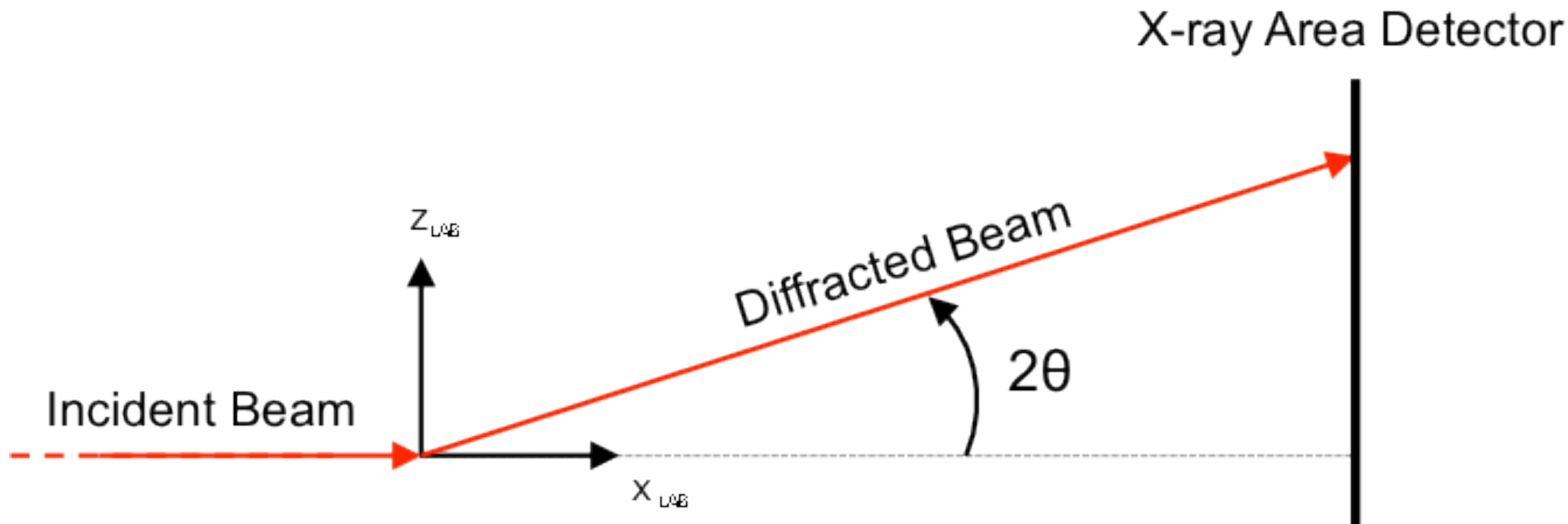

BUILDING A VIRTUAL DIFFRACTOMETER

(AND SURVING YOUR FIRST BEAM TIME…)

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These are just the people that have directly helped me but there are dozens of other people who worked on developing these techniques who I don't have space to acknowledge here.

