains

1.3.1 Macro- and Microstrains

There are a few different kinds of stressors, described by their order.

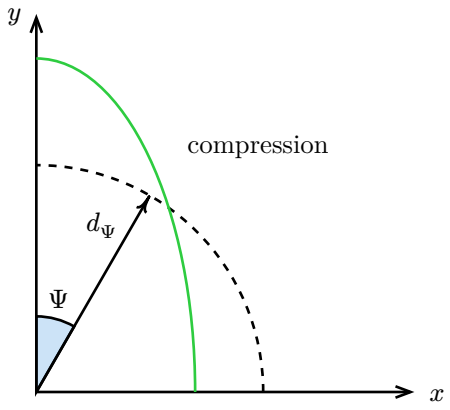
Macro Stress σ^{I}. Homogeneous over several grains.
- Characterized by $\Delta 2\theta$.

Micro Stress σ^{II}. Homogeneous within one grain
- Characterized by $\Delta 2\theta$ and ΔFWHM.

Micro Stress σ^{III}. Inhomogeneous within one grain
- Characterized by ΔFWHM alone.

1.3.2 Lattice Strain Analysis

Consider a lattice under compressive strain will behave like



Definition 1.3.1. The $\sin^2\psi$ method for determining macrostresses uses the "biaxial stress-state":

$$\varepsilon^{hkl}_{\phi,\psi} = 2S_1^{hkl} \cdot \sigma_\phi + \frac{1}{2} S_2^{hkl} \cdot \sigma_\phi \sin^2\psi$$

1.3.3 Oxidation of Bulk Metallic Glass

TODO: Insert info about the research project.

2 Exercises

2.1 Tensile Testing of 4 Alloys

Four alloys were tested from among five possibilities:

- AISI 304 (18/10 austentic stainless steel)
- UHB (heat treatable steel)
- CuZn39Pb3 (or MS 58, a particular type of brass)
- Impax Supreme (tool steel)
- AW 6082 (a precipitation hardenable aluminium alloy)

2.3 Glossary