Three-dimensional polychromatic microdiffraction studies of mesoscale structure and dynamics

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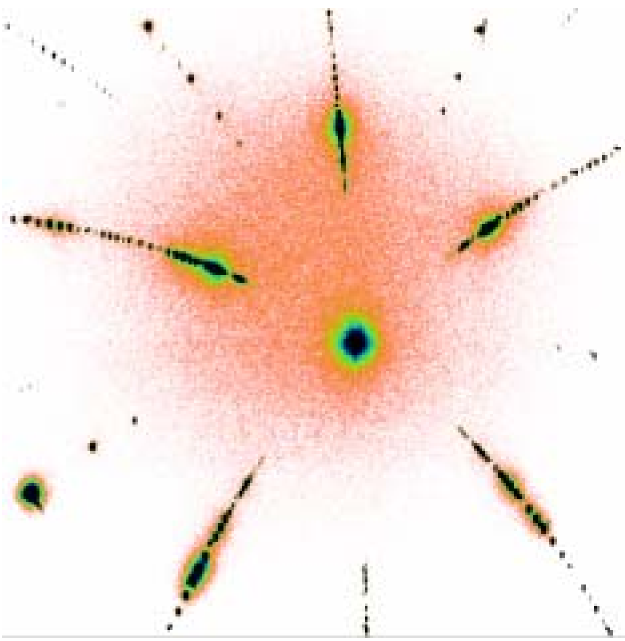
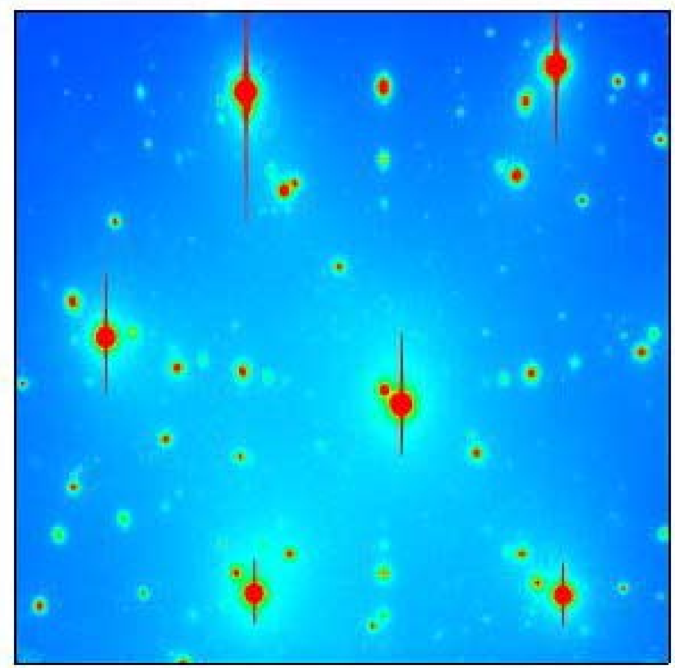
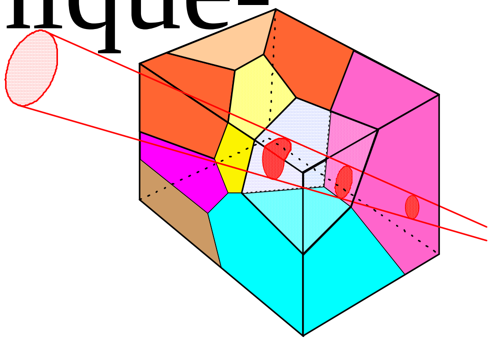




3D polychromatic microdiffraction important emerging technique-

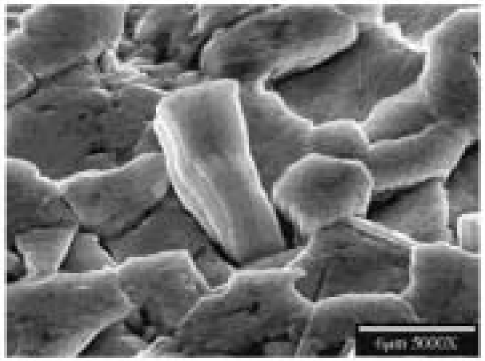


- Fundamentally new direction in materials research
- Unprecedented-direct test of mesoscale modeling
- Addresses long-standing fundamental problems

