UNIVERSITY OF OXFORD

DEPARTMENT OF MATERIALS

FHS MATERIALS SCIENCE

PART II HANDBOOK

2026-27

1. Forward

1.1. Statement of Coverage

This document is a supplement to the Final Honour School of Materials Science handbook. It applies to students starting Part II of the Final Honour School, MEng in Materials Science in Michaelmas term 2026. The information in this handbook may be different for students starting in other years.

1.2. Version

Version	Details	Date
Version 1.1	Update to *7.2. Hours of Working and Lone Working (Offices and Laboratories)* Added section *16.6 Past Part II Project Reports.*	October 2026
Version 1.0	Handbook published	September 2026

1.3. Disclaimer

The Examination Regulations relating to this course are available at **2023-24, Honour School of Materials Science.** If there is a conflict between information in this handbook and the Examination Regulations then you should follow the Examination Regulations. If you have any concerns please contact **undergraduate.studies@materials.ox.ac.uk**.

The information in this handbook is accurate as of September 2026. However, it may be necessary for changes to be made in certain circumstances, as explained at **Potential course changes**. If such changes are made the department will publish a new version of this handbook together with a list of the changes and students will be informed.

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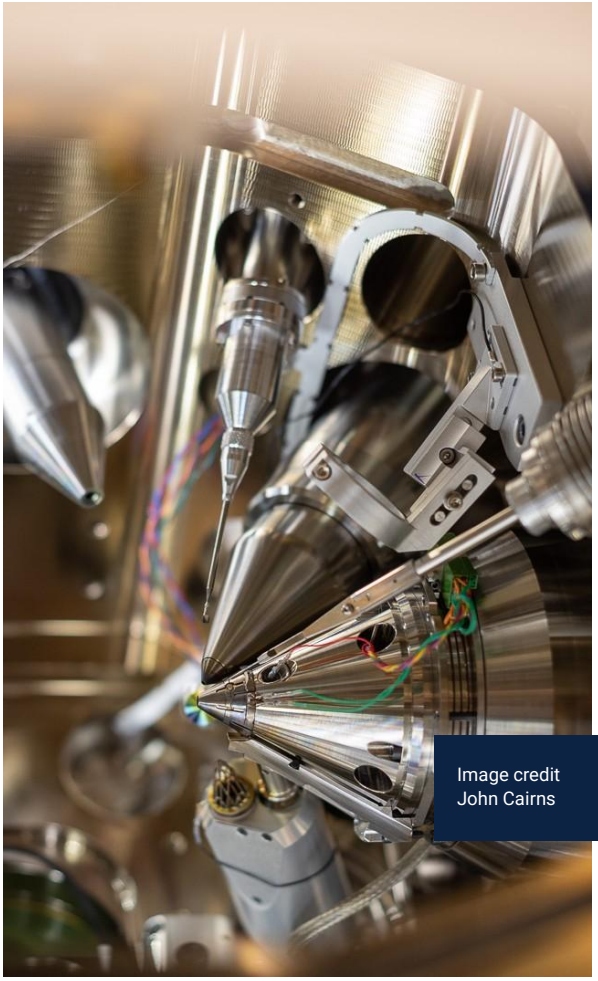
2. Introduction

Welcome to Part II of the Final Honour School MEng in Materials Science.

This handbook contains information specific to the Part II. It is a supplement to the handbook for the FHS in Materials Science course, which contains more general information.



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John Cairns

3. Part II Organisation and Contacts

3.1. Part II Project Organiser

Prof James Marrow

Room 10.15, 21 Banbury Road

Phone: (2)73938

james.marrow@materials.ox.ac.uk

(Please e-mail me in the first instance)

3.2. Administration for Part II Projects

Education Support Team

Ground Floor, Hume-Rothery Building

undergraduate.studies@materials.ox.ac.uk

4. List of Part II Projects 2026-27

Student Name	Project Title	Supervisors, Co-supervisor(s)
Gibran Ahmed	The detection, mitigation and correction of errors in quantum computers	Prof. Simon Benjamin
Simeon Ainsworth	Liquid metal corrosion of structural materials for fusion	Prof. David Armstrong
Eliza Beresford	Fundamental Oxidation Behaviour of Engineering & Catalytic Alloys	Dr Paul Bagot Dr Christina Hofer Dr Benjamin Jenkins
Ella Bolland	Direct Prediction of Optical Spectra in Doped Semiconductors with Artificial Intelligence and Machine Learning	Prof. Mingda Li (MIT) Prof. Saiful Islam
Alec Dakin	Correction of Scan Distortion in STEM	Prof. Angus Kirkland Dr Ali Mostaed
Aron Desilva	Defect engineering in diamond for quantum technologies	Prof. Jason Smith
Kathryn Dudley	Materials Joining Challenges for Nuclear Fusion Power Plants	Dr Paul Bagot Dr Christina Hofer Dr Benjamin Jenkins
Xinning Feng	Neighbourhood effects in deformation of Ti alloys	Prof. Angus J Wilkinson
Kuangyi Fu	Design and Simulation of Solar Cells for Electric Mobility Applications	Prof. Sebastian Bonilla
Jack Harper-Hill	Next-generation high-energy cathodes: anion (O/S) redox and disordered rock-salt materials	Prof. Peter Bruce Dr Sofia De Sousa Coutinho
Syed Hassan	Investigating process defects in polycaprolactone electrospun yarns	Prof. Pierre-Alexis Mouthuy Prof. Hazel Assender
James Hopkinson	Fabrication of Oxide based ceramic matrix nano-composites for creep applications at 1100°C	Prof. Marina Galano Prof. James Marrow Dr Talha Pirzada
Shuhui Jin	Degradable and implantable batteries: Sustainable Power Sources for Biomedical Devices	Prof. Malavika Nair Prof. Hazel Assender
An Lam	Fabrication of 2D devices for optical control of atomic spin defects	Prof. Hannah Stern Prof. Jason Smith
Isabel Lesser	3D Printing composite scaffolds with integrated electrospun yarn for soft–hard tissue interfaces	Prof. Pierre-Alexis Mouthuy Dr Andy Gleadall
Amy Li	Solid Electrolyte Interphase in Lithium Solid State Batteries	Prof. Mauro Pasta Dr Ben Jagger
He Lin	Understanding the mechanism of Roll Bonding as an alternative manufacturing route for metallic lattice structures	Prof. Cem Tasan (MIT) Prof. Roger Reed

James List	Exploring phase transitions in 2D materials with machine learning	Dr Zachary Goodwin Prof. Jonathan Yates
Eythan Loche	Architectured Porous Materials for Transpiration-Cooled Rocket Thrust Chambers	Prof. Zac Cordero (MIT) Prof. James Marrow
Louis McAuliffe	Transfer learning in atomistic graph neural networks	Dr Chiheb Ben Mahmoud Prof. Jonathan Yates
James Moses	Irradiation damage of high temperature superconducting thin films	Prof. Susie Speller Dr Clara Barker
Daniel Ning	Plasmon-Enhanced Optical Control of Altermagnetic Memories	Prof. Giuliana Di Martino
Marcus Papa	HR-EBSD Investigation of Hydrogen-assisted Cracking in Steel	Prof. James Marrow
Christopher Parker	Quantification of Free Nitrogen in Steels by Atom Probe Tomography	Dr Christina Hofer Dr Paul Bagot Dr Didier Farrugia
Rohan Patel	Development of MgB2 superconducting wiress	Prof. Susie Speller Dr Guillaume Matthews
Alexander Penny	Upcycling strategies for low-grade aluminium scrap	Dr Enzo Liotti
Ryan Pople	Microstructural control in additively manufactured metals	Dr Tamsin Whitfield Prof. Angus J Wilkinson Prof. David Armstrong
Nattaya Praesaengiam	High-resolution characterisation of wire arc additive manufacturing (WAAM) aluminium alloys for space applications	Prof. Sergio Lozano-Perez Dr Martina Meisnar ESA
Daniel Record	Alloy anodes to enable sustainable, high-energy density Ca-ion batteries	Prof. Robert House
Yilin Ren	Online Slippage Analysis for Adaptive Battery Cycling	Prof. Robert Weatherup Dr Erik Bjorklund Dr Conor Phelan
Samuel Shorrocks	Solid Oxide Electrolysis Cells performance related to grain boundary crystallography	Prof. Tinka Marquardt Prof. Angus J Wilkinson Dr Surabhi (Ceres Power)
Caitlin Smith	Sustainable Routes to Carbon Fibre Production	Prof. Nicole Grobert Dr Barbara Maciejewska
Sebastian Travis	Tin Whiskers	Prof. Angus J Wilkinson Prof. David Armstrong
Zhuoying Wang	DFT investigation of electron energy loss spectroscopy as a way to characterise hydrogen in zirconium alloys	Prof. Rebecca Nicholls Dr Calum Cunningham UK NNL
Zhang Xinyu	Understanding Failure and Degradation in All-Solid-State Batteries	Prof. Peter Bruce Dr Dominic Melvin
Nuan-Yi Zeng	Crystalline-amorphous phase transitions in Na-ion disordered rocksalt battery cathodes	Prof. Robert House

5. Residence Requirements

The Regulations for **PART II of the Examination for the degree of Master of Engineering in Materials Science** (2023-24, Honour School of Materials Science) state:

"Periods of required residence for Part II

- *From the fifth Friday before to the first Saturday following Michaelmas Full Term.*
- *From the second Friday before Hilary Full Term to the Saturday before Palm Sunday.*
- *From the Friday following Easter to the second Saturday following Trinity Full Term."*

These dates can be found at **Dates of term | Oxford University**.

Students undertaking External Part II project are not required to be in residence during the extended Michaelmas and Hilary Terms, but must be in residence for the Trinity Term.

6. Induction Schedule

Monday 14th September 2026, Hume-Rothery Lecture Theatre

09:30 - 10:20 **Prof. James Marrow**

- Welcome and introductions. Purpose and overview of the day.
- The Part II Project

10:20 -10:30 **Claire Wellstood**

- Opportunities for outreach activities

10:30 - 10:40 **Dr. Phani Karamched**

- Electron microscopy training courses

10:40 - 11:40 **JCCG Representatives & Mr Cleveland Williams**

- The workshop and signing up for the workshop practice course. The course is compulsory for all those doing their Part II in the Department.
- Students are to be split into 3 groups with one group going in a tour at a time, whilst the others have coffee

11:40 - 12:20 **Ms Jennifer Scott**

- Safety

Thursday 17th September 2026, Hume-Rothery Lecture Theatre

14:00 - 15:30 **Prof. James Marrow**

- Project Management and the Part II

7. Safety

You will be briefed during the Part II induction by the Department Safety Officer (DSO) on

- Department Safety Policies
- Laboratory Safety Manual
- Personal Risk Assessment
- Risk Assessments and CoSHH.

Further information on Safety Policies and the processes required for risk assessments and approvals to undertake your work are available on **SharePoint**, including the Department Safety Policy and the Laboratory Safety Manual (LSM), which describes codes of practice and safety advice. Some key points are emphasised here.

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John Cairns

7.1. Safety Code of Conduct

As you undertake your project, whether it is modelling or experimental, you are working in a department that contains research laboratories. As noted in the Lab Safety Manual, a research laboratory is a potentially dangerous environment, where without care and attention accidents can occur, many with serious consequences and most are avoidable. Rules therefore must be followed when working in the lab. The actions required from you are straightforward and are in your interest, however the consequences of not following protocols and thoughtless behaviour mean that you put yourself and colleagues in danger. You therefore have a moral and legal responsibility for your safety and the safety of others.

If your project is office-based, you must complete a '**Personal Risk Assessment and Safety Induction Form - Office users'** form, which must be prepared with your supervisor before beginning any work and submitted to the Department Safety Office (DSO) **by the end of -1st week Michaelmas Term**.

If your project requires any laboratory or workshop work, you will be required to declare acceptance of the **Laboratory/Workshop Code of Conduct.** This declaration is recorded through the completion of your '**Personal Risk Assessment and Safety Induction Form for Laboratory and Workshop users'**, which must be prepared with your supervisor before beginning any laboratory work and submitted to the Department Safety Office (DSO) **by the end of -1st week Michaelmas Term**. If you do not comply you may be banned from lab work, as stated in the Departmental Safety Policy.

