

Annexe A: New/Revised Course Content in OBTL+ Format

Course Overview

Expected Implementation in Academic Year	AY2026-2027
Semester/Trimester/Others (specify approx. Start/End date)	Semester 1
Course Author * Faculty proposing/revising the course	Assoc Prof Dong Zhili
Course Author Email	zldong@ntu.edu.sg
Course Title	Diffraction, Imaging & Spectroscopy Techniques
Course Code	MS6023
Academic Units	3
Contact Hours	39
Research Experience Components	

Course Requisites (if applicable)

Pre-requisites	
Co-requisites	
Pre-requisite to	
Mutually exclusive to	
Replacement course to	
Remarks (if any)	

Course Aims

This proposed course aims to bridge the gap using interdisciplinary approaches for students with diverse engineering background. The course mainly explains the fundamentals of (i) diffraction, (ii) imaging and (iii) spectroscopy techniques applied to materials research, especially for analysis of chemical compositions, crystal structures, defects in crystals and other nano features.

One of the key topics in materials science and engineering is structure – property relationship. To understand why a material displays certain behaviours, the first step is to resolve its crystal structure and reveal its structure characteristics. For each analytical technique included in the course, the fundamentals of materials science, the principle of analysis, and the collections of signals will be explained based on the interactions between the incoming beam and the material under examination. Incoming radiations include photons, neutrons, electrons and ions. The signals collected enable us to understand the chemical compositions and structures of materials. It is believed that the course proposed can help students from different engineering disciplines with materials analysis in their research projects.

Course's Intended Learning Outcomes (ILOs)

Upon the successful completion of this course, you (student) would be able to:

ILO 1	Students will understand the principle of each characterisation technique explained in the course, and be able to choose right analytical techniques to obtain data about materials chemical compositions, crystal structures, electronic structures and defects.
ILO 2	Students will understand the advantages of each diffraction technique. They will understand when to choose neutron diffraction, or X-ray diffraction.
ILO 3	Students will be able to conduct quantitative phase analysis using Rietveld refinement. Students will be able to generate crystal structure file (e.g. CIF format) and draw 3D crystal structures.
ILO 4	Students will understand the differences between X-ray diffraction and electron diffraction, and can choose the right technique depending on whether they need to study the local crystal structures or average crystal structure.
ILO 5	Students will be able to identify the material structures and crystal defects using different microscopic techniques.
ILO 6	Students will be able analyse the local chemical compositions and average chemical compositions through spectroscopic analysis.
ILO 7	Students will be able analyse the materials structures through functional group identification or lattice vibration analysis.

Course Content

1. Introduction

- Energy levels in an atom
- Electronic structure of materials

2. Diffraction

- Neutron diffraction & X-ray diffraction
- Quantitative phase analysis and Rietveld refinement
- Electron diffraction vs X-ray diffraction

3. Imaging

- Aberration of optical lens and resolution
- Schematic illustration of confocal and fluorescence microscopes
- Contrast formation in electron microscopes
- Fundamentals of X-ray radiography and CT
- Fundamentals of Atomic Probe Tomography and AFM

4. Spectroscopy

- Fundamentals of Mössbauer spectroscopy and NMR
- X-ray and electron beam analysis techniques: EDX, XRF, EPMA, XPS, XAFS and EELS
- RAMAN and FTIR
- Fundamentals of mass spectroscopy

Reading and References (if applicable)

1. Z. L. Dong, Fundamentals of Crystallography, Powder X-ray Diffraction, and Transmission Electron Microscopy for Materials Scientists, Taylor & Francis / CRC, Published in May 2022.
2. M. Che and J. C. Vedrine, Characterization of solid materials and heterogeneous catalysts : from structure to surface reactivity , Wiley, 2012.

Note: The above listing comprises the foundational readings for the course and more up-to-date relevant readings will be provided when they become available.

Planned Schedule

Week or Session	Topics or Themes	ILO	Delivery Mode	Activities	Readings
1	Fundamentals 1. The structure of the atom and energy levels 2. The electronic structure of crystals 3. Energy levels in a diatomic molecule	1	In-person	Lecture (2 hr 20 min) + Discussion (40 min)	Ref 1 & 2
2	Fundamentals 1. The structure of the atom and energy levels 2. The electronic structure of crystals 3. Energy levels in a diatomic molecule	1	In-person	Lecture (2 hr 20 min) + Discussion (40 min)	Ref 1 & 2
3	X-ray diffraction vs electron diffraction	2&4	In-person	Lecture (2 hr 20 min) + Discussion (40 min)	Ref 1 & 2
4	Neutron diffraction and X-ray diffraction; Practice: Rietveld refinement for quantitative phase analysis	2&3	In-person	Lecture (2 hr 20 min) + Discussion (40 min)	Ref 1 & 2
5	Quantitative phase analysis; Self-study: Small Angle Scattering Discussion session (recap of teaching weeks 1 to 5 topics)	2&3	Online	Lecture (1 hr) + Discussion (2 hr)	Ref 1 & 2

Week or Session	Topics or Themes	ILO	Delivery Mode	Activities	Readings
6	Light optical microscopy: Aberration of optical lens and resolution; Schematic illustration of confocal and fluorescence microscopes	1&5	In-person	Lecture (2 hr 20 min) + Discussion (40 min) Submission of Continual Assessment 1 (CA1): Individual Written Report 1	Ref 2
7	Electron microscopy: Contrast formation in electron microscopes	1&5	Online	Lecture (2 hr 20 min) + Discussion (40 min)	Ref 1
8	More imaging techniques: Fundamentals of X-ray radiography and CT; Fundamentals of Atomic Probe Tomography and AFM	1&5	In-person	Lecture (2 hr 20 min) + Discussion (40 min)	Ref 2
9	Materials analysis based on Nuclear Energy Levels: Mössbauer spectroscopy and NMR	1&6	In-person	Lecture (2 hr 20 min) + Discussion (40 min) Submission of Continual Assessment 2 (CA2): Individual Written Report 2	Ref 2
10	Materials analysis based on energy levels of atoms: X-ray and electron beam spectroscopy techniques	1&6	In-person	Lecture (2 hr 20 min) + Discussion (40 min)	Ref 2

