Computational Challenges in Rich Tomography

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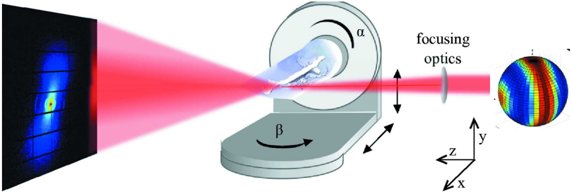
What is Rich Tomography?

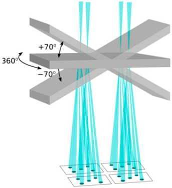
- Typical **scalar** tomographic methods have **one scalar** measurement for each **source** and **detector position**. From this one seeks to recover a **scalar image**.
- **Rich tomography** methods measure higher dimensional data for each source and detector location. For example a
  - polarization state (matrix),
  - spectrum (function of one variable),
  - diffraction pattern (function of two variables),
  - histogram or distribution (function of one variable).

  The image sought can then also have more than one dimension per voxel, for example a
  - function of reciprocal space (three variables),
  - vector such as magnetic field or velocity, or an orientation (line field),
  - tensor such as strain, or
  - the amount of each of a finite number of materials.

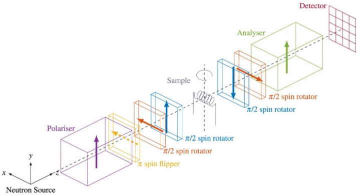
Examples I



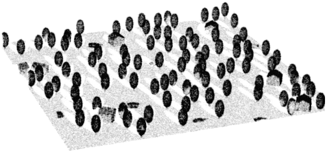
(a) Small angle X-ray scattering tomography, after Liebi[4]. On the right is a reciprocal space reconstruction for one voxel and reciprocal length



(b) Scanning electron diffraction tomography [5].



(c) The set up for Polarimetric Neutron tomography of magnetic fields, after [2].



(d) 3D synthetic apperture radar

ToF neutron spectral tomography I

For neutrons spectroscopy is easy as Time of Flight (ToF), hence speed, is inversely proportional to wavelength.

- Neutrons produced by neutron spallation sources have wavelengths comparable to interplanar lattice spacings. Polycrystalline materials will scatter the incident beam elastically according to Bragg's law.
- Since Bragg scattering can occur only for wavelengths shorter than twice the spacing between the lattice planes, the transmitted neutron spectrum exhibits characteristic abrupt increases in the transmitted intensity at these wavelengths.

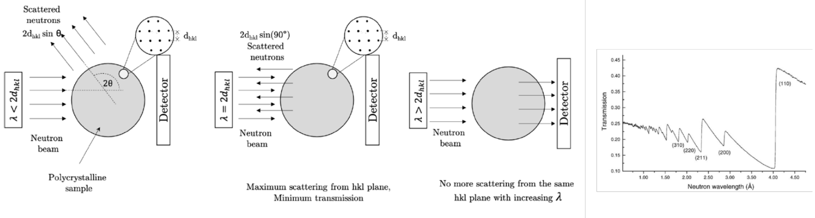


Figure: Principle of Bragg edge transmission technique and transmission spectrum of neutrons through 2.5 cm of iron powder displaying characteristic Bragg edges. Figure from[3].

ToF neutron spectral tomography II

- Pulsed neutron source emits a broad spectrum of wavelengths.
- Neutrons reach the sample and then the detector at different times according to their energy.
- The relation between spectral fingerprint and crystalline properties allows identification of polycrystalline materials and characterisation of their properties such as phase, texture and strain.

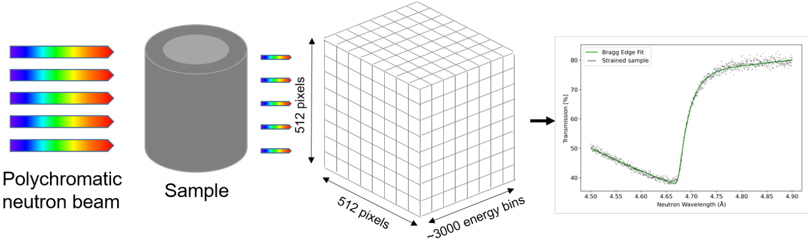


Figure: Implementation of Bragg edge transmission technique. We infer the energy and hence wavelength of each detected neutron from its time of flight from the source to the detector. Right figure from[3].

ToF neutron spectral tomography III

How much data?

Dataset we acquired at IMAT ISIS in November 2019[1].

- MCP detector has 512×512 pixels and measure up to 3000 ToF bins
- Number of projections was 120.
- Total measurement time 32h (15 min exposure)
- Total data (number of equations before regularization) $\approx 10^{11}$.

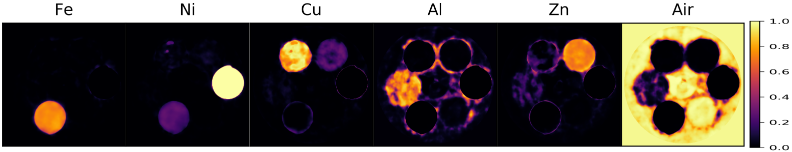
Acquisition is extremely slow. The trade-off between the number of measured projections and the number of neutrons per projections is unclear. Golden Ratio angular sampling is beneficial, especially in probable case of hardware failures.

