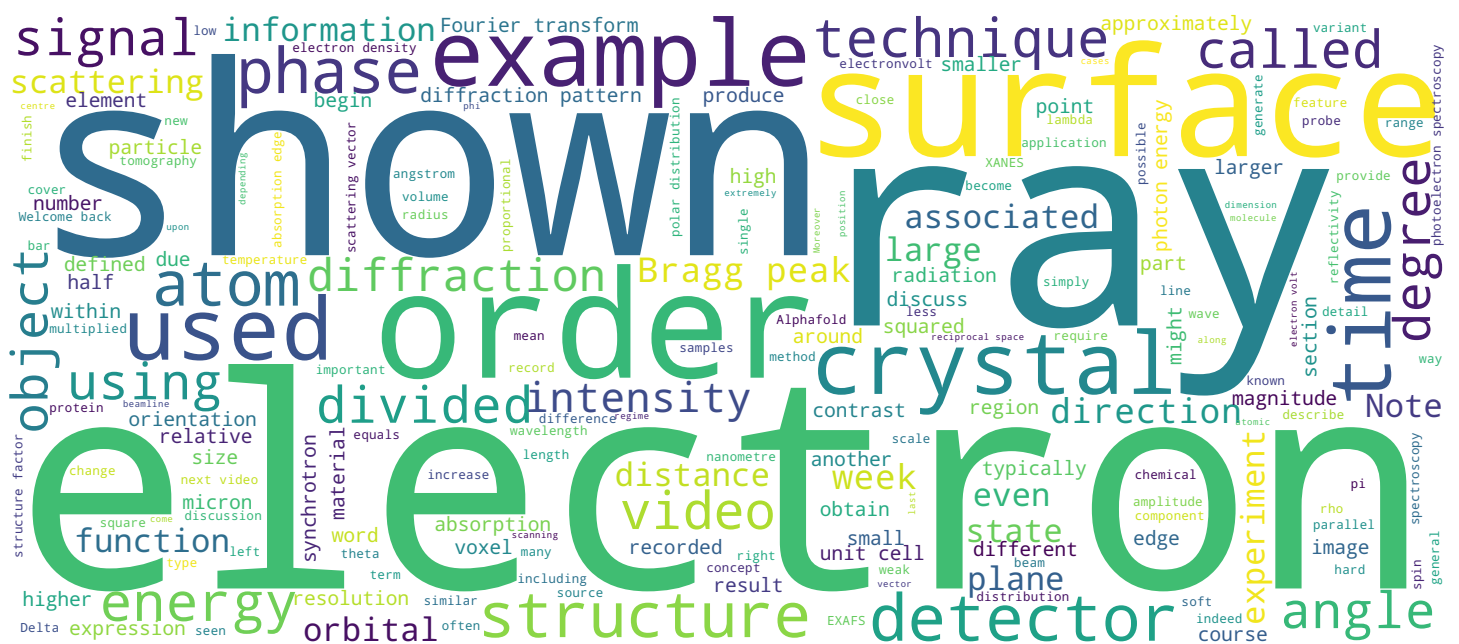


Higher-dimensional imaging

Synchrotrons and x-ray free-electron lasers

Techniques and applications

Prof. Philip Willmott



Search MOOC



Video



Contents and objectives of this video



- Vector ptychography
 - Example
- Scanning SAXS tensor tomography
 - Example

Hi again. In this penultimate video of the entire course, we consider higher dimensional imaging based on scattering methods. We will look at vector ptychography and scanning SAXS tensor tomography, providing examples in both cases.

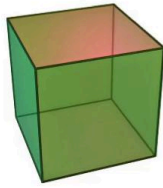
Notes

Summary

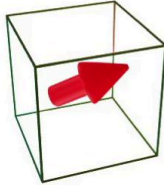


0m 11s

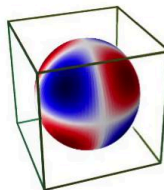
From scalar to vector to tensor



- “Standard” CXDI, ptychography, laminography yield scalar properties for each voxel
 - e.g., electron density



- Progress to directional properties in each voxel
 - Magnetic direction
 - Piezoelectricity
 - ...