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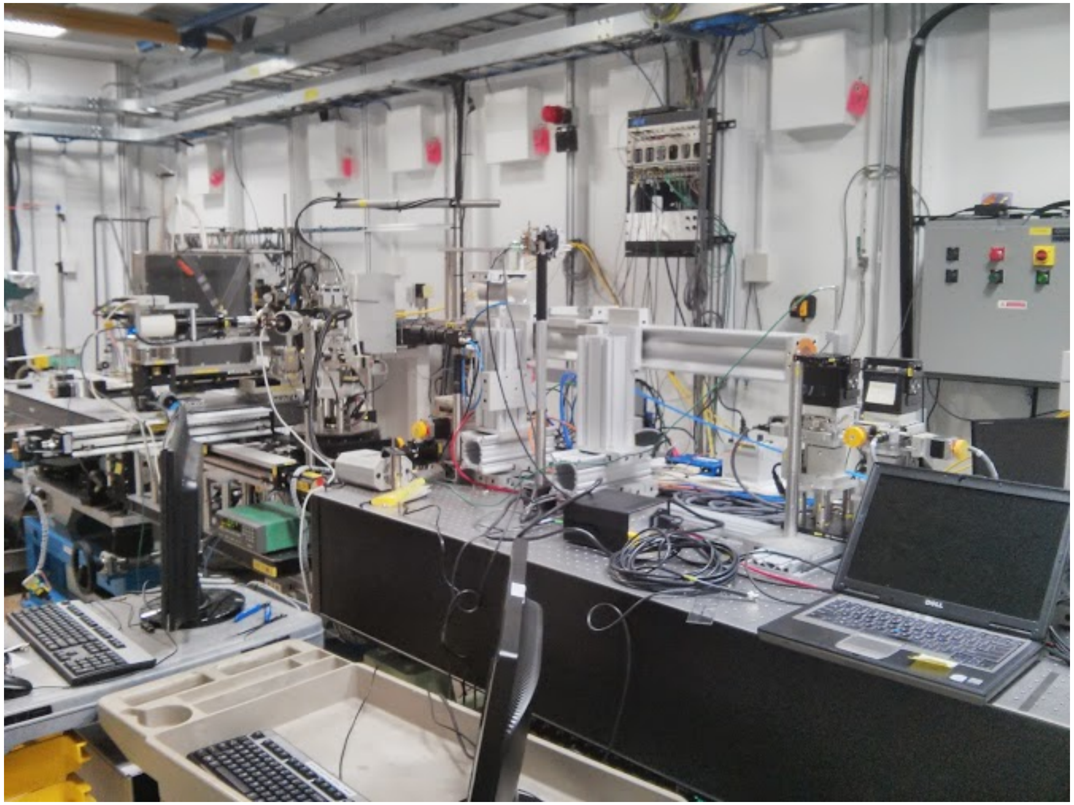
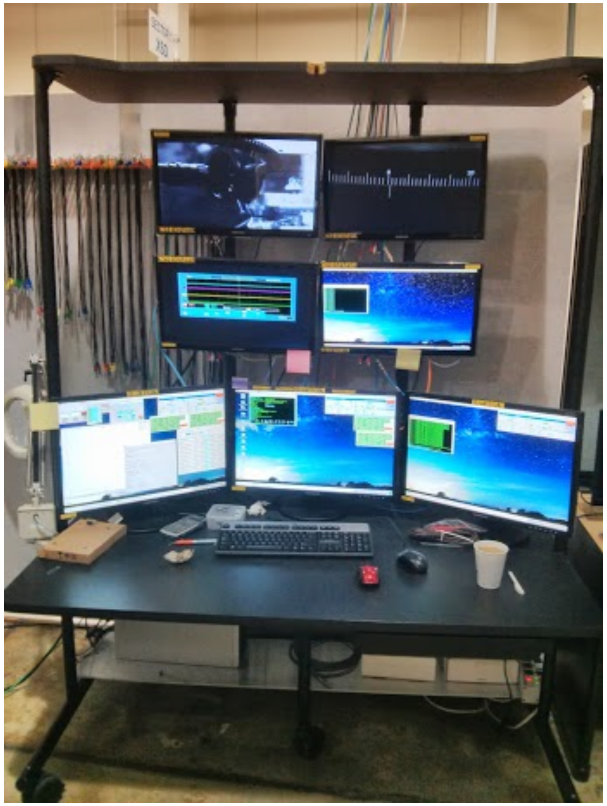
SYNCHROTRONS CAN BE PRETTY INTIMIDATING:





Sector 1-ID E-Hutch at the APS

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DON'T WORRY ABOUT IT:

- There are amazing beam line scientists on hand to help you.
- There is a strong (but small) community that is always willing to help you.
- Some very smart people have done a lot of hard thinking and solved most of the really difficult problems.
- As a result, there is a wide range of sources available to help you understand analysis techniques (the hand out has some references).
- There are even some software packages available that will do a lot of the work for you:
    - FABLE
    - HEXRD
    - Fit2D
    - …

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THAT BEING SAID…

- Beam time can be tough.
- Synchrotron facilities generally run 24/7 during up time.
- If you aren't collecting data then those expensive photons are wasted.
- Ideally you need a team of people (4-5) that are willing to put in very long hours.