Laboratory/Workshop Code of Conduct

- I will never work in any way that endangers myself, or my colleagues, and will always work in accordance with the University Policy Statements and other relevant safety documents.
- I will abide by local lab safety rules set by the Laboratory Supervisor of the laboratory I am working in. When working in labs outside the department of Materials, I will provide risk assessments for this and abide by local rules of the host departments.
- I will comply with the Laboratory Safety Policy as set out in the Department Safety Policy, the Lab Standards and Hazardous Substances Standards as explained and set out in the Laboratories Safety Manual.
- I will provide approved COSHH and risk assessments for all experiments BEFORE starting, and work strictly in accordance with these documents.
- I will always clean up after myself. This means when a lab session is finished, the work space must be cleaned and returned to its original condition.
- I will at all times while working in 'wet labs' (labs that use chemicals), wear correct personal protective equipment and appropriate dress and sensible footwear: safety glasses must be worn, properly fastened lab coat, clothes covering legs and arms, shoes that enclose the foot and are not porous. When working in other types of labs, I will adhere to the local lab rules.
- I will never store or consume food and drink in laboratories.
- I will not wear headphones / earphones when working in a lab of any type.
- I will consult my supervisor whenever I have doubts about procedures.
- If I am pregnant I will inform my supervisor as soon as possible so that the risk of possible exposure to teratogens can be assessed and eliminated. Early action is vital because the foetus is most at risk in the first three months of pregnancy.
- I will report all accidents or potentially dangerous incidents online on IRIS, and all equipment failures/faults to the appropriate people.
- If I need to leave my work space for a time, I will leave an overnight equipment form and unattended experiment card with my name, contact number, date and duration of use.
- When I leave the lab/s, I will ensure that my experiment set up is left in a safe state and I will comply with end of day procedures to ensure the lab/s are left in a safe condition at night.
- To keep good records of procedures and safety considerations.

7.2. Hours of Working and Lone Working (Offices and Laboratories)

As a Part II student, you are an Undergraduate Student on an Integrated Masters course. The University does not permit you to work in laboratories outside normal working hours (8 am to 5 pm, Monday to Friday). You should note that microscopy (e.g. optical, electron and X-ray) takes place in a laboratory environment, and any session you book in the DCCEM must end by 5 pm.

Part II students are also not permitted to undertake laboratory work outside the designated

Part II working periods. University vacation periods are intended to provide students with an appropriate period of rest and recuperation, and laboratory work must not be scheduled during these periods.

Part II students must not be left unsupervised in laboratories at any time. The Academic Supervisor or Co-Supervisor may provide the required support themselves or nominate one or more suitably competent members of technical staff, postdoctoral researchers or DPhil students. Where the required level of support identified in the Part II Personal Risk Assessment is temporarily unavailable, the student must pause the activity until it is restored.

Full information, inclusive of the Part II Personal Risk Assessment, Guidance Notes and other information on H&S requirements can be found **here**. Please ensure you familiarise yourself with these documents and pages.

Office Work

You can work in an office environment outside normal working hours (5pm to 10pm Monday to Friday, 8am to 10pm, Saturday to Sunday). This requires an 'Out of Hours and Lone Working Request' signed by your supervisor. Please contact **dso@materials.ox.ac.uk** for more information.

Part II students must understand that they are required to finish their work and leave the Department by 10 pm. They must plan their work accordingly to ensure they are ready to leave by this time.

Students should know who to call in an emergency out of hours. Students can:

- **For a critical medical or fire emergency:**
    1. call **999 immediately**,
    2. followed by University Security Services on **01865 272999**.
- **For a non-life-threatening emergency or where urgent assistance is required:** call University Security Services on **01865 272944**.

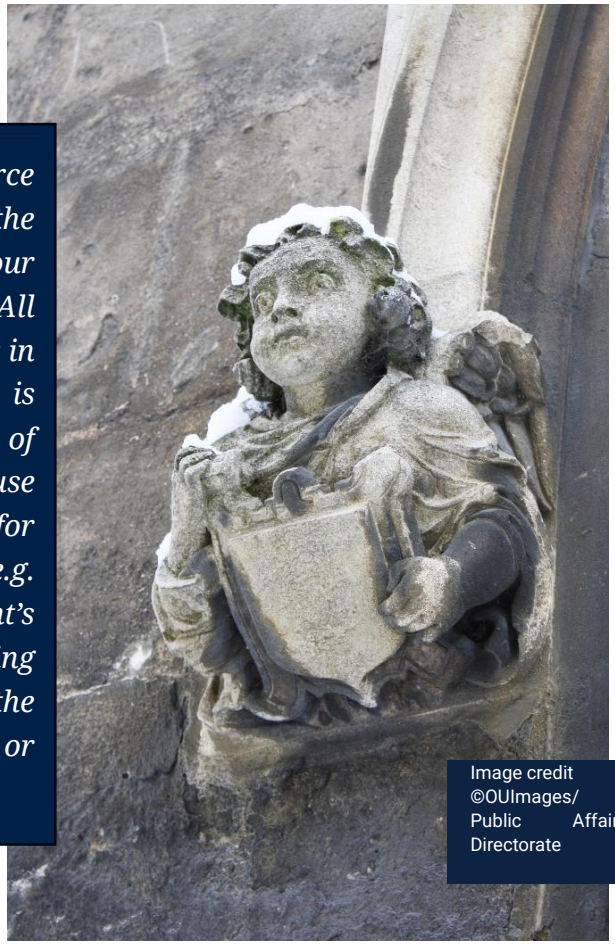
Please refer to the **Department Safety SharePoint** pages or contact the Department Safety Team for guidance.

8. Plagiarism

You will be required to complete the Avoiding Plagiarism online training before you start your Part II Project.

The University definition of plagiarism is as follows:

"Presenting work or ideas from another source as your own, with or without consent of the original author, by incorporating it into your work without full acknowledgement. All published and unpublished material, whether in manuscript, printed or electronic form, is covered under this definition, as is the use of material generated wholly or in part through use of artificial intelligence (save when use of AI for assessment has received prior authorisation e.g. as a reasonable adjustment for a student's disability). Plagiarism can also include re-using your own work without citation. Under the regulations for examinations, intentional or reckless plagiarism is a disciplinary offence."



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You must read the **Student Disciplinary Procedure (Academic Cases)**.

You must always indicate to the examiners when you have drawn on the work of others; other people's original ideas and methods should be clearly distinguished from your own, and other people's words, illustrations, diagrams etc. should be clearly indicated regardless of whether they are copied exactly, paraphrased, or adapted. This includes the use of artificial intelligence.

Failure to acknowledge your sources by clear citation and referencing constitutes plagiarism. The University reserves the right to use software applications to screen any individual's submitted work for matches either to published sources or to other submitted work. Any matches might indicate either plagiarism or collusion. Although the use of electronic resources by students in their academic work is encouraged, you should remember that the regulations on plagiarism apply to online material and other digital material just as much as to printed material.

The University regards plagiarism as a serious matter. Cases will be investigated and penalties may range from deduction of marks to expulsion from the University, depending on the seriousness of the occurrence. Even if plagiarism is inadvertent, it can result in a penalty.

Useful information on plagiarism can be found on the **Study skills and training pages.**

9. Use of Artificial Intelligence (Gen AI)

The Department of Materials encourages the experimentation with, and confident use of, generative artificial intelligence (Gen AI or AI) tools by undergraduate students. However, this must be within the use permitted by the University and Departmental policies (see **Appendix A**).

The Part II thesis is a summative assessed coursework element, and the permitted use of AI is **Category 4**. This means that substantive use of AI is permitted as an integral part of the assessment, and a declaration of any substantive use of AI tools and technologies must be submitted with the thesis. Guidance on what constitutes permitted substantive use of AI tools, and impermissible use, is given in **Appendix B**.

The declaration statement should include the following information:

1. Name and version of the generative AI tool e.g. ChatGPT5, Copilot
2. Publisher (name of company that provides the Gen AI system) e.g. Microsoft, OpenAI
3. Brief description of the way in which the tool was used (e.g. background research, refining code)

The declaration statement must include a formal declaration that any Gen AI use complies with University, divisional and departmental guidance, where and how Gen AI has been used in preparation of the thesis and summarising how specific uses of Gen AI will be referenced in the text.

An example declaration suitable for a Part II thesis could be:

I used Generative AI (ChatGPT5, OpenAI) as a writing support tool. Its use was limited to improving grammar, enhancing readability, refining academic language, generating outlines for chapters, suggesting alternative wording, and assisting in the summarization of scientific literature. ChatGPT was also occasionally used to explain scientific concepts to improve my understanding of topics addressed in this research. All outputs produced by these tools were carefully reviewed, verified, and substantially revised by me before being incorporated into the thesis.

The bioinformatics pipeline was implemented in Python using the pandas, NumPy, SciPy, and matplotlib libraries. Generative AI (ChatGPT5, OpenAI) was used to assist in developing and debugging portions of the analysis scripts and to suggest efficient implementations of standard data-processing functions. This has been described in the Methods chapter of my thesis. No AI-generated code was used without independent testing and verification. All methodological decisions, quality-control procedures, statistical analyses, and interpretation of findings were undertaken by me.

I have ensured that all factual statements, citations, and references have been checked against the original sources and that the final content complies with the ethical standards, academic integrity policies, and guidelines of the University of Oxford and Department of Materials.

10. Training Courses and Workshops

All these training courses and workshops are compulsory, unless noted otherwise. Please consult the **Lecture List** for the schedule.

If you are undertaking an external Part II project, you will be given access to recordings of the in-person workshops and training.

If you encounter any difficulties accessing the online training courses, contact undergraduate.studies@materials.ox.ac.uk.

10.1. Avoiding Plagiarism (Michaelmas term)

You must read the University Guidance on Plagiarism:

⚠ Click ***HERE*** to read the *University Guidance on Plagiarism*

You must pass the online training course on **Avoiding Plagiarism.**

⚠ *Click **HERE** to take the course.*

The objectives of the **Avoiding Plagiarism** training course (duration ~50 minutes) are to:

- Define plagiarism and describe different types of plagiarism
- Recognise and describe key terms relating to plagiarism
- Understand the importance of referencing
- Compile accurate citations and references
- Correctly paraphrase and acknowledge others' work
- Make better use of referencing software to manage your citations and references
- Develop strategies to help you avoid plagiarism in your own work.

A pass mark of 80% is required – you can repeat the course until you achieve this.

On successful completion of the **Avoiding Plagiarism** training course, download your certificate and upload it to the Canvas submission portal. This must be done by **5pm on Friday of -3rd Week, Michaelmas Term.**

You must include a copy of your pass certificate in the Mandatory Final Chapter of your thesis.

10.2. Health and Safety Basics (Michaelmas term)

It is compulsory to complete the **Health and Safety Basics** online training within one month of starting the Part II project.

⚠ *Click **HERE** to take the course.*

The objectives of this training are:

- Understand how and why health and safety is managed in the University
- Overview of common health and safety hazards to look out for at your workplace
- Know what action everyone can and should take to work safely
- Overview of environmental compliance

On successful completion of the **Health and Safety Basics** training, append your certificate to your **PMF1 Project Management Form**.

You must include copy of your pass certificate in the Mandatory Final Chapter of your thesis.

10.3. Information Skills for Part II students (Michaelmas term)

This workshop covers information skills for Part II students and an introduction to Reference Management.

10.4. Ethics & Sustainability (Michaelmas and Hilary terms)

These workshops aim to support critical thinking for the material issues that you will face in your careers. The first workshop in Michaelmas Term uses case studies to discuss sustainability and ethical considerations. The second workshop in Hilary Term is intended to help you explore the ethics and sustainability issues associated with your own projects. Your thesis requires a reflective account (<1000 words) on the ethical and sustainability considerations of your project.