- Tensor properties within a voxel also possible
 - Full 3D spatial distribution of given property within voxel

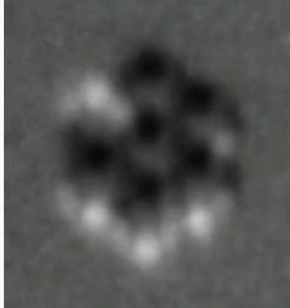
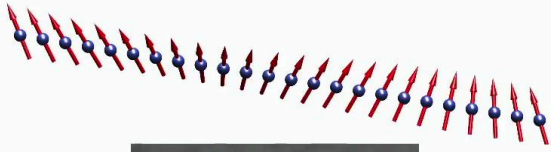
What do I actually mean with higher dimensional? In normal tomography, each voxel is associated with a scalar property, in other words, a property having magnitude only. Typically this might be the electron density. However, many material properties have both magnitude and direction, and as such are vector properties. Obvious examples include magnetism and piezoelectricity. Now lastly, full tensor properties can be represented in which a distribution of vector properties can be recorded within the pixel volume.

Notes

Summary



Vector PXCT – nanomagnetism



- 3D study of nanoscale magnetic materials
 - Basic research
 - Spintronics
 - Storage
 - Energy-harvesting industry
- Transmission electron microscopy
 - Limited to depths < 10 nm
- SXR microscopy
 - Limited to depths < 20 nm
- HXR transmission to many microns
 - GdCo_2
 - L-edge of Gd @ ca. 7.2 keV

We begin with vector ptychography, in which the magnetic domain orientation dependent dichroism associated with the p half and p3 halves of the L-edge of magnetic materials under illumination with circularly polarised X-rays can be exploited to generate a vector tomographic reconstruction. Nanoscale magnetism is of great importance not only in basic research, but also in technologies such as spintronics, data storage, and in the energy harvesting industry. Such hard X-ray imaging techniques have a distinct advantage over transmission electron microscopy or soft X-ray techniques due to the former's much larger probing depths, enabling the investigation of macroscopic objects.

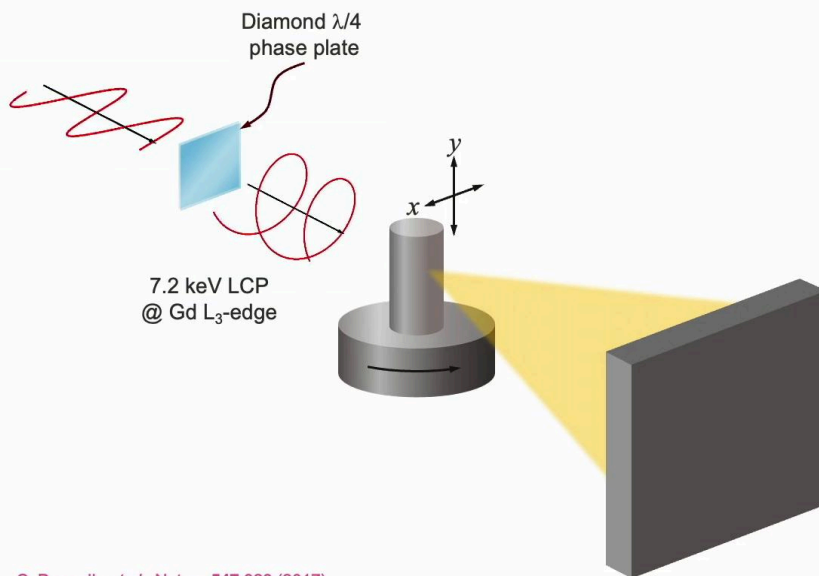
Notes

Summary



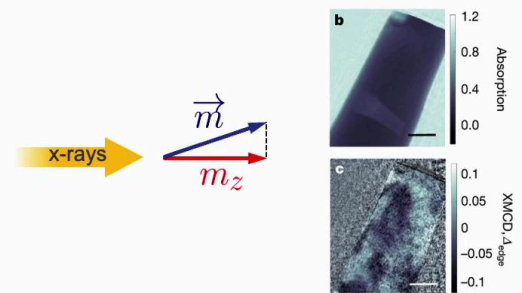
1m 06s

Vector PXCT – magnetism



[C. Donnelly et al., Nature 547 328 \(2017\)](#)

