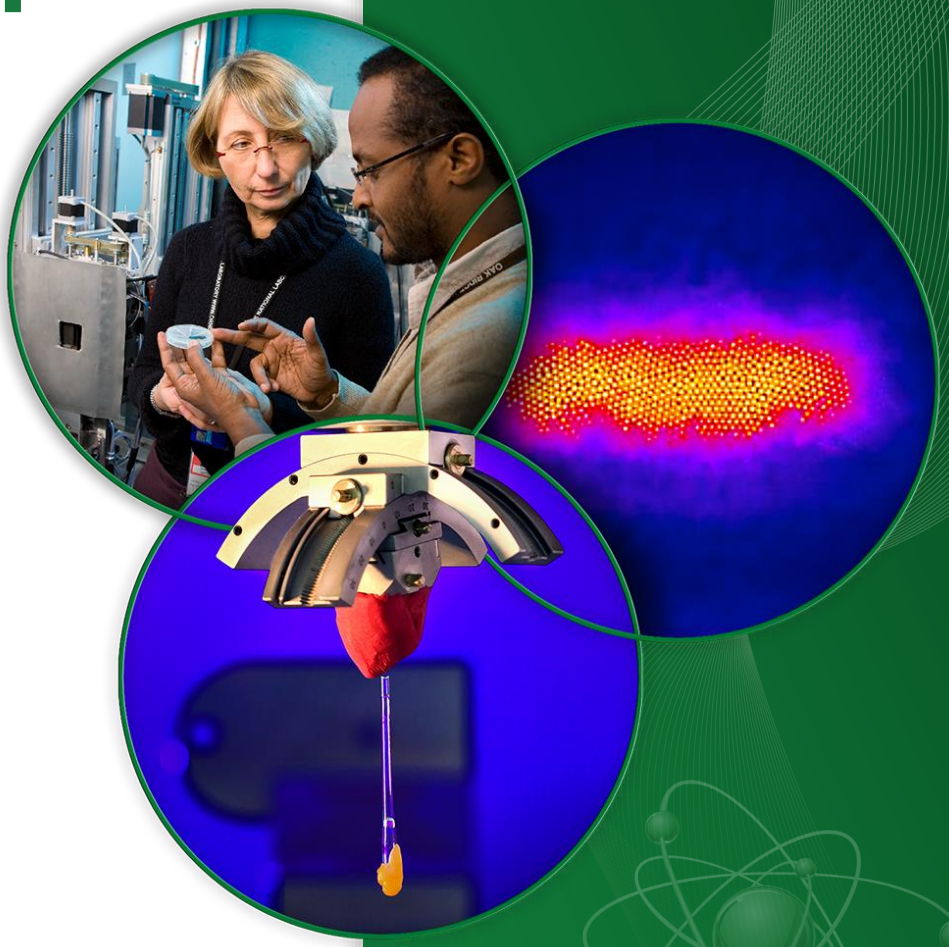
Challenges and opportunities in modeling anisotropic and multiscale data

Ken Littrell

ORNL CEMD



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what are the concerns

- Sample is intrinsically 4-dimensional—at least
  - a volume of sample filled with 3-dimensional scattering objects that
- Measured data on a pinhole instrument is 3 dimensional
  - x,y, and time
- models used in least squares are one-dimensional
  - derived for static objects in correlation space for randomly oriented objects
- multiscale data
  - unless you are on the Ultimate TOF instrument, measured in different configurations
  - may be measured on different instruments
  - may have different probe volumes
  - will be measured at different times

What do “we” do now about anisotropy?

- ignore it
  - if your pattern looks isotropic and your sample is slowly varying, you’re probably safe
  - if you’re seeing anisotropy, not such a good idea
- wedge average or single-q annular plots
  - good if anisotropy is well-described, like for separating nuclear and magnetic scattering,
  - catches the highlights nicely
  - loses resolution through rebinning
- fit 2-d data
  - to what model?

How do “we” handle multiscale data

- usually just string it together
  - “looks better” for users and presentation
  - line it up/ superimpose with a selected scaled data set
  - Rex Hjelm: It actually shouldn’t line up
  - especially at the ends of the overlap region or if there are sharp features
- try to fit the data simultaneously
  - resolution effects
- fit (and present) the data piecewise
  - important for time-series data measured in different configurations
  - doesn’t explicitly connect correlations between behavior on different length scales

What should we be doing

- Adrian Rennie: why don't you fit the data you have?
  - 2-d patterns changing with time
  - sparse, event-mode data sets
- Agreed, but how and to what?
  - 2-d models and their theoretical basis
  - constrained simultaneous fits
  - fitting methods for comparing expected event probabilities with observed events to separate models

Comments/notes

- highly oriented rods, lamellae numerics
- basic structure from microscopy
- RMC
- analytical models have limitations
- harmonics have symmetry. where does it break?

rolled steels

- Parallel/perp to field
- highly oriented rods or lamellae (Hayter)

focusing sans

- colloidal systems
- multiscale data
- butterfly pattern

highly ordered system

- rheosas—spot data
- colloidal crystals
- cubic-hexatic (Kansas)
- similarity to residual stress
- Prdhomme/Princeton D. Scneider/brookhaven pluronincs under shear
- Wolff's talk

Q resolution for time of flight

- Hjelm 1988 J Appl cryst v21 p618
- Journal of neutron research v6 p79 1997
- Long pulse—width important!
- event mode resolution
- Absorption correction debeer/lambert relevance
- anomalous transmission