MSE 675 Advanced Analysis of Structure and Dynamics of Crystalline and Non-Crystalline Matter

Textbook: "X-Ray Diffraction", B. E. Warren (Dover, NY, 1990), "Underneath the Bragg Peaks: Structural Analysis of Complex Materials", T. Egami and S. J. L. Billinge (Pergamon Press, Oxford, 2003; 2012), copies distributed in the class.

Recommended reading: "X-Ray Diffraction Procedures", H. P. Klug and L. E. Alexander (John Wiley, New York, 1974)

Instructor: Prof. T. Egami (egami@utk.edu)

Time: Wed 2:30 – 4:55

Synopsis:

The purpose of this course is to introduce graduate students in materials science, physics, chemistry and biochemistry to modern methods of characterization of structure and dynamics using x-rays and neutrons. In the last two decades synchrotron based radiation sources (synchrotron radiation sources and spallation neutron sources) have revolutionalized the scattering methods to characterize atomic structure and dynamics in solids and liquids, including surfaces. Starting from the basics, this course covers theories and practices necessary to carry out and utilize these advanced techniques.

Outline:

1. Introduction
    - 1.1 Bragg's law, reciprocal space, diffraction vector.
    - 1.2 X-ray diffraction; generation of x-rays, detection of x-rays, interaction of x-rays with matter
    - 1.3 Neutron scattering; generation of neutrons, detection of neutrons, interaction of neutrons with matter
2. Diffraction theory
    - 2.1 Scattering theory, partial wave analysis, phase-shift
    - 2.2 Wave interference, form factor, structure factor,
    - 2.3 Crystallographic analysis, powder and single crystal analysis, the Rietveld method, magnetic scattering
    - 2.4 Small angle scattering, theory and practice, FT technique
    - 2.5 Surface scattering, truncation rod, thin films
3. Local structure by pair-density function (PDF) analysis
    - 3.1 Fourier-transform of structure function, local structure of glasses, liquids and disordered crystals, PDF modeling
    - 3.2 Anisotropic PDF analysis
    - 3.3 Partial PDF and chemical order
4. Inelastic scattering of neutrons and x-rays

- 4.1 Tools: Triple-axis spectrometer for neutrons and x-rays, pulsed neutron chopper spectrometer
- 4.2 Theory: Dynamic structure factor, dynamic PDF, Van Hove function
- 4.3 Examples: Phonons and magnons, local excitations
- 4.4 Dynamics of liquids and glasses

5. Advanced Techniques
   - 5.1 Resonant x-ray scattering
     Combining spectroscopy and scattering, resonant inelastic x-ray scattering
   - 5.2 X-ray Mossbauer resonance
   - 5.3 Coherent scattering and speckle pattern
   - 5.4 Neutron spin-echo method
   - 5.5 X-ray laser spectroscopy
6. Modeling
   - 6.1 Classical molecular dynamics
   - 6.2 Ab-initio molecular dynamics
   - 6.3 Other methods