- GdCo₂ pillar, 5 μm diameter
 - Rotate and scan x- and y-directions
- Circular polarized x-rays sensitive to component of magnetization in the propagation direction
- Rotating the sample therefore changes the absorption coefficient
 - \Rightarrow domain contrast
 - In contrast to standard absorption in lensless imaging



In the presented example, a gadolinium copper two pillar of five micron diameter was tomographically investigated using circular polarised radiation. The sense of that radiation, either left or right circularly polarised light, causing different scattering and absorption responses. The system is dichroic. This, in combination with the dependence of this dichroic contrast on the orientation of the magnetic axis, yielded a three-dimensional image with domain contrast.

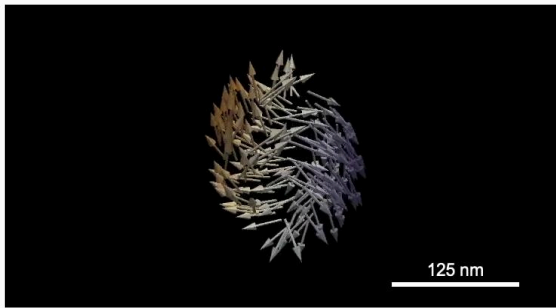
Notes

Summary



2m 00s

Vector PXCT – magnetism



[C. Donnelly et al., Nature 547 328 \(2017\)](#)

- “Magnetic vortices” form when electron spins swirl in a circle within a plane
 - At the centre of the circle, swirl becomes tighter and tighter – “Bloch point”
 - Eventually magnetization at the core tilts out of the plane
 - Prior to this work, magnetic vortices widely studied in 2D systems, but remained only a theoretical prediction in 3D
- Vortices shown to be surprisingly stable to both temperature and externally applied magnetic fields
 - Stability thought to be provided by pinning to domain walls

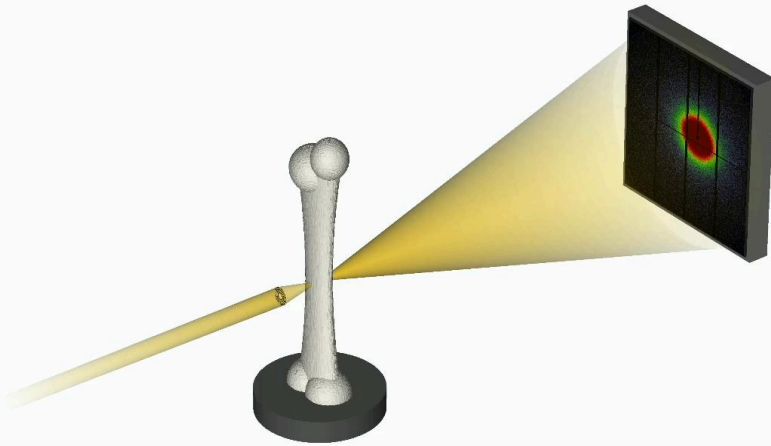
It was observed that magnetic vortices arise when electron spins swirl in a circle within a plane. At the centre of the circle, the swirl tightens like water going down a plughole. This is known as a Bloch point. At some point the magnetism needs to tilt out of the swirling plane. This is the first time that magnetic vortices have been seen in 3D systems. They were shown to be surprisingly stable to both increases in temperature and the application of external applied magnetic fields, which has been proposed to be due to their pinning to domain walls.

