Materials Science 465: Advanced Electron Microscopy & Diffraction

Northwestern University, McCormick School of Engineering

Winter Quarter 2026

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Office Hours: Friday, 10:00 AM - 11:20 PM or by appointment

Prerequisites: Graduate standing in Materials Science, Physics, Chemistry, or related field; basic programming experience in Python/MatLab; undergraduate courses in electron microscopy or materials characterization

Course Philosophy

This advanced graduate course embraces McCormick's "whole-brain engineering" approach by integrating rigorous theoretical foundations in electron microscopy with cutting-edge computational methods and machine learning techniques. Students will develop both analytical thinking through deep understanding of imaging theory, dynamical diffraction, and electron crystallography, and innovative computational approaches through algorithm implementation and automated analysis pipeline development. The course emphasizes the synthesis of fundamental physical principles with modern data science methods to address complex materials characterization challenges.

Course Description

This course provides an advanced exploration of electron microscopy through a computational and data-centric framework. It integrates fundamental imaging and diffraction theory with modern programming, simulation, and artificial intelligence methods used in materials characterization. Students will develop quantitative and practical skills in analyzing transmission electron microscopy (TEM), scanning transmission electron microscopy (STEM), and multi-dimensional data using Python-based environments.

Topics include multislice and Bloch-wave simulations, dynamical diffraction modeling, diffraction pattern interpretation, and AI-driven image analysis for atomic structure, defect detection, and phase identification. Emphasis is placed on reproducible research workflows, automated data processing pipelines, and integration of physical modeling with data-driven methods. Through a series of programming assignments and a major computational project, students will gain the ability to bridge theoretical understanding with computational implementation for advanced materials research.

Learning Objectives

By the end of this course, students will be able to:

1. Master advanced EM data analysis techniques for S/TEM using modern Python libraries

2. Implement machine learning algorithms for automated electron microscopy image segmentation, pattern recognition, and defect detection
3. Perform computational simulations, including multislice calculations and Bloch wave theory applications.
4. Develop reproducible research workflows using version control, data management best practices, and industry-standard computational tools
5. Critically evaluate current literature and emerging AI/ML methods in electron microscopy
6. Design and execute independent computational projects addressing real materials science challenges

Course Information

Meeting Times:

- Lectures: Monday & Wednesday, 11:00 AM - 12:20 PM
- Room: Technological Institute LG72
- Office Hours: Friday, 11:00 AM - 12:20 AM (or by appointment)
- Format: 2 lectures per week + office hours

Course Materials

Required Textbooks

- **Primary Reference:** Course notes and Jupyter notebooks provided via GitHub repository
- **Computational Methods:** Kirkland, E.J. (2020). *Advanced Computing in Electron Microscopy* (3rd ed.). Springer International Publishing.

Supplementary Materials

- Recent research papers provided as PDFs.
- Online documentation for py4DSTEM, HyperSpy, and ASE
- Video tutorials from software development teams
- Conference presentations from MLSTEM and related workshops

Course Schedule & Assignments

All course materials, code, and datasets will be available in NU-MSE-LECTURES/465-WINTER2026

Week 1 (January 5-9): Foundations and Environment Setup

Monday: Overview of modern computational microscopy

- Historical context and evolution of computational microscopy
- Data types in EM: image, diffraction, and multimodal
- Introduction to open-source tools used in this course

Wednesday: Setting up Computational Environments

- Installing Python, Jupyter Lab, and essential libraries
- Version control and GitHub workflows
- Best practices for data organization and reproducible research

Assignment 1: Environment setup and dataset exploration

Week 2 (January 12–16): Core Tools for Microscopy Data Analysis

Monday: Python Ecosystem for EM Data

- Navigating HyperSpy for multi-dimensional datasets
- Introduction to py4DSTEM and 4D-STEM data handling
- Data visualization in Jupyter using Matplotlib and HyperSpy

Wednesday: Structural Metadata and Data Preprocessing

- Using ASE for atomic models and crystal data management
- Data calibration, alignment, and normalization
- Integration of pyXEM, HyperSpy, and ASE workflows

Assignment 2: Implement virtual detector and diffraction analysis workflow

Week 3 (January 19–23): Image Processing and Classical Analysis Methods

Monday: Image Processing Foundations

- Image filtering and noise reduction techniques
- Real-space and FFT-based contrast enhancement
- Histogram equalization and normalization

Wednesday: Classical Image and Diffraction Analysis

- Morphological operations and segmentation methods
- Template matching and particle identification
- Diffraction pattern analysis using pyXEM and py4DSTEM