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THESE WILL BECOME YOUR BEST FRIENDS:

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Previously, the barrier to entry was…

- The extremely difficult nature of the experiments!

Now, the barrier to entry is…

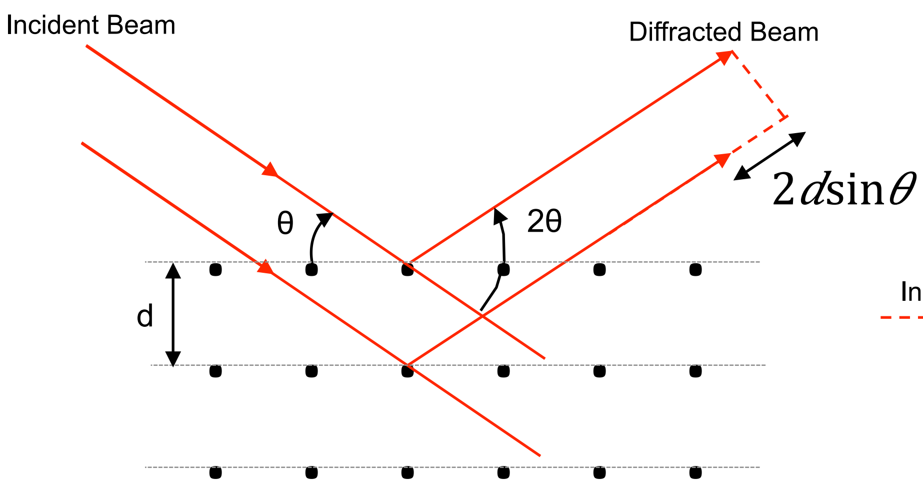
- Understanding different aspects of the problem
- Developing analysis techniques
- Having the toolsets to tackle the problem!

The handout / tutorial is designed to give you the toolset you require to tackle the problem

GENERAL HIGH ENERGY X-RAY DIFFRCTION MICROSCOPY (HEDM) POINTS:

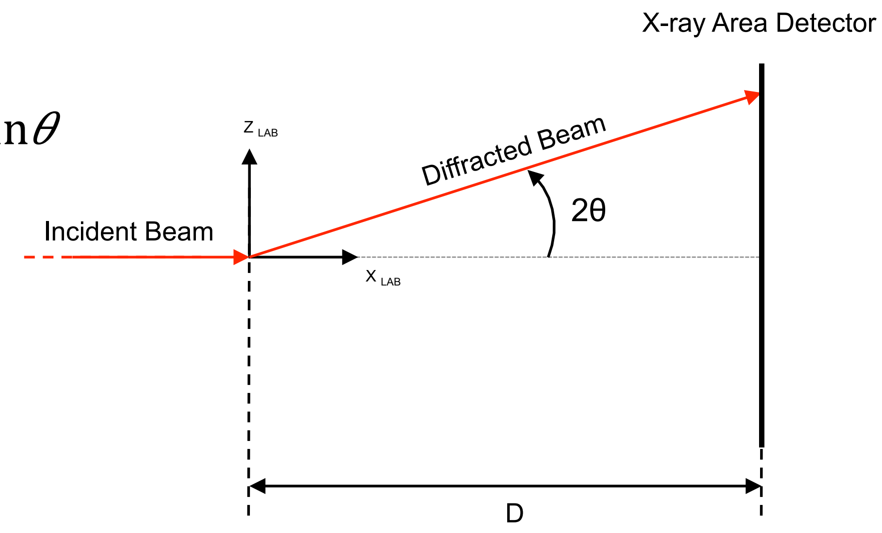
- Use synchrotron x-rays
- All techniques based on Bragg's Law
- Assume kinematic diffraction (generally)

Bragg's Law



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

Simplified Experimental Setup



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HEDM EXPERIMENTAL TECHNIQUES:

- **Strain pole figures experiments:**
  - Fiber averaged lattice strains
  - High lattice strain resolution
  - No spatial information
- **Far-field experiments:**
  - Orientation, position and lattice strains from individual grains
  - High lattice strain resolution
  - Low spatial resolution
- **Near-field experiments:**
  - Orientation and position from sub-grain regions
  - No lattice strain information
  - High spatial resolution

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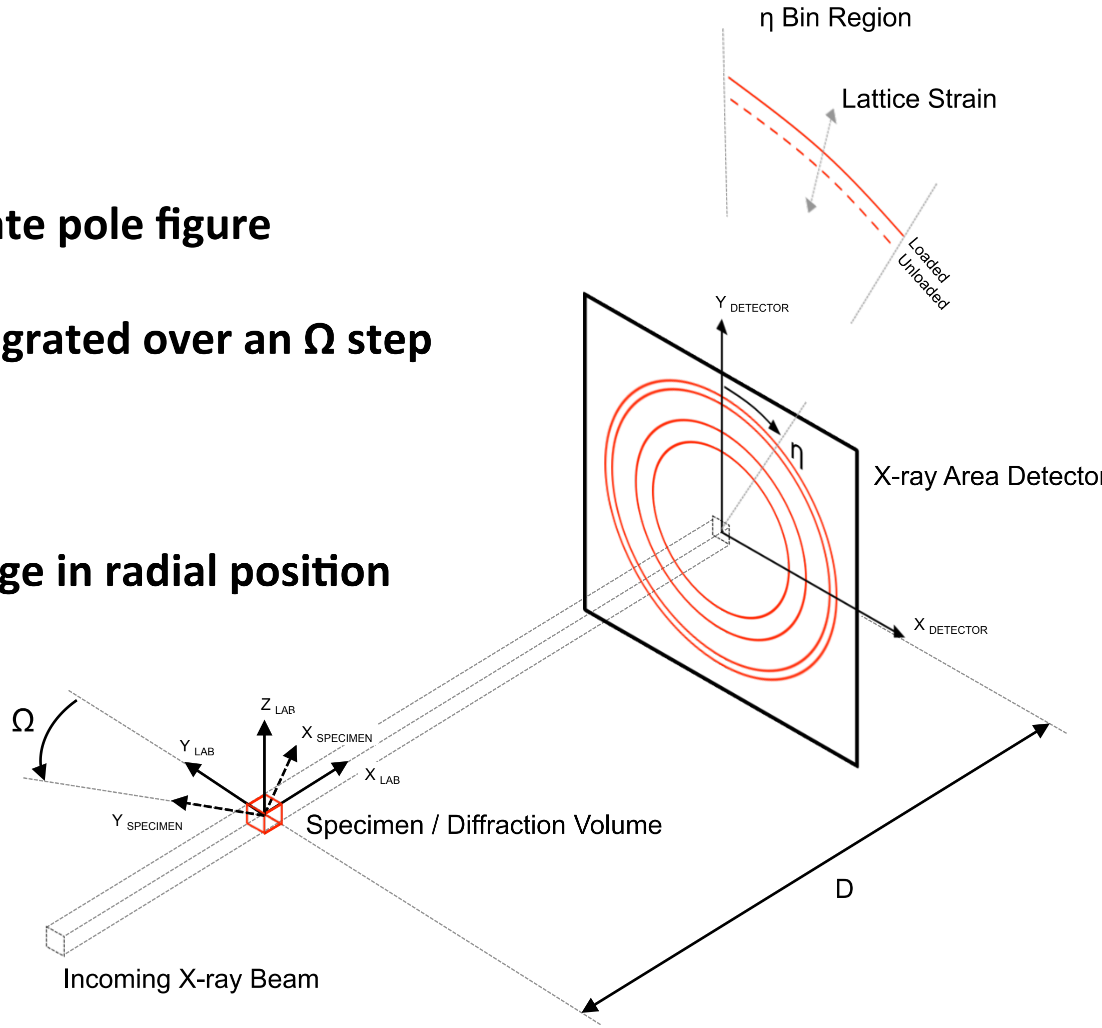
STRAIN POLE FIGURE EXPERIMENT:

- Powder diffraction rings
- Specimen rotated in Ω to populate pole figure
- Intensity of diffracted beam integrated over an Ω step
- Detector binned into η regions
- Lattice strain measured via change in radial position
- Back projection
- Analysis is complicated
- Computationally cheap



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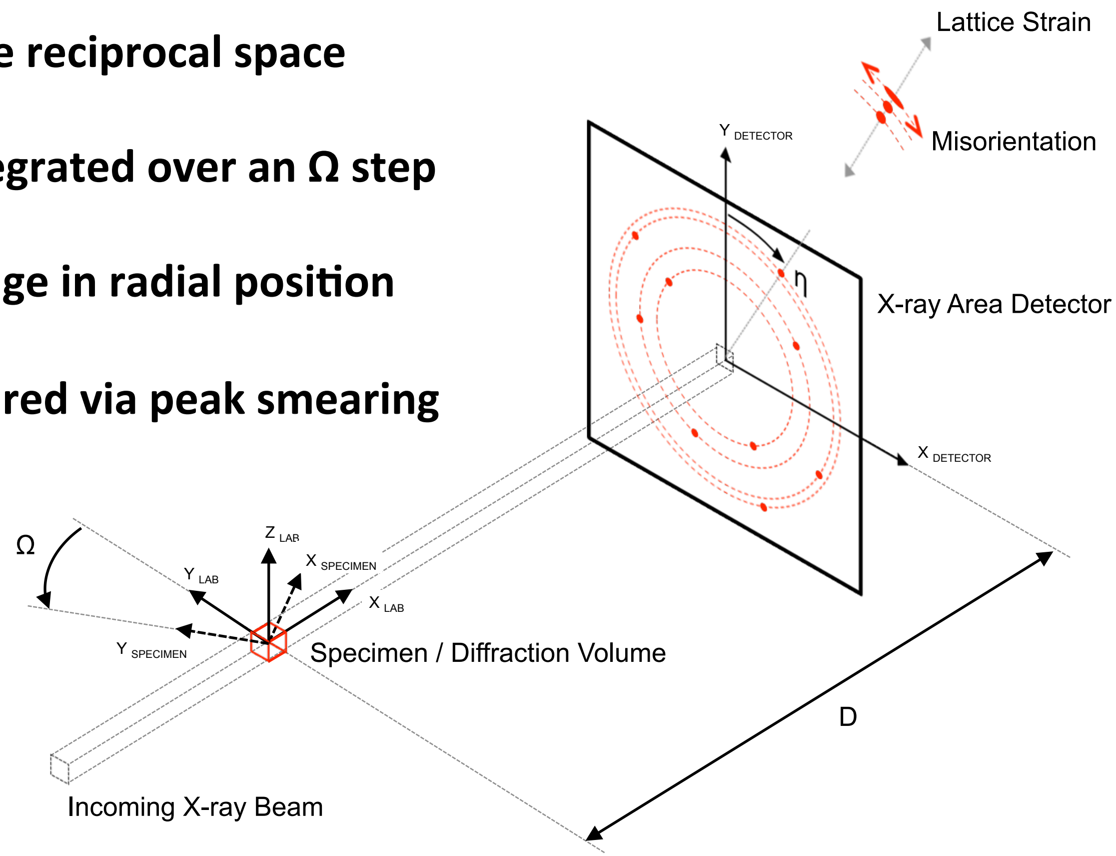
FAR-FIELD EXPERIMENT:

- Multiple diffraction peaks from individual grains
- Specimen rotated in Ω to sample reciprocal space
- Intensity of diffracted beam integrated over an Ω step
- Lattice strain measured via change in radial position
- Misorientation evolution measured via peak smearing
- Back projection
- Analysis is complicated
- Computationally cheap