Notes

Summary



Scanning SAXS tensor tomography



- SSTT
- In each voxel (x, y, z) study a tensor property
 - Physical size
 - Intensity distribution
- Requires six degrees of freedom

In scanning SAXS tensor tomography, we up the game still further. For each and every voxel, we obtain tensor properties. Now tensors can come in different flavours and complexity. In SSTT, we want to describe a certain physical property's spatial distribution for each voxel. This results in a three-dimensional distribution for each voxel, and thus requires six degrees of freedom to obtain this information.

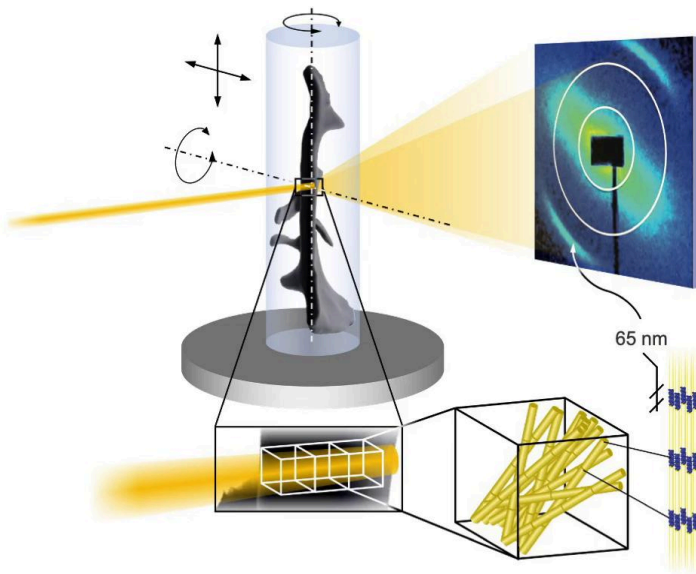
Notes

Summary



3m 13s

SAXS tensor tomography



- $I(\theta, \phi, x_s, y_s, x_d, y_d)$
 - Tensor property
- Within a given voxel @ (x, y, z)
 - $I(Q, \theta, \phi)$
- Detector sees integrated signal of all voxel contributions along direction of propagation
 - Separate using tomographic methods

Now these are obtained in an SSTT experiment by two translations x_s and y_s and two rotations theta and phi of the sample, plus the pixel positions x_d and y_d on the detector. With this information, one can generate for each voxel a polar distribution of the intensity for a given scattering vector. Because the detector sees the integrated signal from all voxels lying in the path of the incident beam, tomographic methods are applied in order to separate these.

Notes

Summary



3m 47s

SAXS tensor tomography

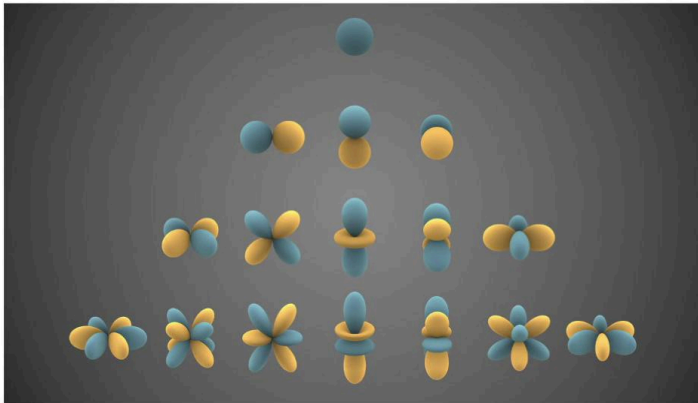
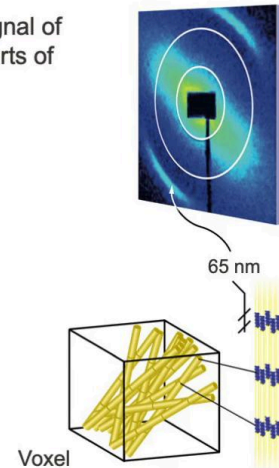