Assignment 3: Classical image segmentation pipeline

Week 4 (January 26–30): Machine Learning for Microscopy

Monday: Fundamentals of ML in EM

- Supervised and unsupervised learning overview
- Feature extraction and labeling strategies
- Model evaluation metrics for microscopy data

Wednesday: Deep Learning Architectures and Applications

- CNN and U-Net for EM image segmentation
- Data augmentation and noise robustness
- Introduction to AtomAI for physics-informed ML

Assignment 4: Develop a neural network for atomic-level pattern recognition

Week 5 (February 2–6): Multislice and Image Simulation Techniques

Monday: Multislice Fundamentals

- Principles of electron scattering and multislice theory
- Implementation using abTEM and Prismatic
- GPU acceleration for image simulation

Wednesday: Image Simulation and Model Validation

- Effects of thickness and atomic number
- Frozen phonon calculations for thermal diffuse scattering
- Comparison of simulated and experimental images

Assignment 5: Multislice simulation of image contrast versus thickness

Week 6 (February 9–13): Dynamical Diffraction and Bloch Waves

Monday: Dynamical Diffraction Theory

- Two-dimensional channeling and Bloch-wave concepts
- Ewald sphere construction and reciprocal lattice mapping
- Diffraction contrast mechanisms

Wednesday: Computational Implementation of Bloch Waves

- Solving eigenvalue equations for Bloch coefficients
- Comparing dynamical and kinematic predictions
- Application to zone-axis diffraction patterns

Assignment 6: Compute diffraction intensities using Bloch-wave model

Week 7 (February 16–20): 4D-STEM and Quantitative Analysis

Monday: Processing and Analysis of 4D-STEM

- py4DSTEM workflow and data structure
- Center-of-mass (COM) and differential phase contrast (DPC)
- Quantitative strain and electric field mapping

Wednesday: Advanced 4D-STEM Applications

- Ptychography and phase reconstruction
- Integration of 4D-STEM and spectroscopy data
- Machine learning-assisted pattern analysis

Assignment 7: Full 4D-STEM analysis workflow

Week 8 (February 23–27): Electron Crystallography and AI-assisted Structure Analysis

Monday: Fundamentals of Electron Crystallography

- Bulk structure solution and refinement
- Charge density analysis
- Limitations of dynamical vs. kinematic approaches

Wednesday: AI for Automated Structure Analysis

- Machine learning for diffraction pattern classification
- Feature extraction and clustering with pyXEM and AtomAI
- Automated phase and defect identification

Assignment 8: AI-based crystallographic classification project

Week 9 (March 2–6): Integration and High-Performance Computing

Monday: Integrating Simulation, Experiment, and ML

- Designing end-to-end analysis workflows
- Combining multislice output, 4D-STEM data, and ML analysis
- Case studies in energy, semiconductor, and catalyst materials

Wednesday: High-Performance Computing for Microscopy

- Cluster computing for large-scale datasets
- GPU parallelization and optimization
- Reproducibility and scalability in research workflows

Assignment 9: Mini-integration project with simulation and ML components

Week 10 (March 9–13): Final Projects and Future Trends

Monday: Final Project Presentations I

- Computational project presentations by students
- Peer feedback and scientific discussion

Wednesday: Final Project Presentations II and Course Reflection

- Continued student presentations
- Discussion on autonomous and closed-loop microscopy
- Future research directions and professional pathways

Final Project Due: Technical report, GitHub repository, and oral presentation

Important Dates:

- January 5: First day of classes
- January 19: No classes (Martin Luther King Jr. Day)
- February 13: Last day to drop a class
- March 21: End of Winter Classes

Course Deadlines:

- All programming assignments are due by 11:59 PM on the due date
- Project proposal due Week 5
- Final project presentations: Week 10
- Final projects due March 21

Assessment

- Weekly Programming Assignments (8 total): 35%
- Major Computational Project: 40%
- Project proposal (5%)
- Progress presentation (10%)
- Final project and repository (25%)
- Project Presentation: 15%
- Participation and Peer Review: 10%

Major Computational Project (40%)

Students will conduct an independent computational project implementing advanced EM analysis methods to address real materials science challenges.