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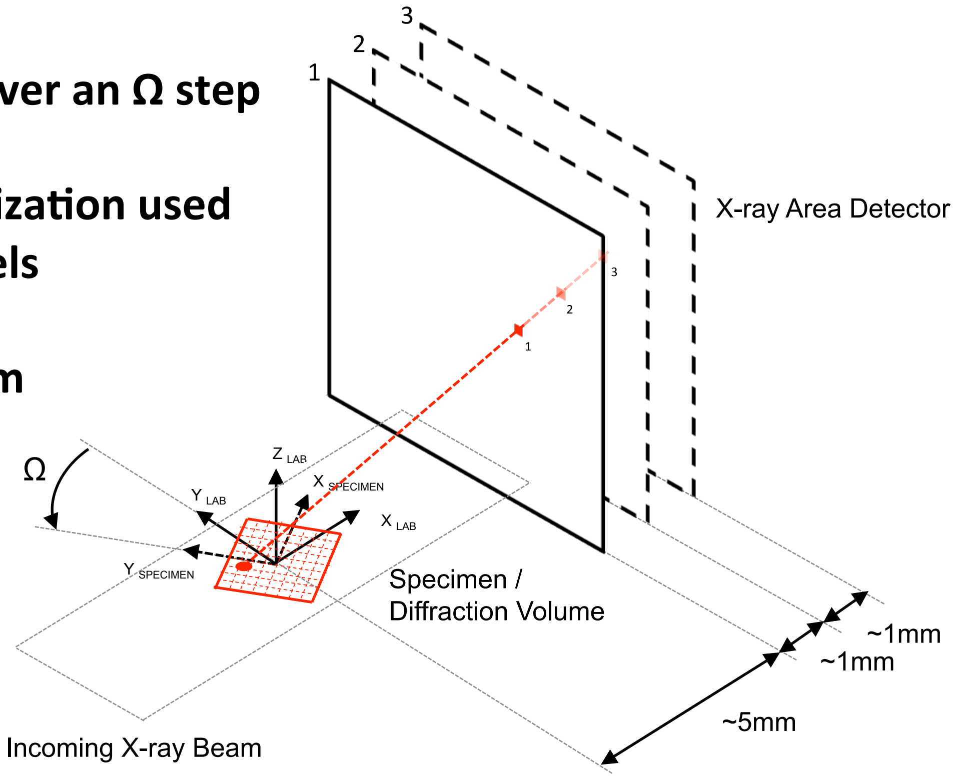
NEAR-FIELD EXPERIMENT:

- Multiple diffraction peaks from sub-grain regions
- Specimen rotated in Ω to sample reciprocal space
- Intensity of diffracted beam integrated over an Ω step
- Forward projection + Monte Carlo optimization used to determine orientation of discrete voxels
- Multiple detector positions + planar beam
- Forward projection
- Analysis is (relatively) easy
- Computationally expensive



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THE OVERALL COMBINED HEDM VISION:

- **Near-field experiments**
  - Orientation
  - Position
  - Sub-grain resolution

Orientation distribution
Orientation
Position

- **Far-field experiments**
  - Orientation
  - Position
  - Strain (and therefore stress)
  - Single grain resolution (centroids)

Orientation distribution

- **Lattice strain pole figures experiments**
  - Orientation distribution function
  - Strain (and therefore stress)
  - Fiber averaged resolution