Image: [Inigo quilez](#) Creative Commons

- Any distribution $I(\theta, \phi)$ can be described as a linear combination of spherical harmonics Y_l^m
- Angular distribution of intensity of given Q-value(s) associated with certain SAXS features
 - e.g., 65-nm signal of mineralized parts of collagen fibrils



This polar distribution was generated using so-called spherical harmonics. These are expressions also used to express the different wave functions of an electron within a hydrogen atom, that can be summed up as a linear combination to describe any angular distribution of given scattering vector values associated with certain SAXS features. The main scattering feature of interest in the particular experiment here was the anisotropic ring, associated with a length of 65 nanometres, produced by mineralised parts of the collagen fibrils in the bone.

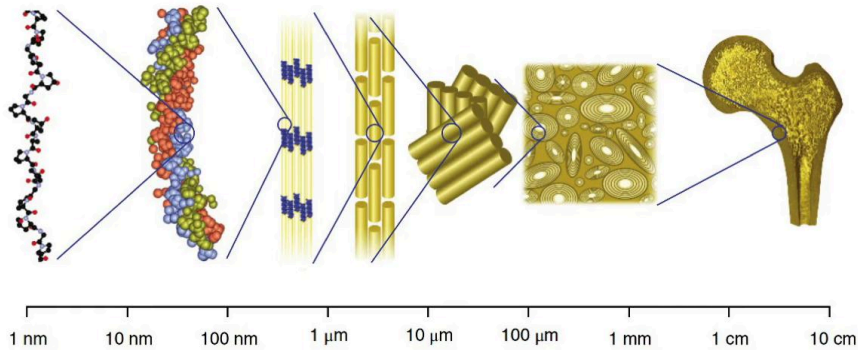
Notes

Summary



4m 26s

SAXS tensor tomography – example: down to the bone



- Biology
 - Principle of hierarchical ordering
 - Maximize functionality
 - Strength
 - Robustness
 - Minimize weight and energy cost
- Bone
 - Multiple length scales
 - Collagen molecules (nm)
 - Microfibrils
 - Fibrils
 - Lamellae
 - Osteons (mm)

See M. Liebi *et al.*, <https://doi.org/10.1038/nature16056>

Bone structure is a classic example of hierarchical ordering in biology, an evolved nested architecture driven by the biological need for high strength and robustness at a minimum cost to weight and energy cost. Consequently, bone contains features at multiple length scales from the basic molecular building blocks of collagen all the way up to ellipsoidal and cylindrical osteons on the millimetre scale.

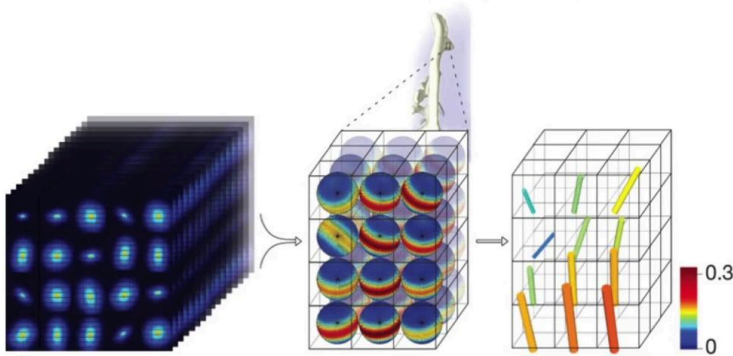
Notes

Summary

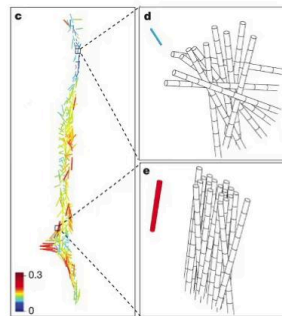


5m 05s

SAXS tensor tomography – example



- Human trabecular (spongy) bone
- Pencil beam $\phi = 25 \mu\text{m}$
- Concentrate on 65-nm feature of mineralized collagen microfibrils
- $> 10^6$ SAXS patterns
 - Reconstruct 3D reciprocal-space map for each voxel
 - Model using spherical harmonics
 - Provides representation of nanoscale structure distribution
- From reconstruction
 - Main ultrastructure orientation depicted by orientation of the cylinder
 - Degree of orientation the orientation of the cylinder illustrated by
 - Colour: indicating the ratio of anisotropic scattering to total scattering
 - Length of the cylinders: total scattering intensity