Workshop 1: Understanding paradigms for considering sustainability

- Climate change
    - Impacts of the greenhouse effect and albedo, and primary sources of anthropogenic climate forcing
    - Basic climate metrics including radiative forcing, GWP, GTP
    - Overview of renewable technologies to combat climate change (and key material challenges - catalysts, battery materials, super-alloys, cryogenic & superconducting, fusion materials, recyclability of these...)
    - Basic understanding of how bio-based material sources may reduce or increase emissions
    - How technology, market and economics are distinct from sustainability
- Critical minerals

    - The factors that contribute to a mineral / material being defined as critical
    - Where critical minerals are used and why
    - The material science challenges raised by these factors (e.g. reduction, substitution, circularity)
- Circular economy
    - Meaning of "circular economy", and Braungart & McDonough Butterfly Diagram or similar to explain the concept
    - Understanding end of life at start of life as a key design factor
    - Design principles to reduce material use, design for maintenance, repair and recycling, design for right life (application in Team Design Project / 4th year project)
- Toxicity
    - Where emissions occur in material supply chains with human and ecological toxicity impacts (examples to raise awareness of ethics in sourcing)
    - Restricted substances regulations and effect of toxic additives on end of life
- Social impacts
    - Accounting for upstream and downstream social impacts, inc slavery, child labour, fair wages/ working hours, health & safety, etc.
    - How regional culture affects perception of social impacts

Workshop 2: Tools and rules for assessing and implementing sustainable solutions

- Life cycle assessment (LCA)
    - Reasons for doing LCA
    - Core understanding - Impact categories (midpoint/endpoint), methodologies, product category rules
    - Goal & scope, boundaries, functional unit, inventory analysis (inputs & outputs), interpretation
    - Data collection challenges and potential for automation
    - Carbon footprinting and Streamlined LCA
    - Prospective LCA - esp considering changes in upstream material supply chain, fuels and electricity sources, market uptake
- Further tools and methods
    - D4S/Ecodesign methodology integrated into D4X
    - Managing variability, e.g. stochastic design, especially for integrating bio / recycled content
    - Managing conflicting factors, e.g. Pareto front
    - Digital thread / twin / passport as powerful emerging tools
- Regulatory drivers
    - Current summary of relevant regulations around ecodesign, end of life, toxicity, etc - understanding that its constantly changing
- Business models and influence
    - Sustainable solutions must be economically viable, or sufficiently incentivised by policies to be viable
    - How business models can support or hinder circularity or other more sustainable solutions
    - Influencing business models, supply chain, standards, regulation and policy

10.5. Engineering Context (Michaelmas term)

The materials science paradigm is to reveal and rationalise the extreme complexity of materials behaviour so that it is better understood and new knowledge is generated. But also included in the field of materials is the more applied aspect of materials engineering. This implies a materials engineering context which – for a well-rounded Part II project – needs to be acknowledged. Here, one is referring to the application of the new materials knowledge for the benefit of humankind and our planet. Experience shows that it is often the materials engineering aspect which determines whether a new materials solution is taken up commercially.

In your thesis you will need to identify the engineering (or scientific equivalent) context of your work. This should include reflection on the engineering implications of your project findings, as well as covering engineering context in a generic manner for the project topic.

These concepts are addressed in this workshop, where you will have the opportunity to ask questions. If, later on in your project, you need further guidance on how to address the Engineering Context of your particular project, the Part II Organiser may be approached for advice.

10.6. Scientific Presentation: Posters (Michaelmas term)

The objective of this workshop is to help you to design a poster to communicate the Engineering Context (or equivalent) of your Part II project to a non-expert audience. The initial training workshop will be followed by online 'drop-in' support during week 5 where you may obtain advice on your draft poster.

You must submit your final poster as a **pdf** via Canvas by **5pm on Friday of Week 5, Michaelmas term**.

The posters will be printed by the Department of Materials at A2-size and displayed at a social event in Michaelmas term Week 6 that will be open to Year 3 and Year 4 students on the Materials MEng course. Further details on time and location will be provided. Attendance at this event is not mandatory but is strongly encouraged.

Part II student will be given online access to up to 5 posters to review (by end of week 6). You will receive a summary of this qualitative peer-feedback on your poster. **Completing these reviews is mandatory.**

You must include a copy of your submitted poster (A4 size), and your written reflection (<500 words) on how you might improve the poster after considering the feedback, in the Mandatory Final Chapter of your thesis.

10.7. Research Integrity: Introductory Core Course (Michaelmas term)

All students must pass the online training course on **Research Integrity: Introductory Core Course**

⚠ *Click **HERE** to take the course.*

You are recommended to complete this before **Week 6 Michaelmas Term**, and to record this in your PMF2 Project Management Form

The objectives of the **Research Integrity: Introductory Core Course** training course (duration ~250 minutes – *it does not need to be completed in a single session*) are to:

- To provide new researchers and research students with an introduction to good practice in research
- To introduce issues that should be considered when planning, conducting and reporting research
- To guide researchers through the lifecycle of a research project
- To provide further information about what constitutes research misconduct and what to do if this is suspected

There are eight modules for this course, for evidence that you have completed the core course, you will need to take and pass the quizzes at the end of each module and score an overall pass mark of 80% or over. You can take the quizzes multiple times.

You must include copy of your pass certificate for the Research Integrity: Introductory Core Course in the Mandatory Final Chapter of your thesis.

10.8. Scientific Writing (Michaelmas term)

This one-day course aims to provides a sound grounding in the core skills needed to produce accurate and effective scientific writing in your thesis. It includes critique of readability in relevant papers, use of tenses in academic papers, writing with impact, concise writing, grammar and proof reading and scientific table and chart techniques.

Students undertaking External Part II projects do not need to attend this training session but will be given access to the course materials.

The objectives are to:

- Develop understanding of the characteristics of scientific writing; write in simple, clear and concise scientific English.
- Develop knowledge of how to write grammatically correct English.
- Improve proof reading skills; organise the sections of a scientific paper effectively.
- Develop a scientific argument with appropriate language that conveys the message effectively.
- Make effective use of charts and tables.

10.9. Research Integrity: Intellectual Property (Hilary term)

All students must pass the online training course on **Research Integrity: Intellectual Property.**

Click HERE to take the course.

You are recommended to complete this course (60 minute duration) before **Week 6 Hilary Term**, and to record this in your PMF3 Project Management Form

The objectives of the **Research Integrity: Intellectual Property** training course (duration ~30 minutes) are to:

- Define 'intellectual property' as it relates to research
- Explain when and how researchers can copyright their research
- Explain when and how researchers can patent their research
- Discuss some of the limitations on intellectual property protection in research
- Explain the steps that should be taken to establish ownership of intellectual property
- Explain how intellectual property is managed in the UK
- Provide examples of the emerging issues associated with copyright and the patent protection of research.

Following the completion of this course, you will need to book onto the **Research Integrity: Intellectual Property Quiz**. Once you have passed the quiz, you will then be sent an email certificate of completion of the course.

You must include copy of your pass certificate for the Research Integrity: Intellectual Property Quiz in the Mandatory Final Chapter of your thesis.

10.10. Scientific Presentation: Talks (Hilary term)

The workshop will cover the key principles of planning and delivering a successful talk and help to build your confidence in preparation for the Part II Talks that will be held in Trinity Term.

Students undertaking External Part II projects do not need to attend this training session but will be given access to the course materials.

The objectives are to

- develop an awareness of what makes a presentation effective.
- understand why planning and practice are crucial to the success of a presentation.
- have the confidence to choose and use a variety of techniques to engage the audience
- practiced delivering a short presentation and gain constructive feedback.

11. Postgraduate and Part II Lectures

You are strongly encouraged to attend any postgraduate lectures that you consider useful or interesting. Please consult the **Lecture List** for details.

Image credit
John Cairns

In particular, if you are planning to do any X-ray diffraction work then you should view the recorded 'X-ray diffractometry' course given by Prof. Susie Speller. Contact **undergraduate.studies@materials.ox.ac.uk** for details.

If you wish to use any of the electron microscopes you must first receive training (and attend the relevant lectures), co-ordinated by Dr. Neil Young. Your supervisor will advise on this.

12. Consumables and Equipment

12.1. Stores

The Department of Materials Stores is on the ground floor of the Hume-Rothery Building. Stores is self-service and accessible via university card. The stores stock a broad range of general goods from stationery to lab ware (e.g. pens, lab coats, sample boxes, tweezers, notebooks, cleaning materials, gas cylinders, sample stubs, etc)

See **Stores and Workshops | Department of Materials**

You must agree requests for consumables, materials, equipment etc. with your supervisor. They will advise you how to order items. Your supervisor will give you an account code for minor items to be obtained from the Departmental Stores (to a total of £250). You should not disclose this account code to others.

12.2. Ordering Materials and Equipment

The materials and equipment that you need for your project should already be available, but projects can change direction or need more resources.

If the items are not held in stores you will need to order it with a **Purchase Order**.

Advice on how to request a purchase order is at **Purchasing | Department of Materials**.

You must **NOT** place a purchase order directly with a supplier.

You **MUST** get your supervisor to approve the order and confirm where the funding is coming from (it will be returned otherwise!).

Where possible, you should use a supplier with whom the University already has an account. Setting up new accounts is very costly, and GREATLY SLOWS the ordering process. Items can only be ordered online (Amazon etc) in special circumstances.

12.3. Printing

You have an allocation of £75 to use the Departmental Printers (2p per sheet A4 monochrome, 4p per sheet colour). See **Materials Printing | Department of Materials.**

13. Student Representation

Part II students are represented on both on JCCU (Joint Consultative Committee for Undergraduates) and JCCG (Joint Consultative Committee for Graduates), which provide a route for direct termly feedback to the Part II Organiser, the Director of Undergraduate Studies and the Head of Department

JCCG Coffee is a free weekly opportunity to meet the postgrads and each other informally. It alternates between Holder Coffee Room and Begbroke. Watch out for emails.

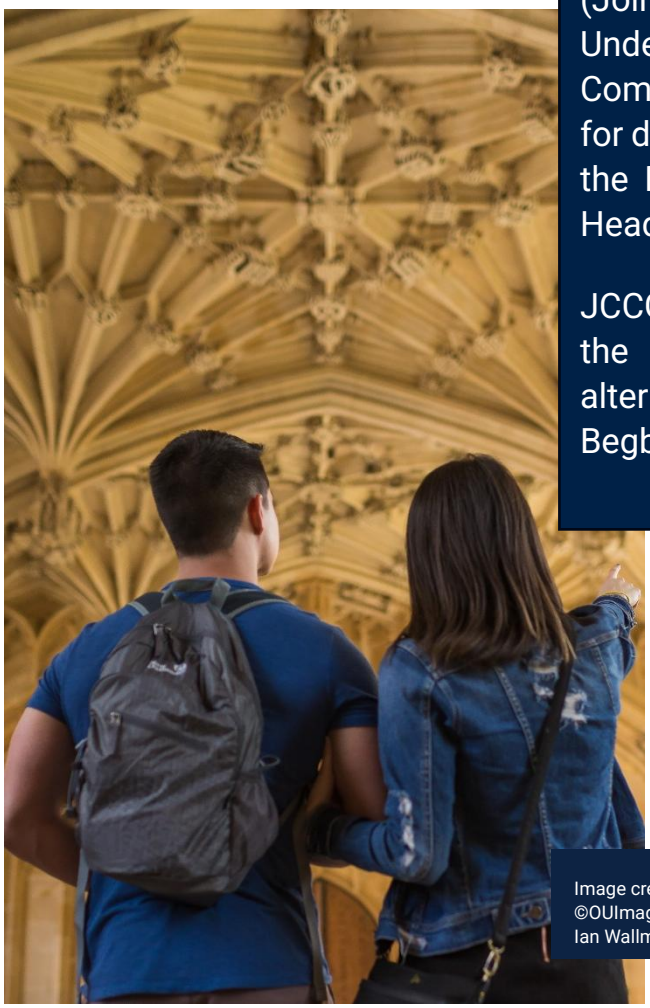


Image credit ©OUImages/ Ian Wallman

14. Supervisors and Supervision

14.1. Supervisors

Your Part II supervisor(s) must be one of the following:

- a professor who is a member of one of the Faculties in the Physical Sciences;
- a reader or university lecturer or senior research officer who is a member of one of the Faculties of Physical Sciences;
- a person listed in a Register of Part II Supervisors to be maintained by the Faculty of Materials.

A supervisor may be a postdoctoral researcher, if this has been approved by DMAC (Department of Materials Academic Committee) on behalf of Faculty and entered into the Register of Part II Supervisors. Your supervisor cannot be a DPhil student, although you may be supported in your research by DPhil students.

14.2. Supervision

The following teaching norm has been adopted by the Faculty of Materials for the supervision of Materials Science Part II projects:

"Responsibility for the project rests with the student, who should be proactive in seeking support and guidance when necessary and in making use of existing written resources.

Part II students should expect to hold regular meetings with their supervisor. These will normally be held at least every two weeks for the duration of the project but significantly more intensive support is usual in the initial and final stages of the project. The support given by the supervisor at these scheduled meetings may include formal discussion of research, feedback on the student's derivations, analyses of results, thesis drafts etc. that have been read by the supervisor and direction to relevant literature."

You are entitled to receive thorough formative feedback on one draft of your thesis provided that it is submitted to your supervisor significantly in advance of the deadline for submission of the thesis to the Examination Schools; feedback may not be possible if the draft thesis is submitted later than two weeks before this deadline. If a first draft is submitted to your supervisor well in advance of the final deadline then he or she is permitted, but not required, to provide limited feedback on revised drafts.