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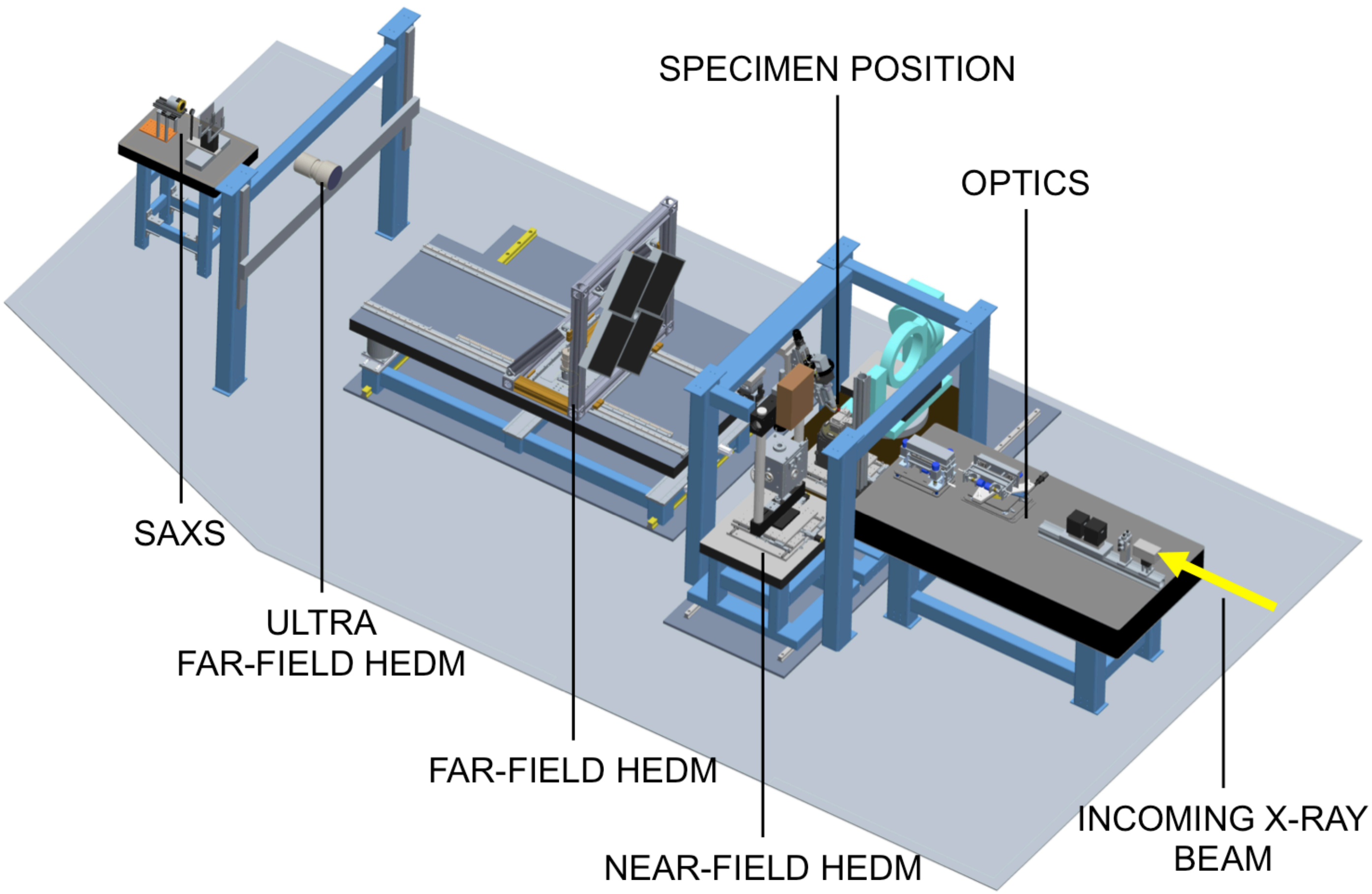
THE OVERALL COMBINED HEDM VISION:



Sector 1-ID E-Hutch at the APS (coming online soon)