In the example given here, a human trabecular or spongy bone was investigated using a pencil beam with a diameter of about 25 microns, which thus defined the voxel size. The experiment concentrated on the 65 nanometre feature of those parts of the collagen microfibrils that mineralise in order to increase strength and rigidity. More than one million SAXS patterns were recorded. Via description of the intensity polar distribution as a sum of spherical harmonics, 3D reciprocal space maps were generated for each voxel. This was depicted by the orientation, length, and colour of cylinders. Clearly, the orientation and length correspond to the orientation in space and strength of the mineralised collagen signal. The colour describes the degree of anisotropy, red indicating very strong anisotropy, blue, little or none.

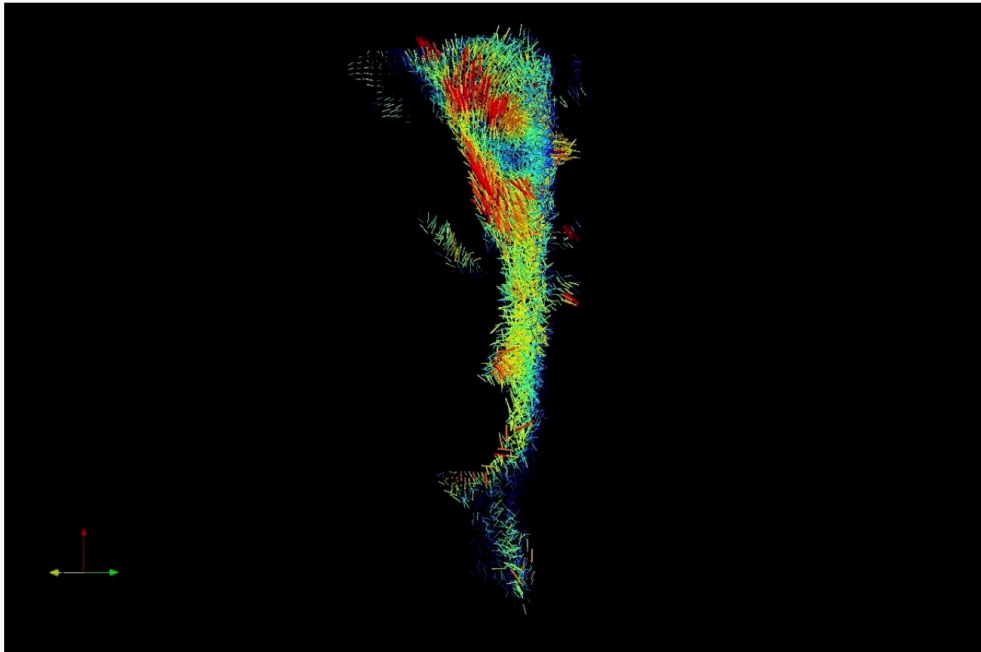
Notes

Summary



5m 35s

SAXS tensor tomography – example



This is summarised in this mesmerising movie. There are regions, for example, in the broad fanlike upper section of the sample, where the bone has a marked anisotropy, almost certainly due to these parts experiencing forces in real life in a particular direction; while other regions, such as down the main shaft and towards the bottom, exhibit anisotropies that are weak or non-existent.

Notes

Summary

6m 36s



In the next video...



In the next video and final video of this course, we discuss X-ray photon correlation spectroscopy. See you in the home straight.

Notes

Summary



7m 04s