Project Duration:

- Weeks 5-10, with the proposal due in Week 5 and final submission in Week 10

Project Components:

- Individual project integrating multiple course concepts (EM analysis + ML + computational methods)
- GitHub repository with well-documented code
- Technical report ($\approx$ 10 pages) in research article format
- Professional presentation of results

Example Project Topics:

- Automated defect analysis in 2D materials using deep learning
- ML-enhanced ptychography reconstruction algorithms
- Real-time 4D-STEM processing pipeline development
- Physics-informed neural networks for electron scattering
- High-throughput crystal structure identification

Deliverables:

- GitHub repository with complete implementation
- Technical report ($\approx$ Up to 10 pages, research article format)
- 15-minute conference-style presentation

Evaluation Criteria:

- Technical rigor and innovation (40%)
- Code quality and documentation (25%)
- Scientific insight and analysis (20%)
- Presentation and communication (15%)

Programming Assignments (35%)

Weekly hands-on assignments designed to build progressive computational skills in microscopy and data analysis:

1. **Environment Setup and Data Exploration** (Week 1): Configure Python and Jupyter environments, initialize GitHub repository, and explore a sample EM dataset.
2. **Microscopy Data Analysis Tools** (Week 2): Use HyperSpy and py4DSTEM to visualize and process diffraction and 4D-STEM data; create a virtual detector.
3. **Classical Image Processing** (Week 3): Implement filtering, FFT-based transformations, and segmentation for image enhancement and feature extraction.
4. **Machine Learning for Microscopy** (Week 4): Build and train a simple CNN or U-Net model for atomic-resolution image segmentation using AtomAI or PyTorch.
5. **Multislice Image Simulation** (Week 5): Perform electron scattering simulations using abTEM or Prismatic; analyze image contrast as a function of thickness and tilt.
6. **Dynamical Diffraction and Bloch-Wave Modeling** (Week 6): Compute diffraction intensities using a simplified Bloch-wave model and compare to multislice results.
7. **4D-STEM Quantitative Analysis** (Week 7): Execute a complete py4DSTEM workflow including COM, DPC, and strain mapping from real or simulated datasets.
8. **Crystallography and AI Integration** (Week 8): Develop a machine learning workflow for automated diffraction pattern classification and structure analysis.
9. **Integration Mini-Project** (Week 9): Combine simulation, experimental data analysis, and ML methods into a unified computational pipeline.

Whole-Brain Computational Approach

This course integrates analytical and creative thinking through:

- Rigorous algorithm implementation and mathematical formulation
- Creative problem-solving in experimental design and data analysis
- Innovation in machine learning applications to materials science
- Critical evaluation of emerging AI/ML methods in electron microscopy
- Development of novel approaches to automated materials characterization
- Integration of physics-based knowledge with data-driven methods

Professional Development

Students will gain exposure to current computational research through:

- Skills directly applicable to careers in computational materials science
- Experience with industry-standard tools and workflows
- Training in reproducible research practices

Course Policies

Prerequisites and Preparation

Students should have completed undergraduate courses in materials characterization or electron microscopy and demonstrate proficiency in linear algebra and statistical methods.

GitHub Repository and Code Sharing

Each student maintains a personal GitHub repository for the course, organizing assignments and project work. Code should be well-documented, include appropriate citations. All repositories must be public by the end of the quarter to facilitate knowledge sharing.

Collaboration Policy

Collaboration on assignments is encouraged through peer code reviews and discussion forums. However, submitted code must represent individual work with proper attribution. The final project may be completed in teams of 2-3 students with instructor approval.

Late Assignment Policy

Programming assignments may be submitted up to 48 hours late with a 10% penalty per day. Extensions are available for documented emergencies or technical difficulties. The final project deadline is firm due to presentation scheduling.

Academic Integrity

Students are expected to comply with Northwestern University's Academic Integrity Policy.

- All work must represent original effort with proper citation of sources, code libraries, and collaborators
- Plagiarism of code or written work violates Northwestern's academic integrity policies
- Students are encouraged to use online resources and documentation but must understand and be able to explain their implementations
- **Large Language Model (LLM) Usage:** Students may use LLMs (e.g., ChatGPT, Claude, GitHub Copilot) to assist with coding assignments, but must clearly cite their usage, demonstrate full understanding of the generated code, and provide written explanations of the reasoning process and implementation steps

- Proper attribution of data sources and collaborations is required
- Honest reporting of computational results and limitations is expected

Accessibility and Support

Northwestern University is committed to providing equitable access. Students with documented learning differences should contact AccessibleNU to discuss accommodations. Office hours provide individual consultation on projects and career guidance in computational materials science.

This course follows the Northwestern University Syllabus Standards. Students are responsible for familiarizing themselves with this information.

This course prepares students for the rapidly evolving field of AI/ML-enhanced electron microscopy, providing both theoretical foundations and practical skills essential for modern materials research and industrial applications.