Formal meetings with your supervisor will be in many cases supplemented by brief discussions of particular aspects of the research on an ad hoc basis, as required for the investigation to progress smoothly. Further support will be given in the techniques required for the student to carry out their research. Examples include the use of equipment and the performance of experimental techniques, training on modelling software and computer programming and tuition in mathematical methods.

You should note that (i) it is in the nature of research that not all projects require the same type or level of support, and (ii) for some projects the supervisor will personally deliver specialist training, whilst for others such training will be provided by informal mentors or via scheduled Departmental training courses."

14.3. Feedback

Supervisors are encouraged to provide written feedback each term via the University of Oxford Teaching Management System (TMS).

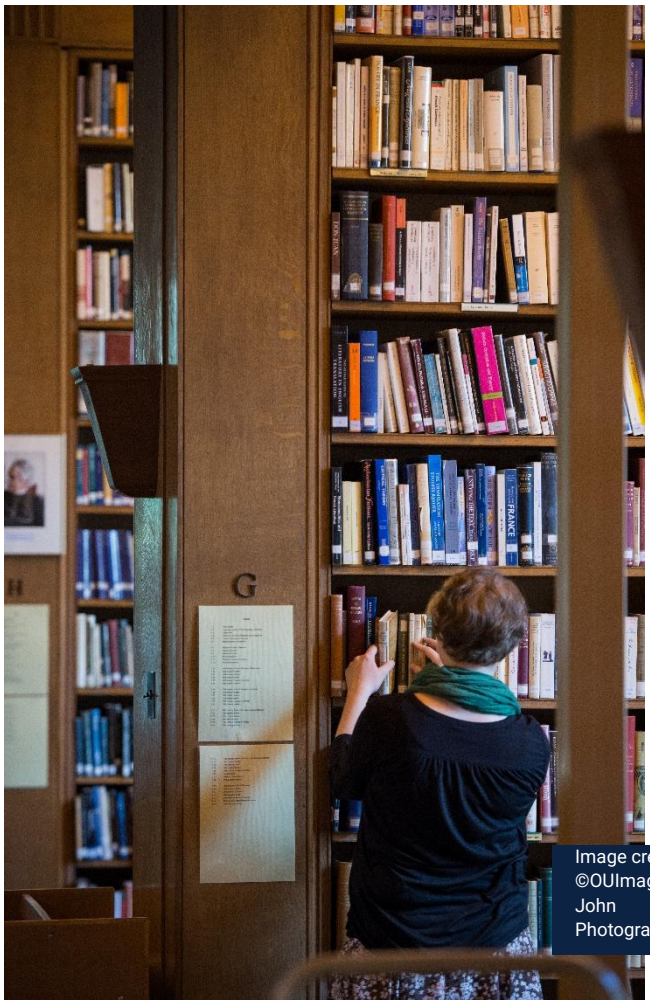


Image credit ©OUImages/ John Cairns Photography

15. The Part II Talks

You will be required to give a talk on your Part II project at a mini-symposium in Trinity Term, usually over two days in Week 2. All Part II students are required to attend and give a talk on their Part II Project. There are no exemptions. The aim is to give you experience of giving an oral presentation.

Each talk will last 12 minutes + 3 minutes for discussion. All members of the Department are invited.

The talk is **not** examinable! Part II examiners are allowed to attend **only** presentations of projects that they supervise, with the exception of the Part II Organiser who attends all talks.

You will receive brief, confidential, feedback about your talk from the Part II Project Organiser.

The talk should be aimed at non-specialist scientists. It should include a brief description of the engineering relevance of your project. Should your talk include content which refers to potentially exploitable intellectual property (IP) it is vital that you alert the Part II Project Organiser to this **in advance** who will arrange for a non-disclosure undertaking to be signed by all external people who may be present. An example of this form can be found at **Appendix C**.

You should note the following guidelines and advice:

- The time scheduled for each talk and associated questions is 15 minutes. This time limit will be strictly enforced.
- The talks are for YOUR benefit, primarily to give you some experience of talking in front of an audience, and there is an Ironmongers' Company prize for the best Part II talk. The judges will include representatives from the Department and the Ironmongers' Company.
- The talk should be pitched at the level of a non-specialist scientist. Make sure that you put your work into context before launching into specific results. Why is the field interesting, what has been done before, what is special about what you have attempted to do? Try to make your talk understandable and interesting to an educated lay person or someone at the level of a first year undergraduate.
- Practice your talk beforehand. You are allocated 15 minutes but make sure you FINISH YOUR TALK IN 12 MINUTES to allow for questions and the change around between speakers. There will be the opportunity to sign up for practice slots in the lecture theatre.
- Familiarise yourself with the controls for projectors and lights in the lecture theatre. To ensure a smooth handover, please ensure that your presentation has been copied to and runs from the main computer in the lecture theatre (this needs to be done in the break before your timetabled session), or ensure that your laptop is running and can be attached directly to the projector without any delays (it is your responsibility to check the right connections are available).
- Don't just turn up for your talk and then leave. Lend each other your support and attend for the full programme of talks.

16. The Thesis

16.1. Submission Deadline

You must submit your Thesis via **Inspera** by **4pm on Monday of Week 7, Trinity term**.

16.2. Required Content

The Exam Regulations (**2023-24, Honour School of Materials Science**) specify the required content for the Part II Report on the Investigations. This report is known within the Department of Materials as the **Part II Thesis**.

The objectives of the Part II Thesis are:

- To review and critically evaluate scientific and technical literature
- To present the methodology, results, discussion and conclusions of the Part II research project
- To present the engineering context of the Part II research project and its findings
- To demonstrate and reflect on the management of the research project, including health, safety and risk management
- To reflect on the ethical and sustainability considerations relevant to the project and its outcomes

The length of the main report of thesis (Parts A and B) is <12,000 words, of which the expected length of the literature review (Part A) is between 2,000 and 4,000 words. In addition, the thesis must have a mandatory final chapter (Part C) that is maximum of 3,000 words in length. The word counts include the abstract and captions for tables and figures. The references, title page, data tables, acknowledgements and table of contents are excluded from the word and page count, as are the appended research poster, PMF forms, Risk assessment forms and pass certificates. You should state the word counts for the main report (Parts A and B) and the final chapter (Part C) on the title page of your thesis.

The mandatory final chapter (Part C) must include all the following elements

- Accounts on
    a. Engineering/scientific context of the research project's findings (<500 words)
    b. Project management with project management forms (<1,500 words)
    c. Health, safety and risk management (<500 words)
    d. Ethical and sustainability considerations (<1,000 words)
    e. Peer feedback on Research Poster and A4 copy of poster (<500 words)
- Pass certificates for
    a. Health and Safety Basics
    b. Avoiding Plagiarism
    c. Research Integrity: Introductory Core Course
    d. Research Integrity: Intellectual Property

If you feel that you have an exceptional case for exceeding the word and/or page limit, and you wish to seek permission to do so, both you and your supervisor should contact the Part II Project Organiser who will put your case to the Chair of Examiners. Such a case should be made at the earliest possible stage. The Examiners will enforce the word limit strongly, and any thesis submitted over the word limit may be subject to penalties.

The purpose of the above word and page limits is to prevent the excessive inclusion of material that is unnecessary for development of the key argument(s) of the thesis. Material which is additional to the main body of the thesis, e.g. further detailed data, computer programs and similar material may be included in **appendices**. However, whilst Examiners are required to consider the main body of the thesis, whether they read appendices is entirely at their discretion.

16.3. Default Structure and Content for a Part II Thesis

The Part II thesis reports on a substantial research project and as such it is appropriate that it is structured in a similar manner to a traditional-style PhD thesis in Materials Science, but taking account of the short duration of the Part II project.

Your supervisor will guide you on any variations to the structure outlined below that might be appropriate for a thesis in the research area of your particular project.

- Title Page
- Declaration of use of Generative AI
- Abstract
- Acknowledgements
- Table of Contents
- Optional brief scene-setting chapter
- Literature Review chapter
- Apparatus, Experimental/Computational Methods and Background Theory chapter
- Results & Discussion chapter(s)
- General Discussion and Conclusions chapter
- Special chapter for Part II, to cover accounts of Engineering/Scientific context, Project Management, Ethical & Sustainability considerations, and Health, Safety & Risk Assessment
- References

It is important that the thesis is considerably more than just a narrative of what you have done. As well as the content outlined below, do indicate when you have provided creative input to the project direction and/or evidence of how you have steered or driven the project. For example, be clear on the reasoning that underlies decisions taken on what experiment(s) to do next, or changes to experimental methodology, in the light of the results of your previous experiments and/or your understanding of the literature.

Clearly describe the aims and objectives of your research. Remember, an **aim** is the broad, long-term goal of a project, answering the question, "What do I want to achieve?" An **objective** is a specific, measurable step taken to reach that aim, answering the question, "How exactly will I get there?

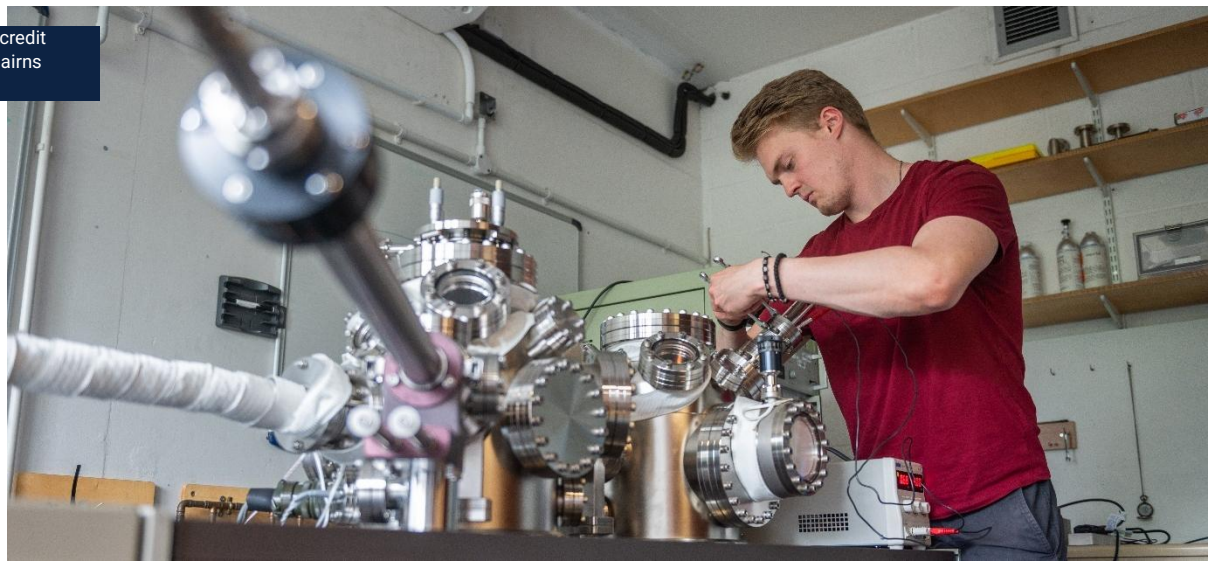
Your literature review should be a systematic, well organised and comprehensive summary of the relevant literature. It is important that you critically appraise this literature. For example, are there flaws or limitations in some of the previous work; do you agree with the authors' conclusions; do all previous reports on related topics fully agree, or are there differences; if the latter do you agree with the authors' explanations of the differences (if the authors do not comment on these differences can you suggest reasons why the differences might exist)? Your review, and the logical argument that you develop within it, should establish the hypothesis of your project.

In your apparatus, methods & theory chapter include brief explanations of why these particular approaches are the most appropriate. It should be clear whether you have used established methods, or have developed new methods of your own. Do not go into detail about methods or instruments where you are using routine applications or for which the underlying theory or calculations are standard topics in undergraduate text books. Remember to provide enough information that someone else could repeat your study.

In your results section, you should consider the errors and uncertainties in your measurements, analyses and calculations. Quantify these where possible. Use this understanding of your errors when determining if trends or changes that you observe in your experiments or simulations are statistically significant, and when deciding how precisely to report your results. There is some useful guidance on how to quantify and report errors in Appendix E.

Following the presentation of your results, you should include a critical discussion of these results: what do they mean, how do they compare and contrast with, and extend, the previously published work in this field. Finally draw succinct conclusions from your work and comment briefly on potential applications and future work.