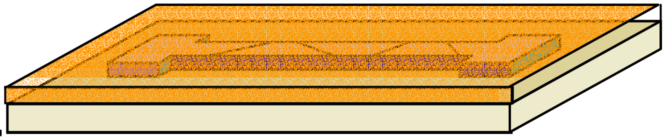
- Programmatic effort only possible at APS
  - requires synchrotron radiation - advanced x-ray optics
  - emerging capabilities only possible with intense 3rd generation source and continued progress

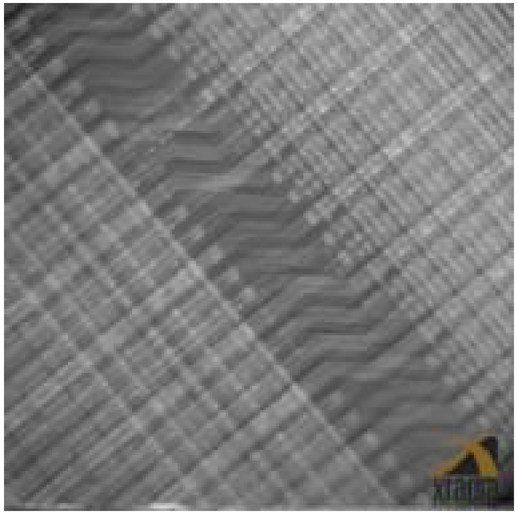
Will become an essential technique for x-ray synchrotron sources.

Virtually all materials influenced by structure and properties at *mesoscale*

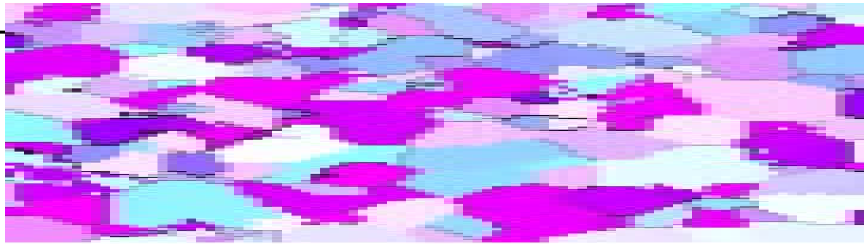


- **Electronic/electro-optic materials**
  - **Thin polycrystalline films/implanted layers defects/anisotropic domains**