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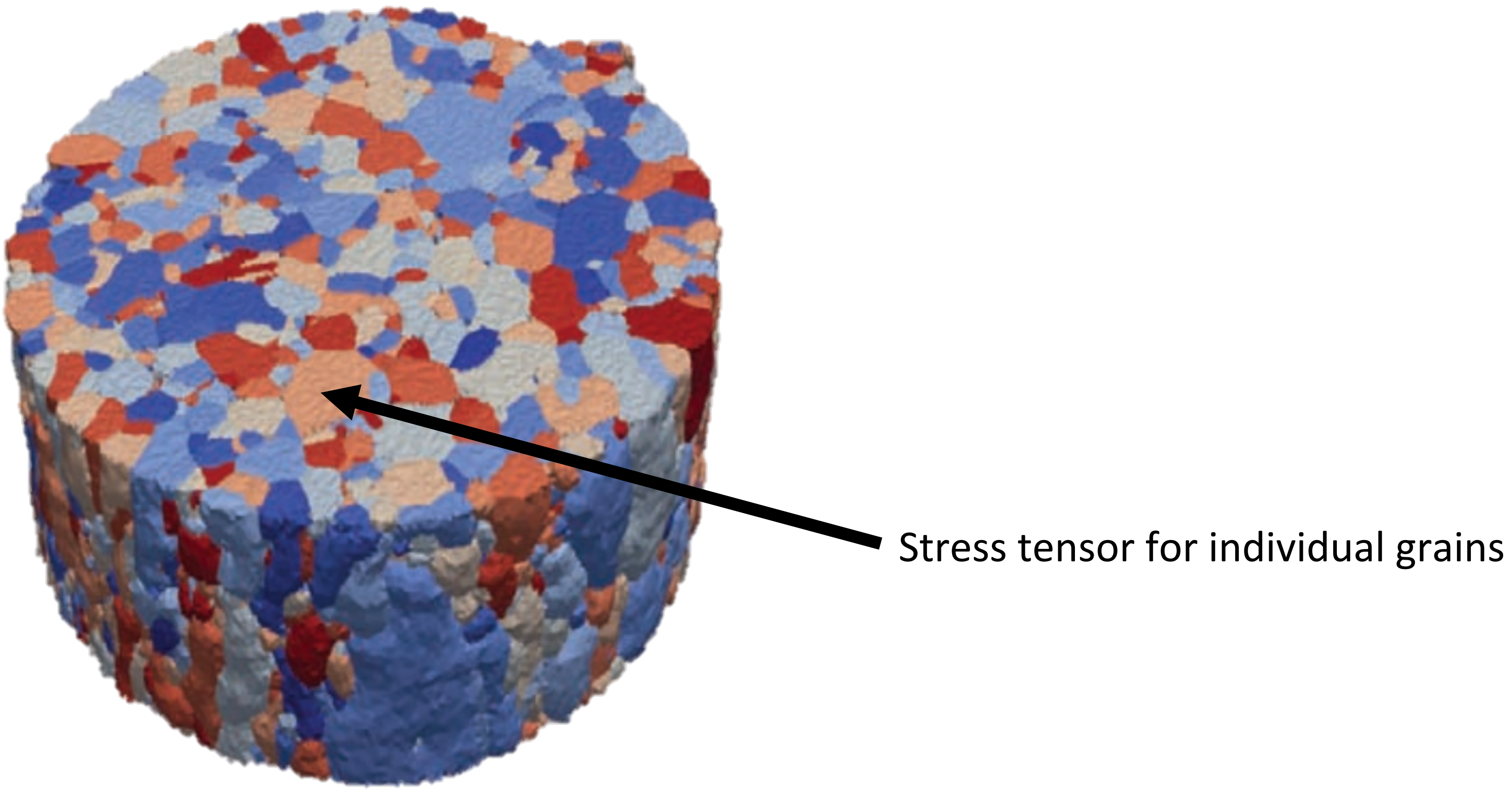
THE OVERALL COMBINED HEDM VISION:



Example near-field HEDM reconstruction of a polycrystalline specimen of pure Nickel, with colours indicating different crystallographic orientations, diameter = 1mm

Miller et al., 2012, "High-energy Needs and Capabilities to Study Multiscale Phenomena in Crystalline Materials", Synchrotron Radiation News

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WHAT YOU NEED TO BE ABLE TO DO HEDM EXPERIMENTS:

- Good experiment
- Instrument corrections / errors
- Rotations, orientations and transformations
- Stress and strain
- Diffraction
- <u>Combining it all together</u>

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STRUCTURE OF THE TUTORIAL:

- **Rotations and orientations**
- **Stress and strain**
- **High-energy x-ray diffraction (powder)**
- **High-energy x-ray diffraction (single crystal)**
- **In-situ high energy diffraction tensile test**

The idea of the handout and tutorial is to give you a structured, step-by-step framework for building up the basic toolsets you require to analyze HEDM data sets, whether they are near-field, far-field or lattice strain pole figures.

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QUESTIONS?

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