Image credit
John Cairns



16.4. What are the Examiners looking for in a Good Part II Thesis?

"Let's start with the obvious. What the examiners most want to see is high quality scientific work, professionally carried out and well presented. There is not a requirement in the regulations that you should discover something entirely new and revolutionary. You only have nine months to carry out your project, and one of the essences of scientific research is its unpredictability. You may run into unexpected difficulties, or the project may not work out at all in the way you anticipated. It may even happen that other people are working on the same scientific problem, entirely unknown to you, who publish their results shortly before you complete your own work. You have no control over such events. For this reason, the examination regulations require only that you submit a report on your investigations. Tell us what you did. If it worked, that's great. If it didn't, tell the examiners why, and if appropriate, suggest how the project might be improved or redesigned to get better results. If you find that other people have duplicated your work, you should include a critical comparison of your work and theirs. If the various results agree, that's good: if not, that's interesting – try to explain the reasons for the discrepancies.

Now to some details. The Part II year forms part of your training for the M.Eng. degree, and for subsequent Chartered Engineer status. Thus there are a number of professional skills that you should be acquiring during the year, and for which training will be provided. These include experimental and/or computational abilities, literature searching, data analysis, oral and written presentational skills, and project management. Your Part II thesis should demonstrate what you have learnt in a number of these areas. For example:

- *Your literature survey should be concise and critical, and you should include mention of what databases or other information sources you have used in compiling it.*
- *An engineering context of your work also needs to be included.*
- *Full information should be given about the materials that you study – their source, purity, full composition, prior thermal and mechanical treatments, etc.*
- *The reproducibility of experimental measurements should be stated, and an estimate of experimental errors and uncertainties should be included alongside the results.*
- *Analysis of the statistical significance of experimental results should be included whenever appropriate.*
- *Where computer modelling has been used, an assessment of the reliability of the model and the accuracy of the calculations should be attempted.*
- *A short discussion of project management aspects of your research must be included, describing the evolution of the aims and objectives of the work, the chronology of what was actually done, and the reasons for any changes of strategy as the year progressed.*
- *The thesis should contain a clear summary of the main results and conclusions and (where appropriate) should identify key objectives for further work.*

One aspect of the Part II which is not formally assessed for examination purposes is your development of oral presentational skills. You will give a talk about your project at a

Departmental 'mini-symposium' which is held shortly after Easter, and there is a prize for the best presentation on that occasion. But the examiners will not take this oral presentation into account when awarding your degree. The reason is simple – some people are naturally much better talkers than others! For the same reason, although you will have a viva voce examination following the submission of your thesis, you will not be marked for your presentational skills on that occasion. The purpose of the viva is to establish that you fully understand the subject matter of your thesis, that you are conversant with the workings of the equipment or computer models that you have used, and that you have a good critical appreciation of the significance of your results.

In assessing the thesis, the examiners will seek information from the project supervisor(s) about the extent of your interaction with other people, the nature of your specific contributions to the overall research, and about the effects of factors outside your control. But it is important not to let the existence of this form of evaluation distort your behaviour pattern. Don't hide away in a corner and refuse to talk to anyone about your work for fear of being penalised at the end of the year. Teamwork is vital, and discussing plans and ideas with colleagues is a very important and enjoyable aspect of research – it's just that, at the end of the year, the examiners have to try to establish what contribution you have made to the overall work of the research group of which you have been a member.

Have a great year – the Part II should be one the most enjoyable parts of the whole course."

Prof.G D W Smith (Chair of Part II Examiners 1999-2000)

16.5. Marking the Thesis

The Part II Thesis contributes a weight of a maximum of 1/3 towards the total mark for the whole degree.

Your thesis will be read independently by two internal examiners or one internal examiner and an assessor, who will each allocate a provisional mark before the viva. The marking guidelines used by the examiners are given in **Appendix D**. Those two marks are declared to all the examiners present before the vivas begin. Each thesis will be inspected by one of the two External Examiners.

A viva voce examination is held for all Part II students. The viva voce examination is normally held during **Week 10 of Trinity Term and your attendance is mandatory**.

The purpose of the viva is to clarify any points the readers believe should be explored, and to ascertain the extent to which the work reported is the candidate's. A discussion involving all examiners present is held after the viva. In arriving at the agreed mark the Examiners will take into account all of the following, (i) the comments and provisional marks of the original markers, (ii) the candidate's understanding of their work as demonstrated during the viva and (iii) the opinion of the external examiner who has seen the thesis.

It must be stressed that in order to preserve the independence of the Examiners, you are not allowed to make contact directly about matters relating to the content of the exams or the marking of coursework. Any communication must be via the Senior Tutor of your college, who will, if they deem the matter of importance, contact the Proctors. The Proctors in turn communicate with the Chair of Examiners. If you have any queries about the Examinations or anything related to the Examinations, for example, illness, personal issues, please don't hesitate to seek further advice from your College tutor, or one of the Department's academic support staff.

For further details, please see the **FHS Examination Conventions**.

16.6. Past Part II Project Reports

Past Part II project reports are available for students to consult. Details of the reports available and how to request access are provided on Canvas.

17. Project Management

The Part II Project is the first time that you have to focus on a full-time, self-driven piece of work for such a lengthy period. You are expected to take control of, and responsibility for, your own projects. For some this can be a daunting prospect. To help you, and to provide some development of what is a useful generic skill, there is a workshop on project management as part of the Part II induction programme and there is a formal Part II project management process which all students must undertake.

17.1. Why is project management important?

Setting goals: Identifying your goals and objectives at the beginning of your project helps you to focus and remain focused on what you aim to achieve. You wouldn't want to get on a flight to New York only to realise half-way across the Atlantic that actually you should have been going to Paris!

You have a pre-determined, fixed deadline. Planning what tasks you need to carry out, how long each will take, and the order in which you will do them will help you to understand if your goals are realistic, and to achieve them efficiently and on time. Avoid 'two steps forward, one step back…'

Planning resources. A carefully planned sequence of tasks will mean little if you haven't thought about what you will need to carry out each of those tasks. Identifying what resources you will need (consumable items, equipment bookings, technical staff time, training etc), and having them in place at the right time is crucial. Consider also the availability of resources when scheduling your activities..

Assessing and mitigating risks. It is in the nature of research that things can and do go wrong, e.g. suppliers fail to deliver, a technician that is helping you falls ill, or an instrument breaks down. Many of these things are outside of your control, but thinking in advance about the risks to the success of your project will help you to plan what to do if something does go wrong. Expect the unexpected.

Monitoring progress. Having a pre-determined project schedule provides you with a means of continuously monitoring your own progress. Setting yourself milestones also helps you to keep on track. Although 'following your nose' can be fun, it's easier to navigate by checking where you are in relation to landmarks on a map.

Self-control. If left unchecked, your scientific curiosity may lead you along a variety of side-paths, some of which will be dead ends, and some of which may lead to very interesting but irrelevant outcomes. Effective project management will help you to resist that temptation, or at least help you to consider any risks to your project, and to re-plan, if you do decide to take a detour.

17.2. The Part II Project Management Process

Throughout your Part II you are required to complete three **Project Management Forms**. Once these have been signed off by your lead supervisor, and by the deadlines detailed below, submit them as pdf documents via Canvas.

You should downloaded the forms from Canvas. Examples are included in this handbook for reference. When completing the forms, you may wish to consider that you will need to include a copy of each in your thesis, so you should ensure they are legible and succinct! If you are undertaking an external Part II project, note that both your local supervisor and your Oxford supervisor will need to review and sign-off these forms.

The Part II Project Organiser will review the forms, and if your project is falling on stony ground then the Part II Project Organiser will invite you for a discussion, possibly with your supervisor.

Project Management Form 1 (due Friday, Week 0 Michaelmas Term) asks you to set out what you expect to achieve during your project, how you expect to achieve it and what resources you will need to achieve it.

Project Management Form 2 (due Friday, Week 6 Michaelmas Term) and **Project Management Form 3** (due Friday, Week 6 Hilary Term) provide you with an opportunity to reflect on your progress, and to describe any difficulties you are experiencing and how you intend to resolve them.

Please take the management of your project and the completion of the Project Management forms seriously. Be honest with yourself and with us. Don't tell us what you think we want to hear. By all means discuss the completion of the forms with your supervisor, but you should not allow them to influence your responses unduly.

Please do not feel that you have to wait until the next Project Management form is due before you can raise any issues that you are concerned about. Your supervisor is normally your first port of call, but you should feel free to discuss any matters of concern with the Part II Project Organiser at any time.

17.3. Compulsory Final Chapter of the Part II Thesis

This chapter must contain reflective accounts of your project management, the Engineering/scientific context of the research project's findings, your health, safety & risk assessment processes, the ethical & sustainability considerations relevant to your project and its outcomes, and the feedback on your research poster.

The chapter **must** also include copies of your pass certificates for the training in **Health and Safety Basics**, **Avoiding Plagiarism**, and **Research Integrity** (Core course and Intellectual Property).

17.3.1. Project Management

Assessment of your ability to manage your project is an integral part of the Examiners' overall evaluation of your thesis. The Examination Regulations require that your Part II thesis includes a compulsory final chapter on the project management aspects of your investigation. The chapter should include a reflective account, of no more than 1,500 words, of how you managed your project and copies of the three project management forms which you may refer to in the reflective account.

It is important that you provide in this compulsory chapter a good description of the way in which you managed your project in order that the scientific fruits of your labour could be realised. The following are some ideas that might help you to plan this chapter, although they are not exhaustive and should not be considered as a template:

- Remind the Examiners of your initial objectives and what milestones you set yourself to achieve along the way. Note down whether you achieved those milestones in time. If not, why not?
- Were your early results in-line with your original hypothesis/objectives, or did they suggest an alternative path for your project (as much as we can plan, research projects often turn out to have a strong evolutionary element).
- In the early stages, did you think about what might go wrong and have a set of mitigating back-up plans? Did the things you thought might go wrong actually go wrong? Were you successful in putting your predetermined back-up plan into action?
- Did unexpected things go wrong? How did you cope with them?
- Did you plan what resources (raw materials, consumables, access to equipment and laboratories, other people's time) you were going to need in advance? How did you ensure that they were all available to you at the right time? Were there any circumstances outside of your control that put those resources out of reach?
- How did you go about making decisions about your project? Did you take autonomous decisions, or did you take decisions only after consultation with your supervisor(s)? Did you have regular review meetings with your supervisor(s)? Were your meetings more ad-hoc as and when problems arose?
- Describe whether you essentially worked alone or as part of a group. If you worked as part of a group describe your role in that group, and how you ensured other members of your group carried out their roles in helping you achieve your aims.
- You might want to describe how you planned to write your thesis. Did you wait until you had done all of your practical work before starting your thesis, or did you draft sections as you went along? Did you use your lab book to help you write your thesis?
- Finally, you might also like to reflect on the planning and management of your project, and show the examiners that you have used this opportunity as a learning experience for the future; e.g. with the benefit of hindsight are there any aspects of your project that you now realise could have been better planned or managed.

17.3.2. Health, Safety & Risk Assessment

Assessment of your understanding of the appropriate aspects of health, safety & risk assessment for the work carried out in your project is an integral part of the Examiners' overall evaluation of your thesis. In the final chapter, you should include a reflective account, of no more than 500 words, of the hazards associated with your work and the appropriate risk assessments and control measures.

Even those of you carrying out a purely modelling or theory project will have completed a project Risk Assessment that can be commented on in this section, but you are likely to need only a small fraction of the 500 word limit to cover this.

17.3.3. Ethics & Sustainability

Image credit John Cairns

Assessment of your understanding of the ethical and sustainability (including life cycle analysis where appropriate) implications of your project and its potential applications is an integral part of the Examiners' overall evaluation of your thesis. In the final chapter, you should include a reflective account, of no more than 1000 words, of the broad and any specific ethical and sustainability implications of your project and its potential applications.

17.3.4. Engineering/scientific context of the research project's findings

Assessment of your understanding of the Engineering/scientific context of your research project's findings is an integral part of the Examiners' overall evaluation of your thesis. In the final chapter, you should include a reflective account, of no more than 500 words, on the engineering/scientific implications of your project findings, as well as covering the generic engineering context of the project topic.

17.3.5. Research Poster Feedback

Assessment of your ability to evaluate the effectiveness of the methods you use to communicate effectively on complex engineering matters with technical and non-technical audiences is an integral part of the Examiners' overall evaluation of your thesis. You will receive up to five peer reviews of the research poster that you prepared in Michaelmas Term, and you should include a copy of your poster and a reflective account, of no more than 500 words on how you might improve the poster after considering this feedback.