- **Structural materials**
  -

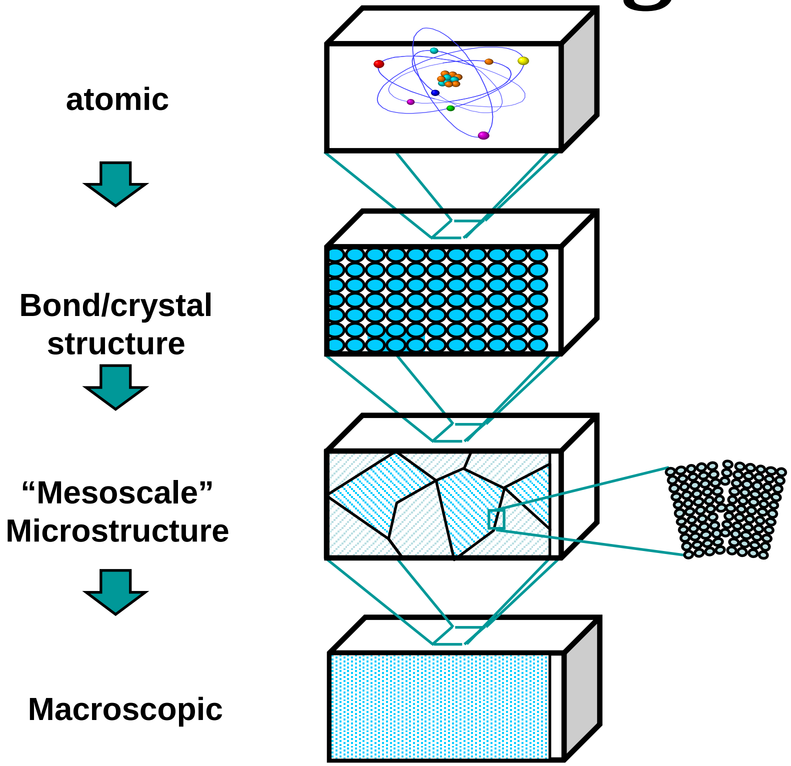


Yet most information -surfaces or property averages

Importance of mesoscale structure/ dynamics→multiscale modeling

- 0.1-100 μm
  - Too *large* - molecular dynamics
  - Too *small* - average behavior

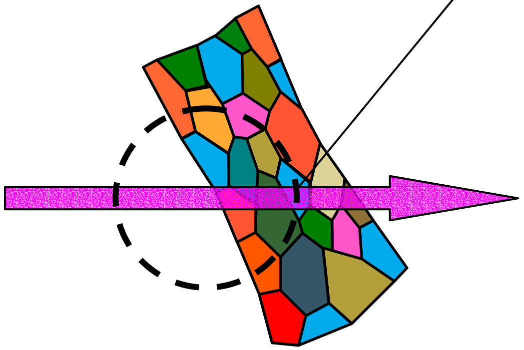
- Models need guidance
  - Grain boundary structure/properties
  - 3D Deformation
  - Elastic response of grain-boundary networks



Experimental measurements are essential to guide/test mesoscale modeling

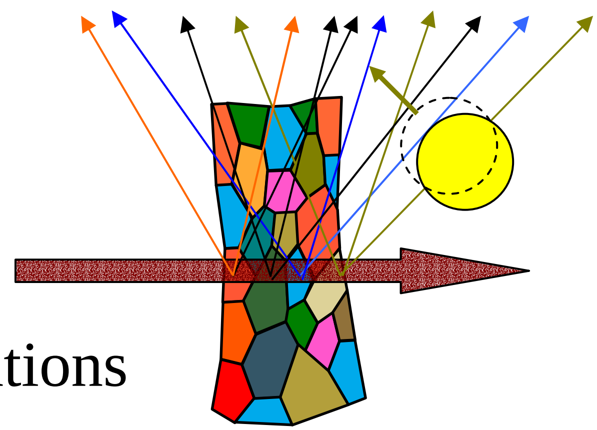
Polychromatic microdiffraction unique advantages

•***No*** sample rotation- high spatial resolution



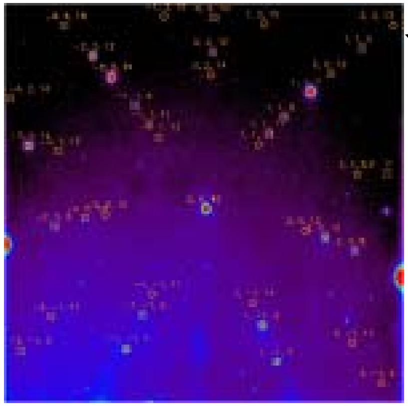
•***Single crystal*** information from every subgrain volume.
J. S. Chung and G.E. Ice J. Appl. Phys. 86 (1999).

•Differential aperture microscopy ***decodes Laue patterns*** along beam
B. Larson et al. Nature 415 (2002).