ToF neutron spectral tomography IV

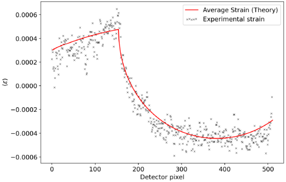
Reconstruction

- Number of counts in each channel depends on wavelength and detector settings. Varies quite significantly across spectrum.
- Noise model in projection data is neither Gaussian nor Poisson.
- In principle, each energy bin can be reconstructed individually however inter-channel correlation has shown significant improvement.
- Alternatively, we can decompose spectral data in individual material maps (prior, simultaneous or after reconstruction)
- In case of strain tomography, we need only a region around Bragg edge with sufficient resolution to extract the cumulative histogram of the component of the strain.

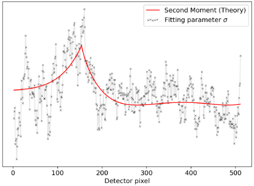
ToF neutron spectral tomography V



(a) Material maps retrieved from ToF tomography[1].



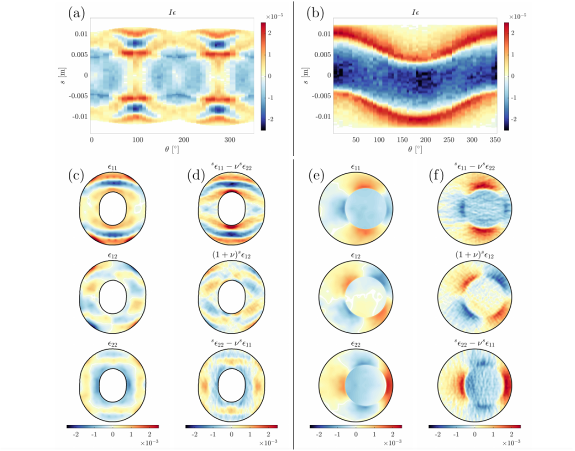
(b) Plot of the average strain in the within the sample as a function of detector pixel[3].



(c) Plot of the variation of the σ fitting parameter as a function of detector pixel for the strained sample[3].

Neutron strain results

Experimental results of Bragg edge strain tomography compared to direct strain diffraction measurements. Data (a),(b). two samples. (c) and (e) direct measurement, (d) (f) reconstructions.



Details see ArXiV:2309.02440 Wensrich et al [6]

Electron Diffraction Tomography I

- A Scanning Transmission Electron Microscope (STEM) scans a narrow beam of electrons, and typically the dark field (diffraction pattern) is used for imaging in materials science, in contrast to eg Cryo-EM for biology.
- With a tilt stage this can be used for STEM diffraction tomography, tilt angle is always limited, typically to $\pm 70^\circ$
- There is a wide range of applications and theory is the same as SAXS except for limited angle.
- Our special interest is strain tomography of a single silicon crystal (eg for electronics)[5]

Electron Diffraction Tomography II

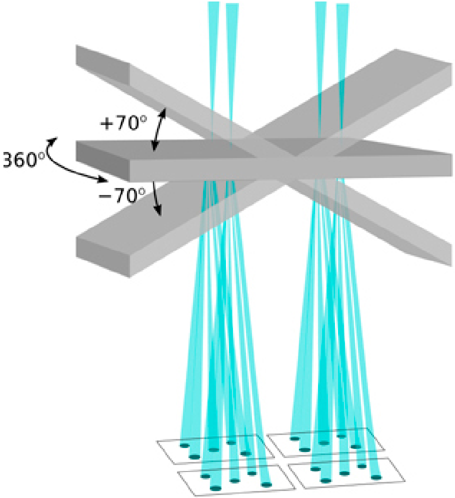


Figure: Scanning Electron Diffraction Tomography tilt sequence after[5], for a single crystal each beam results in a pattern of diffraction spots, blurred by the variation of strain along the beam path.

Electron Diffraction Tomography III

How much data?

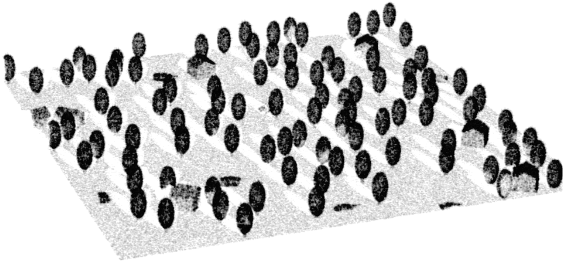
- Typical experiments are on a modest scale at the moment with 40 projections 1000^2 (rebinned to 100^2) sensor and 50^2 beam positions. Total of only 10^9 measurements, but these are early days for this experimental technique
- Limited angle as well as scattering of diffracted electrons remain significant problems.
- Each diffraction spot is essentially a 2D histogram of displacements of atom positions along the beam, blurred by the transfer function of the system. Formulated in this way it is a non-linear problem.

Synthetic Apperture Radar (SAR)

- We are looking at *Volumetric*, ie 3D SAR imaging
- Multistatic: transmitter and receiver in different positions.
- Basic model is integrals over spheroids of constant travel time, with transmitter and receiver at foci.
- Data and image are *complex* as phase is measured
- Polarization can also be measured
- scatterers can be anisotropic
- Multi frequency
- Traditional methods use Fourier domain filtering.

Volumetric SAR

Preliminary results using CGLS/Tikhonov as in CIL show that it is (just) feasible. Image shows a reconstruction from simulated data.



Conclusions

- Rich tomography methods result in potentially huge increases in the scale of reconstruction problems.
- Using theoretical insights and optimal design of experiments we can cut the data size without reducing the relevant information about the image.
- Some problems have a natural product structure and so can be parallelized. However regularization usually breaks that, coupling across layers, frequencies etc, so there are compromises to be made.
- Model based approaches and using a priori information systematically decreases number of unknowns.
- Non-linearity, low count data and the need for uncertainty quantification leads us towards Bayesian (MCMC) methods, which are inherently computationally expensive.

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