17.4. Project Management Form 1

Part II Project Description Form

After discussion with your supervisor YOU should complete this form and submit it via Canvas by Friday of 0th week of Michaelmas Term.

Name: College:

Address for correspondence:

Contact telephone number:

Title of project:

Supervisor:

What are the objectives of the project in order of priority?

List the major milestones that must be accomplished in order to meet the objectives of the project

Are you working essentially on your own or as part of a team? If you are part of a team what is your role, and to what extent is the success of your project dependent on other members of the team?

What resources (equipment, materials, technician support etc.) will you need?

Do you require any training to meet your objectives, e.g. in the use of specific experimental equipment or software, and how are you going to obtain that training?

Complete the following plan for your entire project as you see it now. List each major task

down the left hand column, and for each one draw a horizontal line to indicate the period you expect to allocate to it. For example, the final task, writing your thesis, is shown as occupying mid-April to mid-June.

Task	Oct	Nov	Dec	Jan	Feb	Mar	Apr	May	Jun
Writing up							xxx	xxx	xxx

Have you completed the Health and Safety Basic Training? (Yes/No)

Have you completed the Avoiding Plagiarism Training? (Yes/No)

Has your supervisor completed the Risk Assessment Form for your project? (Yes/No)

Has you sent your Risk Assessment Form to the Department Safety Office? (Yes/No)

Your signature:

Date:

Your supervisor's signature:

Date:

17.5. Project Management Form 2

1st Part II Project Analysis Form

Complete this form and submit it via Canvas by Friday of 6th week of Michaelmas Term

Name:

Title of Project as given in your Project Description:

Refer back to the project plan in your Project Description and list the goals you set for this term. Comment briefly on the extent to which you have achieved them.

Identify clearly any difficulties you have encountered. Are they surmountable in the time available?

State any refinements, modifications or replacements of the original objectives for your Part II project:

Are you intending to change the title of your project? If so, state the new title:

Have the training needs you identified in the Project Description been met, and have you identified any further training requirements?

Tick the appropriate box. Do you have

	None	Some	Sufficient
Results			
Analysis of results			

Do you have any other comments you wish to make?

After looking at the project plan in your Project Description complete the following project plan for the remainder of your Part II.

Task	Dec	Jan	Feb	Mar	Apr	May	Jun

General comments by the supervisor:

Your signature:

Date:

Your supervisor's signature:

Date:

17.6. Project Management Form 3

2nd Part II Project Analysis Form

Complete this form and submit it via Canvas by Friday of 6th week of Hilary Term

Name:

Title of Project:

Refer back to the project plan you made last term and list the goals you set for this term. Comment briefly on the extent to which you have achieved them.

Identify clearly any difficulties you have encountered. Are they surmountable in the time available?

State any refinements, modifications or replacements of the objectives you set for your Part II project:

Are you intending to change the title of your project? If so, state the new title:

What is the title of the talk you will give to the Department?

Have all your training needs for this project now been met?

Tick the appropriate box. Do you have

	None	Some	Sufficient
Results			
Analysis of results			

Do you have any other comments you wish to make?

General comments by the supervisor:

Your signature:

Date:

Your supervisor's signature:

Date:

18. Prizes

18.1. Part II Talks

There is a prize of £450 and a medal from The Worshipful Company of Ironmongers for the best Part II talk in Trinity Term.

18.2. Best Project

The Armourers and Brasiers' Company award a medal and a prize of £250 for the best Materials Science Part II project.

The award is based on the recommendation of the Part II examiners, after the examination of the Part II thesis is completed.

The Armourers like to award the prize and medal at a formal presentation by one of their senior people, on a public occasion.

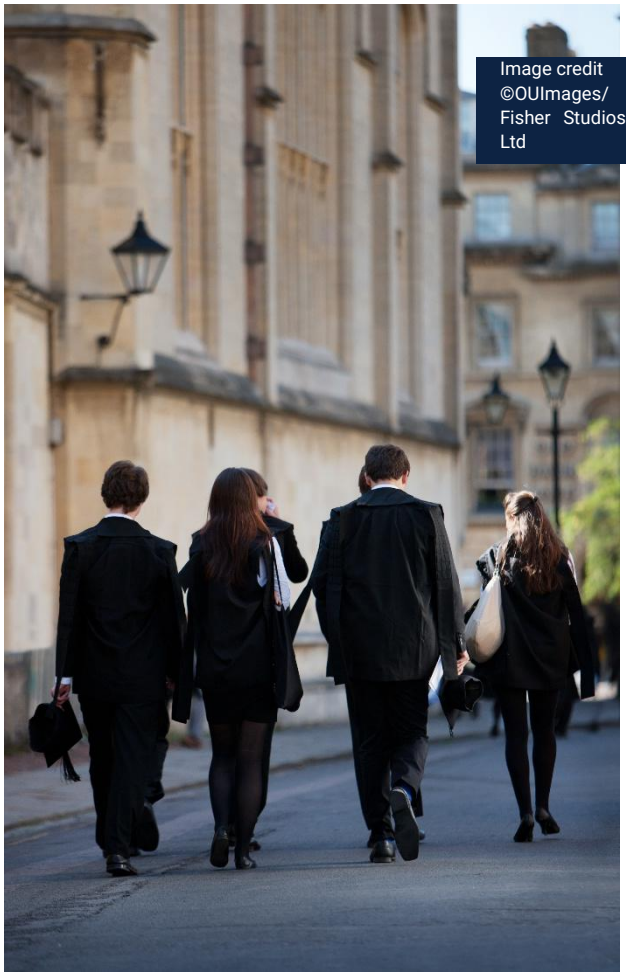


Image credit ©OUImages/ Fisher Studios Ltd

19. Leaving the Department

In the closing stages of the course you will be asked to complete the online Part II Leavers Form.

The form is in three parts:

Part A relates to sponsorship and vacation work whilst on course, and your onward career. This information is very important for various audits and assessments that the University and Department are subject to; for instance accreditation by IOM3.

Part B is a declaration that you have returned your library books and keys and cleared your workspace.

Part C seeks your feedback on the Part II year. As you will know by now, feedback is important to us and we welcome hearing your views about your 4th year experience.

Image credit ©OUImages/ Ian Wallman

20. Appendix A: Policy for students on the use of Artificial Intelligence in Materials Science MEng

*The policy should be read together with the University **Policy on AI use in Summative Assessment** and the guidance in the relevant Undergraduate Handbook.*

The Department of Materials encourages the experimentation with, and confident use of, generative artificial intelligence (Gen AI or AI) tools by undergraduate students.

Students are reminded of the **University guidance** on the use of generative AI tools to support learning. They are reminded that the University's Examination and Assessment Framework states: *"Unauthorised use of artificial intelligence is the presentation of work produced wholly, or in part, by AI as your own. [...] Use of AI in the process of preparing work for summative assessment without authorisation is still academic misconduct, even if the student amends the AI output."* and that they are bound by the university's declaration of authorship for all coursework submissions.

Students must follow the **departmental** and the **university** information security policies and the university's **data protection policy** when interacting with AI.

All coursework in Materials has a ***Category*** that defines permitted AI use:

- Category 1: Prohibited
  - No use at all (i.e. in person exams or 'device-free' classes)
- Category 2: Minimal (default level)
  - Use of spell and grammar checkers, and other non-substantive use, is permitted
- Category 3: Selective
  - Substantive use of AI is permitted in limited and clearly defined ways
- Category 4: Integral
  - Substantive use of AI is an integral part of the assessment.

Using AI for tasks such as assisting non-native speakers with translation, transforming transcribed spoken language to written language by users who face barriers to writing, formatting documents, or improving one's own standard of English or a foreign language is ***not substantive***.

Where substantive AI use is permitted for assessed coursework, students must complete a declaration to confirm their awareness of the category and to declare what substantive use of AI has been made.

21. Appendix B: Guidance for students on the use of artificial intelligence

The Department of Materials encourages the experimentation with, and confident use of, generative artificial intelligence (Gen AI or AI) tools in your studies. AI significantly extends the established tool kit such as search engines, spell-checkers, or debuggers, and opens up new opportunities in collating material, improving your writing, or generating code. However, these wide-ranging and rapidly expanding capabilities require careful consideration in relation to originality, attribution, and good academic practice.

The guidance here should be read together with the **University's guidance** on the use of generative AI tools to support learning. You should note that the University's **Examination and Assessment Framework**, stated: "Unauthorised use of artificial intelligence is the presentation of work produced wholly, or in part, by AI as your own. [...] Use of AI in the process of preparing work for summative assessment without authorisation is still academic misconduct, even if the student amends the AI output." The consequences of unauthorized use through the University's procedure for plagiarism range from mark deductions in minor cases of bad academic practice to expulsion from the university in extreme cases.

You are bound by the university's **declaration of authorship** for all coursework submissions, in which you pledge, among others, "that the work [you] are submitting is entirely [your] own work, except where otherwise indicated".

General considerations for the use of Gen AI

AI can assist, but not replace, your own critical engagement with the subject. You must carefully examine any AI output you build on and be aware of the limitations and pitfalls of the tools you use. These include but are by no means limited to: reproducing information the model was trained on, potentially leading to classical plagiarism and copyright infringement; 'hallucinations', i.e., presenting false information as fact, either through training on erroneous data or incorrect synthesis of correct data, such as made-up references; producing biased or offensive output; code with incorrect syntax or which gives unintended results. Ultimately, you, the student, take full responsibility for the submitted work.

As a broad principle, if it would be inappropriate to ask someone else to do a certain part of the work for you, it will also be inadmissible to use AI for that task. Taking text or mathematics verbatim from AI is strongly discouraged, as it is not reproducible, and cannot be assigned authorship or cited as a permanent source. Any such verbatim passages need to be flagged up explicitly (e.g., in quotation marks) with citation in the style of a "personal communication".

If you use an AI tool to assist you in your writing (e.g., to eliminate grammatical mistakes), it is essential that you scrutinise the result and edit it such that it captures precisely what you want to say.

Always follow the **departmental** and the **university's** information security policies and the university's **data protection policy** when **interacting with AI**. In particular, do not enter private or confidential data into third-party AI tools as they may be stored or passed on to a wider audience, in their original or a processed form, for instance, by being used to train the AI tool.

Permitted use of AI in Coursework

All coursework in Materials has a ***Category*** that defines permitted AI use:

- Category 1: Prohibited
  - No use at all (i.e. in person exams or 'device-free' classes)
- Category 2: Minimal (default level)
  - Use of spell and grammar checkers, and other non-substantive use, is permitted
- Category 3: Selective
  - Substantive use of AI is permitted in limited and clearly defined ways
  - For example: to explore concepts, suggest structure, summarise key ideas
- Category 4: Integral
  - Substantive use of AI is an integral part of the assessment.
  - For example: prompting outputs for critique and improvement using human intelligence

Substantive use of AI is defined as:

- interpret and analyse data (including audio and image files) and texts,
- undertake a literature review or translation,
- identify research gaps,
- formulate research aims,
- develop hypotheses,
- assist with generating ideas or to develop one's own thinking,
- generate code and synthetic data,
- produce documents using other people's work or from transcripts or recordings.

Using AI for tasks such as assisting non-native speakers with translation, transforming transcribed spoken language to written language by users who face barriers to writing, formatting documents, or improving one's own standard of English or a foreign language is ***not substantive***.

Examples of generally ***impermissible*** use of AI:

- substantive original writing by AI, e.g., for an introduction or conclusion section, including verbatim or closely paraphrased use of AI for a literature review;
- improvements to your original writing beyond spelling and grammar, e.g., that bring in domain knowledge or improve a logical argument;

- any use of AI generated code without declaration;
- production of plots by Gen AI, as this may obfuscate the data generating algorithm or the data source, including alteration of data in a diagram;
- asking AI to produce an interpretation of mathematics or data.

Declaration of AI use

Where substantive AI use is permitted for assessed coursework, you must complete a declaration to confirm your awareness of the category and to declare what substantive use of AI has been made.

This declaration must include how the AI tool was interacted with. While it is not generally expected that you give a complete list of individual prompts used, you need to make clear, for instance, whether a piece of code (for example) was constructed through an iterative process with AI by building individual blocks, or fully AI generated.

