CHEN 5838-003: X-ray and Neutron Scattering, Spectroscopy, and Imaging

Description. This course offers an in-depth survey of X-ray and neutron-based materials characterization methods with the goal of providing graduate students sufficient knowledge to apply these techniques to their own research. The fundamentals of scattering will be reviewed to provide context for X-ray and neutron diffraction, small-angle scattering, inelastic scattering and spectroscopy, and imaging. Each technique will be presented with relevant applications in mind for crystalline and amorphous solids and liquids, and students will develop familiarity with data modelling and analysis software. This course will also provide an overview of statistical analysis and model fitting and introduce data analysis methods.

Instructor: Prof. Michael Toney, (he/him/his). Michael.toney@colorado.edu;
Office: N321G Sustainability, Energy and Environment Community (SEEC)

Instructors office hours: Wednesday afternoon 3-4, starting Sept 3rd. After class is generally an excellent opportunity to ask questions, as the instructor will stay around until any questions are answered.

Graders: none.

Communication and Announcements: Class announcements (cancellations, schedule changes, reminders) will be made through Canvas. The instructor will attempt to promptly reply to emails, but do not expect turnaround in under 24 hours.

Lectures: TTh 8:30-945 AM in A104 JSCBB

Special dates: No classes on Oct 9th (reading day); Nov 22nd – 30th (Fall Break). Prof Toney will be on occasional travel, with Dylan Ladd, Erin Dunphy or Keith White filling in.

Text & References:

- "Elementary Scattering Theory: For X-ray and Neutron Users" by D.S. Sivia. Ebook at the library; pdf is posted to canvas
- "Elements of Modern X-ray Physics", by Jens Als-Nielsen & Des McMorrow. Pdf posted to canvas.
- "Elements of X-ray Diffraction", BD Cullity
- "Introduction to solid state physics", Charles Kittel. I will copy relevant chapters.

Website: https://canvas.colorado.edu/

Expectations: ***Attendance at all lectures is expected;*** asking questions and participating in class discussion is required. Occasional absences are understandable, and recorded lectures will be available for viewing for some lectures, but these do not substitute for in-person attendance. If you have to miss more than a few classes throughout the semester, please contact Prof. Toney to discuss. I can almost always make accommodations.

Grading

Participation	10%
Homework (≈8)	45%
Tests (2)	25%
Final Project	20%

Class Participation
Each class will have opportunities to work through and answer example problems and will typically involve working with another student or two.

Homework
About 8 homework assignments will be given throughout the semester for 40% of your grade. The tentative dates are listed in the schedule below and will be announced in class. You can work with partners to complete these, but each student turns in their own homework. Do not copy from lecture notes or use artificial intelligence (AI, e.g. ChatGPT) to answer homework questions. Use of AI is explained below and was discussed in the first class.

Tests
Two tests will be given throughout the semester during class (75 minutes each) for 25% of your grade. The dates are listed in the schedule below and will be announced in class. There is no final exam. Tests are not cumulative.

Final Projects:
The final project for this course is to a deep dive into a X-ray or neutron scattering, spectroscopy or imaging based analysis for a problem of your choice. This is beyond what you would typically do in your research, but is meant to be useful in your PhD. The goal here is for you to go into more depth in a specific example. You are encouraged but not required to discuss your project ideas with Prof Toney. This is 20% of class grade.

More detailed information about the projects will be distributed later in the semester as well as past examples. The grading for the project will focus primarily on depth of knowledge of the specific technique or analysis.

Possible examples include:

- Explanation of multiple scattering in EAXFS and description of multiple scattering paths for your data
- Explanation and quantification of error bars in EAXFS fits, XRR fits, SAXS analysis, PDF analysis

Topics:

- Scattering theory and relevant concepts including Fourier transforms, probability distribution functions, model fitting, and statistical figures-of-merit.
- Instrumentation – lab-based sources, detectors, storage rings, X-ray free-electron lasers.
- X-ray and neutron diffraction from crystals
- Scattering and reflectivity from surfaces, thin films, and single crystals.
- Small-angle scattering.
- Total scattering and the pair distribution function.
- Inelastic scattering and spectroscopy for the study of vibrations and electronic structure.
- X-ray absorption spectroscopy for the study of electronic structure, oxidation states and local structure (XANES, EXAFS).
- Imaging techniques including computed tomography (CT), diffraction microscopy, ptychography and coherent diffraction microscopy.