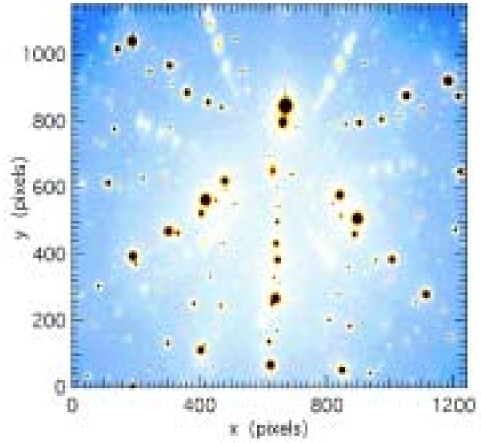
Allows investigation of mesoscale correlations

3DPMD correlates mesoscale structural heterogeneities and driving forces

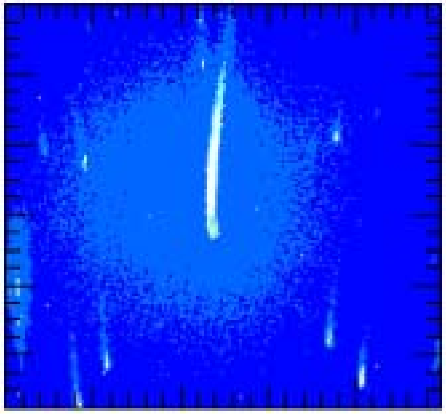


Phase/phase boundaries

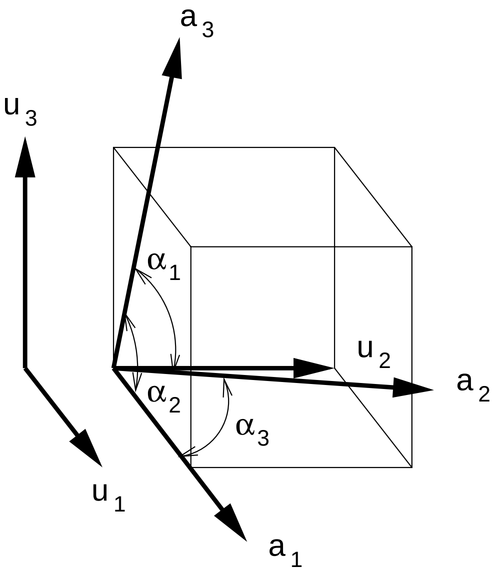
Texture (0.01º)/grain boundaries



Elastic strain (1 x 10^{-4})