I declare that I am aware that this assessed coursework is classified for use of AI tools and technologies (as defined in the course handbook) as below, and I confirm that my work is compliant with that category:

> *Category 1: [Yes/No]: I have not used any AI tools or technologies to prepare this assessment.*
>
> *Category 2: [Yes/No]: I have made no substantive use of AI tools and technologies to prepare this assessment.*
>
> *Category 3: [Yes/No]: I acknowledge the substantive use of AI tools and technologies to prepare this assessment. I entered the following prompts [list of prompts]. The output from these prompts was used to [explain use].*
>
> *Category 4: [Yes/No]: I acknowledge the substantive use of AI tools and technologies to prepare this assessment. This is described within an appendix of the submitted work.*

Example Declarations

Category 3

I declare that my use of generative AI for this practical complies with University, Divisional and Departmental policy and guidance.

I used ChatGPT (GPT-5.6 Sol), published by OpenAI, to help identify relevant background literature and search terms relating to the solidification of aluminium alloys, including the effects of cooling rate and mould material on cast microstructure, grain morphology and dendrite arm spacing. I independently checked the existence and relevance of the suggested sources before

using them. I used the information obtained from these verified sources to develop my own predictions of the microstructures expected in the samples cast in the steel and pre-heated clay moulds.

I also used ChatGPT (GPT-5.6 Sol), published by OpenAI, to help write and debug Python code for processing the experimental temperature–time data, calculating cooling rates, and producing plots from these data. I also used ChatGPT to help identify errors in the Python code when it did not run as expected.

I ran the code myself using the experimental data provided for the practical. I reviewed and understood the AI-generated code and checked that the calculations and plots were appropriate and gave reasonable results before using them in my lab notebook.

I did not use generative AI to write or paraphrase the substantive text of my lab notebook, generate or alter experimental data or figures, or generate scientific interpretations or conclusions. The scientific interpretation, predictions and discussion recorded in my lab notebook are my own work and were not generated by AI.

Category 4

I used Generative AI (ChatGPT5, OpenAI) as a writing support tool. Its use was limited to improving grammar, enhancing readability, refining academic language, generating outlines for chapters, suggesting alternative wording, and assisting in the summarization of scientific literature. ChatGPT was also occasionally used to explain scientific concepts to improve my understanding of topics addressed in this research. All outputs produced by these tools were carefully reviewed, verified, and substantially revised by me before being incorporated into the thesis.

The bioinformatics pipeline was implemented in Python using the pandas, NumPy, SciPy, and matplotlib libraries. Generative AI (ChatGPT5, OpenAI) was used to assist in developing and debugging portions of the analysis scripts and to suggest efficient implementations of standard data-processing functions. This has been described in the Methods chapter of my thesis. No AI-generated code was used without independent testing and verification. All methodological decisions, quality-control procedures, statistical analyses, and interpretation of findings were undertaken by me.

I have ensured that all factual statements, citations, and references have been checked against the original sources and that the final content complies with the ethical standards, academic integrity policies, and guidelines of the University of Oxford and Department of Materials.

22. Appendix C: Non-Disclosure Undertaking for Part II Presentations

In return for the opportunity to attend the presentations given by [Student Name], each of the undersigned agrees with [Company Name] and the University of Oxford that he or she will not use for his or her own benefit or disclose to anyone else any information which is disclosed during the presentation unless [Company Name] first gives its consent in writing.

Each of the undersigned understands that information disclosed during these presentations is confidential and that failure to maintain confidentiality of the information may prevent its owner from obtaining patent protection for the information and may lead to substantial financial loss, including loss to individual students and researchers.

Signed and agreed by:

Print Name:	**Signature**

I confirm that every person attending the presentation has signed this agreement:

Signature:

Name:

Position:

23. Appendix D: MS Part II Thesis: Assessment Report and Marking Guidelines

Examiners should write a report of not more than three pages giving their assessment of the thesis (Parts A, B and C), taking into account the marking guidelines overleaf, and including explicit comments explaining their assessment under ***each*** of the headings.

Name of Candidate	
Introduction *Is the topic well introduced.* *What are the aims and objectives of the project?* *Are these clearly identified in the thesis?*	
Literature Review *Is there evidence of a systematic and comprehensive review?* *Is there evidence of clear critical thinking?* *Is there evidence of appraisal and evaluation of most of the papers cited?* *Is there a clear and logical argument? Is this well rooted in evidence? Is it well organised?* *Is there evidence of critical thought?* *Is the work correctly referenced?* *Comment on whether there are spelling or grammatical errors, use of English and overall style*	
Methods *(including data analysis methods)* *Are the methods and analysis of the data used in the project clearly described?* *Did the candidate develop and new methods?*	
Results	

Are the "raw" results attained clearly described? *Are the results analysed adequately and appropriately?* *If appropriate, are errors handled adequately?*	
Discussion *Are the results properly discussed?* *In relation to the previous work in the area?* *In relation to the aims and objectives of the project?*	
Summary and Additional Comments *What do you consider to be the main achievements of the project?* *Are these clearly identified in the thesis?* *What are the key strengths of the thesis?* *Does the thesis show original thinking on the part of the candidate?* *Are there any areas of minor, significant or serious weakness? Does the thesis show awareness of these?* *Comment on the quality of the report (use of English, clarity of structure, extent to which structure and style follows that normally expected of a research thesis in the field of the research topic, coherent story, overall style, quality of diagrams and figures, use of references to previous work, etc.*	

Name of Candidate	
Part A: Literature Review (quality threshold)	
Is the Literature Review satisfactory?	*Y/N*
Part A	***Pass/Fail***
Give a short justification for this judgement	
Part B: Main Thesis (including Literature Review)	
Mark (%)	
Give a short justification for this mark (refer to Mark Guidelines)	
Part C: Mandatory Final Chapter	
Is the account on the **engineering context** of the research project's findings satisfactory?	*Y/N*
Is the account on the **project management** satisfactory?	*Y/N*
Is the account on the h**ealth, safety and risk management** satisfactory?	*Y/N*
Is account on the **ethical and sustainability considerations** satisfactory?	*Y/N*
Is the **Research Poster** included with a satisfactory accounton the feedback for the poster?	*Y/N*
Is evidence provided for passing all the e-learning courses on **"Avoiding Plagiarism", Research Integrity (core)** and **Research Integrity (Intellectual Property)**?	*Y/N*
All the above must be "Y" to pass: Part C	***Pass/Fail***
Comment on any omissions or failed elements	
Assessor:	*Date*

Marking Guidelines

This marking guide should be used in conjunction with the report form, which asks examiners to comment on the quality of the thesis under a total of several headings – these are the criteria which the candidates themselves have been told will be assessed.

- **90-100%:** Thesis rated very highly in all categories of the assessment guidelines. Typically this would be an extremely high quality thesis showing extensive evidence of original thought, results very well analysed and put in context, very well presented, and with no important deficiencies.
- **80-89%:** Thesis demonstrating very strong performance across most areas, with some minor weaknesses in one or two areas. Typically this would be a very high quality thesis showing evidence of original thought, results very well analysed and put in context, very well presented, but with some minor deficiencies.
- **70-79%:** Very strong overall performance, but with moderate weakness in one area or minor weaknesses in several. Typically this would be a high quality thesis showing some evidence of original thought, results well analysed and put in context, well presented. May be deficient in one or two areas accounting for a minority of the whole.
- **60-69%:** Strong overall performance, but with moderate weaknesses in several areas. Typically the work would have been competently carried out and reasonably well presented and analysed. This mark range should be achievable by an average student with reasonable effort.
- **50-59%:** Satisfactory overall performance, but with serious weaknesses in at least one area. Typically the work would have been carried out mostly with competence, but with some flaws (e.g. errors, misinterpretations). Little evidence of original thought.
- **40-49%:** Poor overall performance with serious weaknesses in several areas. No evidence of original thought.
- **30-39%:** Poor overall performance with serious weaknesses in the majority of areas. The thesis of a candidate who has done little work and has presented this work poorly.
- **<30%** Very poor performance with little or no meaningful content.

24. Appendix E: Treatment of Experimental Errors

Introduction

Results obtained by experiments are never perfectly accurate, and therefore they are only meaningful if their accuracy can be estimated. The accuracy is expressed in the form of a quantity called **the error**, which is a measure of the **lack of accuracy** of the measurement. If the result of an experiment is the magnitude of some quantity, then it is just as important to estimate the error in this quantity as it is to calculate the quantity itself.

The following notes contain a summary of the basic points necessary for undergraduate practical work. For more details, reference should be made to textbooks. An excellent introduction to the subject at an elementary level is **Errors of Observation and their Treatment** by J. Topping (Chapman and Hall).

These notes deal with the estimation of **random** errors (those that are equally likely to occur with positive or negative sign). In any experiment, there might also be **systematic** errors (those that have a bias towards occurring with the same sign). Systematic errors cannot be treated by statistical methods, and it is therefore important to eliminate them at the experimental stage, or to calculate their effect afterwards.

The error in a measured quantity

Suppose a measurement is made of a quantity x whose actual value is x_0. This actual value can never be precisely established by experimental measurements. The result of the measurements might be a quantity x_m. Suppose that the error in x_m has been estimated to be ε. This does not mean that the actual value x_0 is definitely between $x = x_m - \varepsilon$ and $x = x_m + \varepsilon$, and cannot be outside that range. Neither does it mean that x_0 is equally likely to be anywhere in the range $x = x_m - \varepsilon$ to $x = x_m + \varepsilon$. What it does mean is that there is a certain probability p (say 50% or 80%) that x_0 is in the range $x = x_m - \varepsilon$ to $x = x_m + \varepsilon$, and that the probability that x_0 is outside that range is $1 - p$. Moreover, the probability that x_0 is between $x = x_m - 2\varepsilon$ and $x = x_m + 2\varepsilon$ is higher than p, and the probability that x_0 is between $x = x_m - 3\varepsilon$ and $x = x_m + 3\varepsilon$ is even higher. The meaning of x_m is that it is the **most probable** value of x_0. In most cases of practical interest, p varies with x according to a Gaussian law

$$p = A\exp\left[-\frac{(x-x_0)^2}{2\sigma^2}\right]. \qquad (1)$$

Eq. (1) means that the probability that the result of a measurement will be between x and $x+dx$ is $p(x)dx$, and is called the Gaussian or normal distribution. We see that

(i) p is a maximum when $x = x_0$,

(ii) σ is a measure of the 'sharpness' of the peak at $x = x_0$. The smaller σ, the more rapidly p decreases with increasing difference between x and x_0. Therefore, σ is related to the error ε in some way. The relationship between ε and σ is discussed below.

(iii) The total probability must be 1, so that A is given by the condition

$$\int_{-\infty}^{\infty} p\,dx = 1. \qquad (2)$$

It can be shown that this condition gives

$$A = \frac{1}{\sigma\sqrt{2\pi}}. \qquad (3)$$

Of course, to establish the exact form of the probability function would need an infinite number of independent measurements of the quantity x. But even with only a finite number of measurements, we can make a reasonable guess. Suppose we have made n measurements whose results are $x_1, x_2, x_3, \ldots, x_n$. The most likely value of the 'actual result' x_0 is the arithmetic mean x_m of the measurements:

$$x_m = \frac{x_1 + x_2 + x_3 + \ldots + x_n}{n}. \qquad (4)$$

We can therefore regard x_m as the 'result of the experiment'. Now consider the quantities

$$\delta_1 = x_1 - x_m,$$

$$\delta_2 = x_2 - x_m,$$

...

...

$$\delta_n = x_n - x_m. \qquad (5)$$

The δ-s are called the **deviations**, and the best guess we can make for σ is

$$\sigma = \left(\frac{\delta_1^2 + \delta_2^2 + \delta_3^2 + \ldots + \delta_n^2}{n-1} \right)^{1/2} . \qquad (6)$$

The quantity σ is called the **standard deviation**. Note that as we make more and more measurements of x (i.e. as $n \to \infty$), σ does not keep decreasing, but tends to a constant value. It is a measure of how much an individual measurement is likely to differ from x_m. The error, however, is a measure of how much x_m is likely to differ from the 'actual value' x_0, and this error must obviously get smaller as n increases. It is usual therefore to define the error by the expression

$$\begin{aligned} \varepsilon &= \frac{\sigma}{\sqrt{n}} \\ &= \left[\frac{\delta_1^2 + \delta_2^2 + \delta_3^2 + \ldots + \delta_n^2}{n(n-1)} \right]^{1/2} \end{aligned} \qquad (7)$$

which is called the **standard error**.