- Time-resolved scattering and absorption spectroscopy.

Tentative Schedule

Wk	Day	Topic	Reading	Due (tentative)
1.1	Th 8/21	Syllabus, math refresher, introduce scattering theory	Silva Chap 2, pp 19-38, pp 56-59 (math review) and pp 63-67.	
2.1	Tu 8/26	X-ray and neutron sources, instrumentation, detectors	Silva Chap 3.4 & 3.5, Als-Nielsen pp 1&2, pp29-34 (rest of chap 2 is optional)	
2.2	Th 8/28 (Mike out)	Structure of materials (1): Bravais lattices and crystallographic description of crystals; space groups; Wigner-Seitz cell → reciprocal space/Brillouin zones	Kittel Ch 1,	
3.1	Tu 9/2	Structure of materials (2); amorphous solids/liquids and pair distribution function; order parameters, incommensurate structures	Als-Nielson 1.1-1.2, 4.1-4.4	HW1 (structure)
3.2	Th 9/4	Scattering from single atom, molecule, and crystal, kinematic approximation	Sivia 2.3, parts of 2.4, Nature Reviews Methods Primer	
4.1	Tu 9/9	Scattering theory, form factor, differential cross section	Sivia 2.3, parts of 2.4, Nature Reviews Methods Primer	HW2 (diffraction)
4.2	Th 9/11	Diffraction (1): Structure factors and intensity calculations, single crystal diffraction	Sivia 3.3, Fultz 6.1, 6.2	
5.1	Tu 9/16	Diffraction (2): Powder diffraction, Rietveld		HW3 (diffraction2)
5.2	Th 9/18	Diffraction (3): Line-shapes (size/strain effects); Statistics in scattering	Fultz 1.1.3, 1.1.4, 6.6, 9.1.1; Fultz 9.1, 9.2	
6.1	Tu 9/23	Quantitative diffraction (1): Modeling & fitting		
6.2	Th 9/25	Quantitative diffraction (2): Rietveld refinement	Toby, 10.1154/1.2179804 McCusker et al., J. Appl. Cryst. 1999	
7.1	Tu 9/30	Short-range structure: Pair-distribution function, total scattering		
7.2	Th 10/2 (Mike out)	Short-range structure: Single crystal diffuse, incommensurate phases	Fultz/ Simonov and Weber	HW4 (diffraction3)
8.1	Tu 10/7	Midterm Exam		
8	Th 10/9 (no class)			
9	Tu 10/14	Small-angle X-ray scattering (1): form/structure factor		
9	Th 10/16	Small-angle X-ray scattering (2): Quantitative SAXS, comparison to SANS	Witham and Fultz paper on D distribution in LaNixSn(5-x)D6	
10	Tu 10/21	Small-angle X-ray scattering (3): instruments/experimental details, comparison to SANS		HW5 (SAXS/SANS)
10	Th 10/23	X-ray reflectivity (1): optical constants, Snell's law and Fresnel equations	Als-Nielson 3.1-3.6	
11	Tu 10/28	X-ray reflectivity (2): Surface structure factors, roughness	Als-Nielson 3.7,	
11	Th 10/30 (Mike out)	Kinematic diffraction: lattice sums for epitaxial thin films, RSMs		HW6 (surface scattering)

12	Tu 11/4	Surface diffraction and crystal truncation rods	Als-Nielson 4.4.6	
12	Th 11/6	X-ray spectroscopy (1): XANES, EXAFS		
13	Tu 11/11	EXAFS/XANES part 2		HW7 (spectroscopy)
13	Th 11/13	X-ray & neutron inelastic scattering/ instruments (or exafs continuation)		
14	Tu 11/18	Imaging (1): computed tomography		
14	Th 11/20	Imaging (2): computed tomography		HW8 (imaging)
15	Tu 11/25	Fall Break		
15	Th 11/27	Fall Break		
16	Tu 12/2 (Mike out, MRS)	2nd half exam		
16	Th 12/4	Coherent diffraction imaging & ptychography, diffraction microscopy; Time-resolved scattering and diffraction, X-ray photon correlation spectroscopy		
	Due Dec 8th			project

Honor Code

All students enrolled in a University of Colorado Boulder course are responsible for knowing and adhering to the Honor Code. Violations of the Honor Code may include but are not limited to: plagiarism (including use of paper writing services or technology [such as essay bots]), cheating, fabrication, lying, bribery, threat, unauthorized access to academic materials, clicker fraud, submitting the same or similar work in more than one course without permission from all course instructors involved, and aiding academic dishonesty. Understanding the course's syllabus is a vital part of adhering to the Honor Code.
All incidents of academic misconduct will be reported to Student Conduct & Conflict Resolution: StudentConduct@colorado.edu. Students found responsible for violating the Honor Code will be assigned resolution outcomes from Student Conduct & Conflict Resolution and will be subject to academic sanctions from the faculty member. Visit Honor Code for more information on the academic integrity policy.