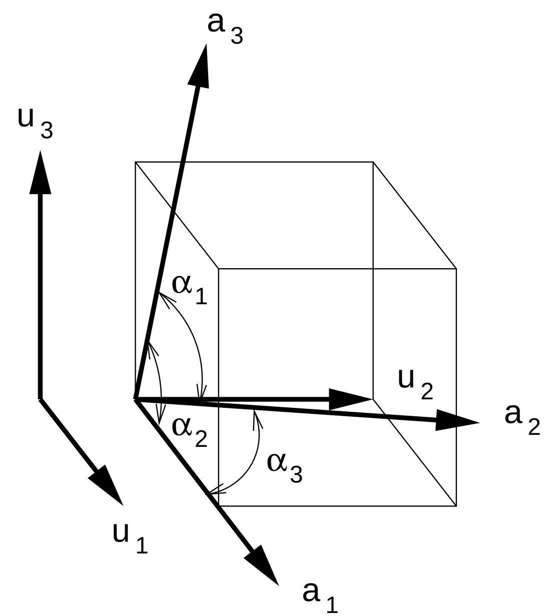
Deformation



Strain is derived from unit cell parameters

$$\mathbf{A_{Meas}=TA_0}$$

$$_{ij} = (T_{ij}+T_{ji})/2-I_{ij}.$$



Accurate measurements require absolute calibration

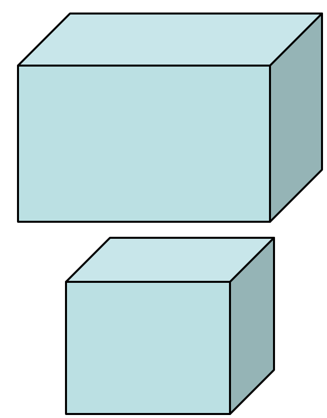
monochromator energy to ~1 eV

CCD to 0.2 pixels ~0.01 degrees

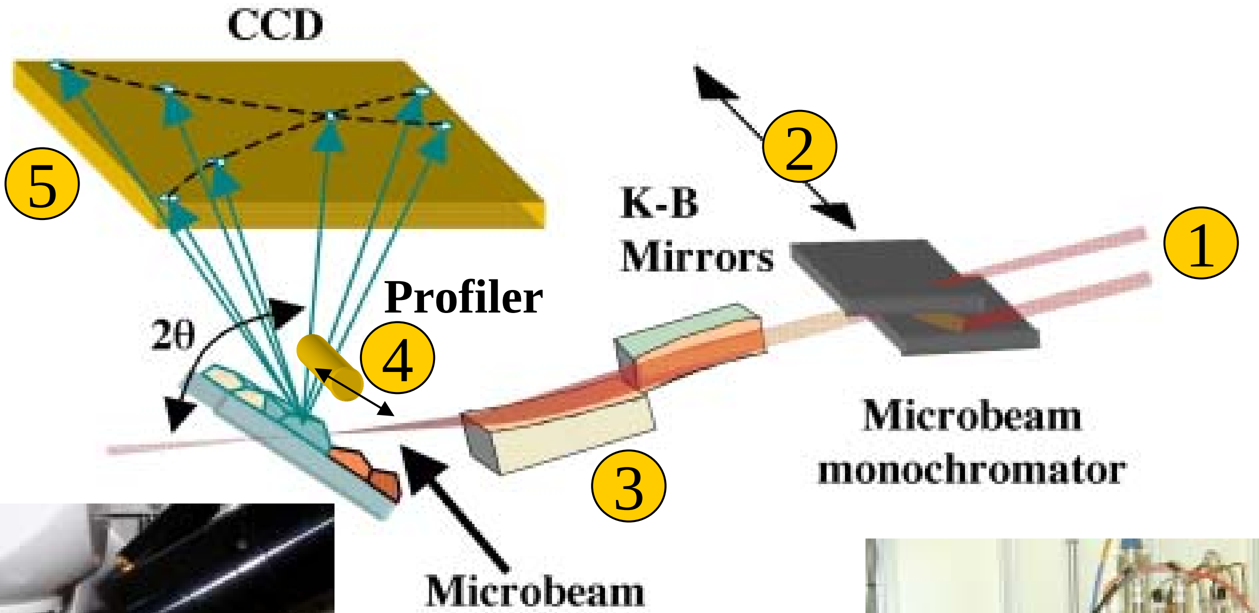
Deviatorial strain tensor from single crystal Laue pattern

4 reflections → deviatoric strain tensor

+ 1 energy → full strain tensor



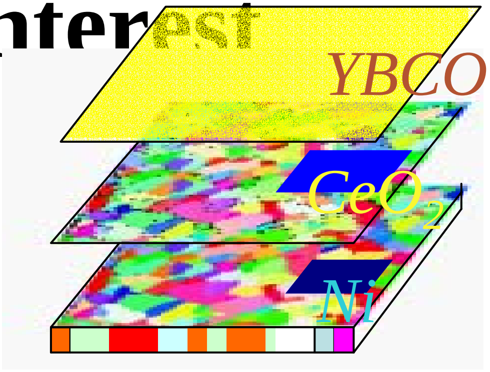
3-D Polychromatic Microscope has 5 key Elements



Operational 3D X-ray crystal m

- 10-22 keV
- Differential aperture microscopy with software

Programmatic mission centered on three areas of long-standing interest

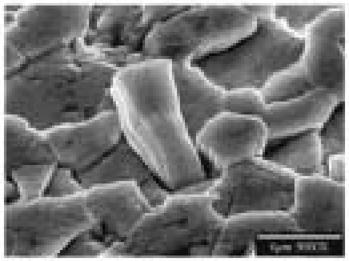


- Grain-growth
  - Epitaxial (near surface)
  - True 3D

- Deformation and strain localization
  - Mesoscale deformation using nanoindents
  - In-situ deformation in polycrystals