Superposition of errors

In many cases, the quantity of interest is not directly measured, but is calculated from a formula that contains several directly measured quantities. In general, we calculate a quantity y from a formula

$$y = f(x_1, x_2, \ldots, x_n) , \qquad (8)$$

where $x_1, x_2, \ldots, x_n$ are the experimentally measured quantities. Suppose we have determined the errors in $x_1, x_2, \ldots, x_n$ by using the formulae in the previous section, having made repeated measurements of each of the quantities. Let the errors in $x_1, x_2, \ldots, x_n$ be $\delta x_1, \delta x_2, \ldots, \delta x_n$ respectively. Then according to the 'chain rule', the error δy in y should be

$$\delta y = \frac{\partial y}{\partial x_1} \delta x_1 + \frac{\partial y}{\partial x_2} \delta x_2 + \ldots + \frac{\partial y}{\partial x_n} \delta x_n , \qquad (9)$$

provided $\delta x_1, \delta x_2, \ldots, \delta x_n$ are sufficiently small. However, if we use this formula to find δy, we would be taking too pessimistic a view of the accuracy of the result. In effect, we would be assuming that all the errors $\delta x_1, \delta x_2, \ldots, \delta x_n$ occur with the same sign. However, since these errors are random, there is an equal probability for each of them to be positive or negative. In order to take this randomness into account, we consider what happens when we square the expression for δy:

$$(\delta y)^2 = \left(\frac{\partial y}{\partial x_1}\right)^2 (\delta x_1)^2 + \left(\frac{\partial y}{\partial x_2}\right)^2 (\delta x_2)^2 + \ldots + \left(\frac{\partial y}{\partial x_n}\right)^2 (\delta x_n)^2$$
$$+ 2\left(\frac{\partial y}{\partial x_1}\right)\left(\frac{\partial y}{\partial x_2}\right)\delta x_1 \delta x_2 + \ldots + 2\left(\frac{\partial y}{\partial x_{n-1}}\right)\left(\frac{\partial y}{\partial x_n}\right)\delta x_{n-1}\delta x_n \qquad (10)$$

Clearly, the squared terms will always be positive, whether the δx-s are positive or negative. However, each of the cross-product terms can change sign if either of the δx-s it contains changes sign. Thus, there is an equal probability for any of the cross-product terms to be positive or negative. We are justified in assuming that the **average** value of each cross-product term is zero. The correct expression for the error in y is therefore

$$\delta y = \left[\left(\frac{\partial y}{\partial x_1}\right)^2 (\delta x_1)^2 + \left(\frac{\partial y}{\partial x_2}\right)^2 (\delta x_2)^2 + \ldots + \left(\frac{\partial y}{\partial x_n}\right)^2 (\delta x_n)^2\right]^{1/2}. \qquad (11)$$

Here are two simple examples of the use of Eq. (11).

1. An aircraft is flying west, and its windspeed indicator registers a speed of $v_1 \pm \delta v_1$. The weather report gives an easterly wind of speed $v_2 \pm \delta v_2$. Then the speed of the aircraft relative to ground is

$$V = v_1 + v_2. \qquad (12)$$

Since

$$\frac{\partial V}{\partial v_1} = \frac{\partial V}{\partial v_2} = 1, \qquad (13)$$

Eq. (11) gives

$$\delta V = \left[(\delta v_1)^2 + (\delta v_2)^2\right]^{1/2}. \qquad (14)$$

This example shows that the square of the error in a sum is equal to the sum of the squares of the individual errors.

2. The unit cell of an orthorhombic crystal is a rectangular parallelepiped. The lattice parameters (lengths of the sides of the unit cell) have been found to be $a \pm \delta a$, $b \pm \delta b$ and $c \pm \delta c$. Then the volume of the unit cell is

$$V = abc. \qquad (15)$$

Since

$$\frac{\partial V}{\partial a} = bc, \qquad \frac{\partial V}{\partial b} = ac, \qquad \frac{\partial V}{\partial c} = ab, \tag{16}$$

Eq. (11) gives

$$\delta V = \left[b^2c^2(\delta a)^2 + a^2c^2(\delta b)^2 + a^2b^2(\delta c)^2\right]^{1/2}. \tag{17}$$

This result can be simplified by using Eq. (15), giving

$$\frac{\delta V}{V} = \left[\left(\frac{\delta a}{a}\right)^2 + \left(\frac{\delta b}{b}\right)^2 + \left(\frac{\delta c}{c}\right)^2\right]^{1/2}. \tag{18}$$

This example shows two important points.

1. The square of the **fractional** error in a product is equal to the sum of the squares of the individual **fractional** errors.
2. In many cases, as in this example (but not in the previous one), it is simpler to relate fractional errors to each other, rather than absolute errors.

The method of superposition of errors outlined here is a most important one, since it is used in nearly all experiments in which quantitative measurements are made. The quantity one is trying to determine is in many cases not directly measured, but is calculated from other, directly measured quantities.

Straight line fitting

In many cases, measurements are made of a quantity y as a function of x, when a linear relationship

$$y = a + bx \tag{19}$$

is believed to exist between y and x. The object is to determine a and b by finding the straight line that is the 'best fit' to the set of measured points. Suppose that n values of x are chosen ($x_1, x_2,..., x_n$), and the corresponding values of y, i.e. ($y_1, y_2,..., y_n$) are measured. We assume that $x_1, x_2,..., x_n$ are accurately known, but $y_1, y_2,..., y_n$ are subject to error. The problem is to find the line that is as near as possible to the points (x_1, y_1), (x_2, y_2),..., (x_n, y_n). There are several methods for finding a line that satisfies this criterion to some extent. The best line is the one found by the **method of least squares**. In this method, we consider the sum of the squares of distances of the points from any given line, measured in the y-direction, and try to find the values of a and b that make this sum a minimum. The distance of the point (x_1, y_1) from a line such as that given by Eq. (19) is

$$d_1 = |y_1 - a - bx_1|, \tag{20}$$

for the point (x_2, y_2), the distance is

$$d_2 = |y_2 - a - bx_2|, \tag{21}$$

and so on. The sum Q we are trying to minimise is

$$Q = (y_1 - a - bx_1)^2 + (y_2 - a - bx_2)^2 + \ldots + (y_n - a - bx_n)^2. \tag{22}$$

The conditions for Q to be a minimum are

$$\frac{\partial Q}{\partial a} = 0 \quad \text{and} \quad \frac{\partial Q}{\partial b} = 0. \tag{23}$$

From the first condition we get

$$-2(y_1 - a - bx_1) - 2(y_2 - a - bx_2) - \ldots - 2(y_n - a - bx_n) = 0, \tag{24}$$

which can be rewritten

$$(y_1 + y_2 + \ldots + y_n) - an - b(x_1 + x_2 + \ldots + x_n) = 0. \tag{25}$$

Since x_1, x_2,..., x_n and y_1, y_2,..., y_n are known, we can calculate the expressions in the brackets. For simplicity we put

$$S_x = x_1 + x_2 + \ldots + x_n, \tag{26}$$

$$S_y = y_1 + y_2 + \ldots + y_n. \tag{27}$$

Then

$$an + bS_x = S_y. \tag{28}$$

Similarly, from the second condition we have

$$-2x_1(y_1 - a - bx_1) - 2x_2(y_2 - a - bx_2) - \ldots - 2x_n(y_n - a - bx_n) = 0 \tag{29}$$

which gives

$$aS_x + bS_{xx} = S_{xy}, \tag{30}$$

where

$$S_{xx} = x_1^2 + x_2^2 + \ldots + x_n^2, \tag{31}$$

$$S_{xy} = x_1 y_1 + x_2 y_2 + \ldots + x_n y_n. \tag{32}$$

We can obtain *a* and *b* from Eqs (28) and (30):

$$a = \frac{S_{xx} S_y - S_{xy} S_x}{n S_{xx} - S_x^2}, \tag{33}$$

$$b = \frac{n S_{xy} - S_x S_y}{n S_{xx} - S_x^2}. \tag{34}$$

It is also important to estimate the error in *a* and *b*. They are given by

$$\delta a = \left[\frac{Q S_{xx}}{(n-2)(n S_{xx} - S_x^2)} \right]^{1/2}, \tag{35}$$

$$\delta b = \left[\frac{n Q}{(n-2)(n S_{xx} - S_x^2)} \right]^{1/2}. \tag{36}$$

Average value of results with different errors

Suppose a quantity *x* is measured independently *n* times, and the results are $x_1 \pm \delta x_1$, $x_2 \pm \delta x_2$,..., $x_n \pm \delta x_n$. In such cases, the arithmetic mean

$$\langle x \rangle = \frac{1}{n} \sum_{i=1}^{n} x_i \tag{37}$$

does not give the best estimate of the result. As the various measurements are not equally accurate, the result is more likely to be close to the more accurate measurements than the less accurate ones. It is therefore better to estimate the result using a **weighted mean**, in which we give **greater** weight to the values whose errors are **smaller**. The weighted mean is

$$\langle x_w \rangle = \frac{\sum_{i=1}^{n} w_i x_i}{\sum_{i=1}^{n} w_i}, \tag{38}$$

where $w_1, w_2,..., w_n$ are the weights assigned to $x_1, x_2,..., x_n$ respectively. It is usual to assume that the weights are inversely proportional to the errors:

$$w_i = \frac{1}{(\delta x_i)^2} \quad (i = 1, 2, ..., n) \quad . \tag{39}$$

The error in $\langle x_w \rangle$ can be calculated in two different ways as the external error or the internal error.

The **external** error δx_E is related to the scatter of the x_i-values about $\langle x_w \rangle$:

$$(\delta x_E)^2 = \frac{\sum_{i=1}^{n} \frac{x_i - \langle x_w \rangle}{(\delta x_i)^2}}{(n-1)\sum_{i=1}^{n} \frac{1}{(\delta x_i)^2}} \quad . \tag{40}$$

The **internal** error δx_I is related to the individual errors δx_i. It can be derived by applying the superposition formula, Eq. (11), to Eq. (38):

$$(\delta x_I)^2 = \sum_{i=1}^{n} \left(\frac{\partial \langle x_w \rangle}{\partial x_i} \right)^2 (\delta x_i)^2 = \left[\sum_{i=1}^{n} \frac{1}{(\delta x_i)^2} \right]^{-1} \quad . \tag{41}$$

The results are **consistent** if δx_E and δx_I are of the same order of magnitude. (For example, if each measurement is thought to be very accurate but the different measurements differ from each other by large amounts, then something must be wrong. Conversely, it is rather an unlikely coincidence if the measurements are thought to be rather inaccurate but the different values are all nearly equal.)

We can define a consistency parameter, $Z = \delta x_E / \delta x_I$, which should be of the order of 1 for the results to be consistent. From Eqs (40) and (41),

$$Z^2 = \frac{1}{n-1} \sum_{i=1}^{n} \frac{x_i - \langle x_w \rangle}{(\delta x_i)^2} \quad . \tag{42}$$

The best estimate of the error in $\langle x_w \rangle$ is either the larger of δx_E and δx_I, or $\delta x = \left[(\delta x_E)^2 + (\delta x_I)^2 \right]^{1/2}$.

Quoting the results and errors

In most experiments, the error itself is unlikely to be known very accurately (unless the result is based on a very large number of measurements of the same quantity). The error should in most cases only be quoted to one significant figure, except if that first figure is 1, then sometimes two significant figures may be given. The error can now be used to find the number of significant figures in the result, and the result should be rounded off accordingly.

The general rule is that the result and error should be quoted to the ***same number of decimals****. For example, a measured interatomic distance could be given as* $a = (0.427 \pm 0.003)$ *nm, or as* $a = (0.43 \pm 0.02)$ *nm, or as* $a = (0.427 \pm 0.013)$ *nm, or as* $a = (0.427 \pm 0.010)$ *nm, or as* $a = (0.42735 \pm 0.00007)$ *nm, depending on the magnitude of the error. But the following examples are incorrect:* $a = (0.42735 \pm 0.003)$ *nm (the last two decimals of the result are not significant),* $a = (0.43 \pm 0.002)$ *nm (not enough significant figures in the result),* $a = (0.427 \pm 0.01)$ *nm (which should be either* 0.427 ± 0.010 *or* 0.43 ± 0.01*),* $a = (0.427 \pm 0.00385)$ *nm (the error should be rounded off to 0.004), and* $a = (0.42735 \pm 0.00385)$ *nm (the error should be rounded off to 0.004 and the result to 0.427).*

The result and error should always be quoted together, as in the first four examples above. The error may sometimes also be quoted as a percentage, which is a convenient way of comparing the accuracy of results obtained by different methods.

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