Week or Session	Topics or Themes	ILO	Delivery Mode	Activities	Readings
11	Materials analysis based on energy levels of molecules: RAMAN and FTIR techniques	1&7	In-person	Lecture (2 hr 20 min) + Discussion (40 min)	Ref 2
12	Instrumentation (Guest lecture by Engineers from ThermoFisher Scientific, Agilent Technologies, PerkinElmer)	1	In-person	Lecture (2 hr 20 min) + Discussion (40 min)	Ref 2
13	Discussion session (recap of teaching weeks 1 to 13 topics) Continual Assessment 3 (CA3): Individual Final Quiz	1-7	In-person	Discussion (2 hr) Continual Assessment 3 (CA3): Individual Final Quiz (1 hr)	N/A

Learning and Teaching Approach

Approach	How does this approach support you in achieving the learning outcomes?
Blended learning with active use of multi-media resources (TEL)	This will permit flexibility of access to learning materials, activities and assessments and can help you develop independent learning and critical thinking skills.
Showing real-world applications	Concepts and features of Diffraction, Imaging & Spectroscopy Techniques discussed here are related to applications in materials analysis.
Weekly Consultation	Weekly consultation hours will be available to encourage discussions that will reinforce students' understanding of various concepts and applications. Instead of providing answers directly to students' queries, they will be guided to think and make intelligent guesses based on sound principles. This approach will cultivate critical thinking.

Assessment Structure

Assessment Components (includes both continuous and summative assessment)

No.	Component	ILO	Related PLO or Accreditation	Weightage	Description of Assessment Component	Team/Individual	Rubrics	Level of Understanding
1	Continuous Assessment (CA): Report/Case study(Continual Assessment 1 (CA1): Individual Written Report 1)	1	N/A	30	Based on the quantitative phase analysis results obtained using the Rietveld refinement software in week 4, write a report. Page count 3-5 pages.	Individual	Holistic	Relational
2	Continuous Assessment (CA): Report/Case study(Continual Assessment 2 (CA2): Individual Written Report 2)	1	N/A	30	Written report on the topic of Microscopy Analysis, page count 3-5 pages. Students will be required to submit the report to Turnitin for plagiarism check.	Individual	Holistic	Relational

No.	Component	ILO	Related PLO or Accreditation	Weightage	Description of Assessment Component	Team/Individual	Rubrics	Level of Understanding
3	Continuous Assessment (CA): Test/Quiz(Continual Assessment 3 (CA3): Individual Final Quiz)	1,2	N/A	40	The assessment will test the students' grasp of concepts and applications. Duration: 1 hour; Short-essay questions; Open-book	Individual	Holistic	Extended Abstract

Description of Assessment Components (if applicable)

Continual Assessment 2 (CA2): Individual Written Report 2

Choose a representative material in your materials related research projects.

Have you examined (Will you examine) the material using microscopy techniques?

What information have you obtained (do you expect to obtain) from your microscopy experiments?

Formative Feedback

- The last 20 minutes of each weekly lecture will be dedicated to a discussion session. Students may ask questions, and the course coordinator will provide feedback as needed.
- Grading and general feedback will be shared with students after each CA.
- Students are encouraged to visit the course coordinator's office during consultation hours to review their papers and discuss any concerns.

NTU Graduate Attributes/Competency Mapping

This course intends to develop the following graduate attributes and competencies (maximum 5 most relevant)

Attributes/Competency	Level
Learning Agility	Advanced
Problem Solving	Advanced
Transdisciplinarity	Advanced
Critical Thinking	Intermediate
Design Thinking	Intermediate

Course Policy

Policy (Academic Integrity)

Good academic work depends on honesty and ethical behaviour. The quality of your work as a student relies on adhering to the principles of academic integrity and to the NTU Honour Code, a set of values shared by the whole university community. Truth, Trust and Justice are at the core of NTU's shared values. As a student, it is important that you recognize your responsibilities in understanding and applying the principles of academic integrity in all the work you do at NTU. Not knowing what is involved in maintaining academic integrity does not excuse academic dishonesty. You need to actively equip yourself with strategies to avoid all forms of academic dishonesty, including plagiarism, academic fraud, collusion and cheating. If you are uncertain of the definitions of any of these terms, you should go to the academic integrity website for more information. On the use of technological tools (such as Generative AI tools), different courses / assignments have different intended learning outcomes. Students should refer to the specific assignment instructions on their use and requirements and/or consult your instructors on how you can use these tools to help your learning. Consult your instructor(s) if you need any clarification about the requirements of academic integrity in the course.

Policy (General)

You are expected to complete all assigned readings, activities, assignments, attend all classes punctually and complete all scheduled assignments by due dates. You are expected to take responsibility to follow up with assignments and course related announcements. You are expected to participate in all project critiques, class discussions and activities.

Policy (Absenteeism)

In-class activities make up a significant portion of your course grade. Absence from class without a valid reason will affect your participation grade. Valid reasons include falling sick supported by a medical certificate and participation in NTU's approved activities supported by an excuse letter from the relevant bodies. There will be no make-up opportunities for in-class activities.

Policy (Others, if applicable)

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