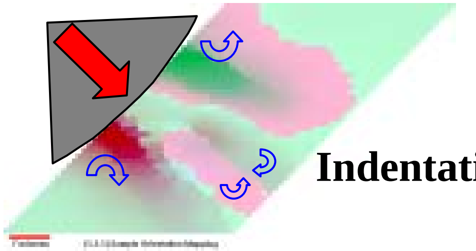
uickTime™ and a Video decompressor are needed to see this picture.

Al Polycrystal



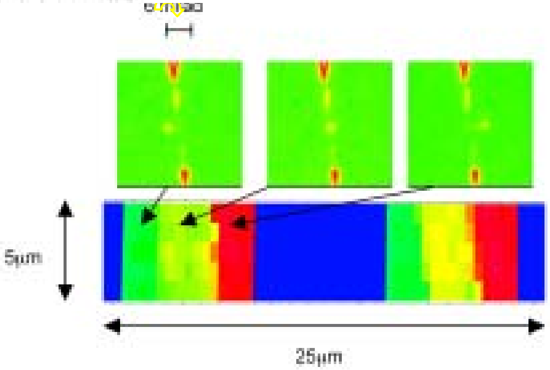
Tin Whiskers

- Fatigue and fracture
  - Thin films
  - Artificial cracks



Indentation

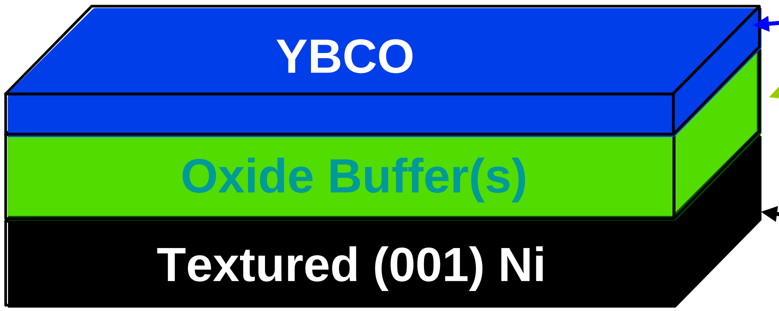
Compelling applications to many materials



GaN on SiC

Rolling-Assisted Biaxially-Textured Substrates (RABiTS) practical approach High T_c Wires

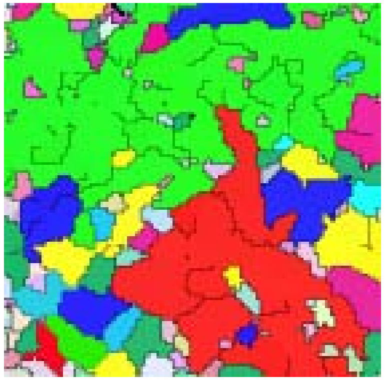
RABiTS Architecture



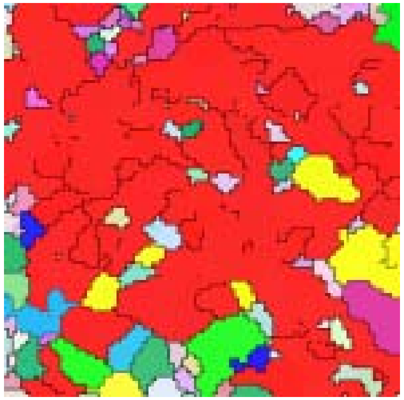
Epitaxial Oxide Buffer(s) and Superconductor

Cube Textured Ni Tape {001} <100>; ~7° Mosaic

- Texture controls current transport
- Texture can be improved by buffer
- Scale-up requires fundamental understanding of epitaxial growth.



Ni



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