Accommodation for Disabilities, Temporary Medical Conditions, and Medical Isolation

If you qualify for accommodations because of a disability, please submit your accommodation letter from Disability Services to your faculty member in a timely manner so that your needs can be addressed. Disability Services determines accommodations based on documented disabilities in the academic environment. Information on requesting accommodations is located on the Disability Services website. Contact Disability Services at

303-492-8671 or DSinfo@colorado.edu for further assistance. If you have a temporary medical condition, see Temporary Medical Conditions on the Disability Services website. If you have a temporary illness, injury or required medical isolation for which you require adjustment, please contact Prof Toney via email to alert us of the illness or quarantine. Please note the FERPA regulations apply, and you do not need to inform us of any diagnosis or potential exposure to COVID-19, if you choose.

Accommodation for Religious Obligations

Campus policy requires faculty to provide reasonable accommodations for students who, because of religious obligations, have conflicts with scheduled exams, assignments, or required attendance, if you cannot make class. See the campus policy regarding religious observances for full details.

Preferred Student Names and Pronouns

CU Boulder recognizes that students' legal information does not always align with how they identify. If you wish to have your preferred name (rather than your legal name) and/or your preferred pronouns appear on your instructors' class rosters and in Canvas, visit the Registrar's website for instructions on how to change your personal information in university systems.

Classroom Behavior

Students and faculty are responsible for maintaining an appropriate learning environment in all instructional settings, whether in person, remote, or online. Failure to adhere to such behavioral standards may be subject to discipline. Professional courtesy and sensitivity are especially important with respect to individuals and topics dealing with race, color, national origin, sex, pregnancy, age, disability, creed, religion, sexual orientation, gender identity, gender expression, veteran status, marital status, political affiliation, or political philosophy.

Additional classroom behavior information

- Student Classroom and Course-Related Behavior Policy.
- Student Code of Conduct.
- Office of Institutional Equity and Compliance.
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Sexual Misconduct, Discrimination, Harassment and/or Related Retaliation

CU Boulder is committed to fostering an inclusive and welcoming learning, working, and living environment. University policy prohibits protected-class discrimination and

harassment, sexual misconduct (harassment, exploitation, and assault), intimate partner abuse (dating or domestic violence), stalking, and related retaliation by or against members of our community on- and off-campus. The Office of Institutional Equity and Compliance (OIEC) addresses these concerns, and individuals who have been subjected to misconduct can contact OIEC at 303-492-2127 or email OIEC@colorado.edu. Information about university policies, reporting options, and OIEC support resources including confidential services can be found on the OIEC website.
Please know that faculty and graduate instructors are required to inform OIEC when they are made aware of incidents related to these concerns regardless of when or where something occurred. This is to ensure the person impacted receives outreach from OIEC about resolution options and support resources. To learn more about reporting and support a variety of concerns, visit the Don't Ignore It page.

Mental Health and Wellness

The University of Colorado Boulder is committed to the well-being of all students. If you are struggling with personal stressors, mental health or substance use concerns that are impacting academic or daily life, please contact Counseling and Psychiatric Services (CAPS), located in C4C, or call (303) 492-2277, 24/7.

No Acceptable Use of AI in this Class

Generative artificial intelligence tools—software that reproduces text, images, computer code, audio, video, and other content—have become widely available. Well-known examples include ChatGPT for text and DALL•E for images. This statement governs all such tools, including those released during our semester together. Keep in mind that the goal of gen AI tools is to reproduce content that seems to have been produced by a human, not to produce accurate or reliable content; therefore, relying on a gen AI tool may result in your submission of inaccurate content. It is the experience if the instructor that AI can be inaccurate in the space of this class. You may use AI tools for help with assignments in this course, but these should be limited to help with math any derivations.