

# MatSE 584: Point and Line Defects

**Fall 2020**

## Schedule

TR 12:30–1:50pm in Zoom / Gather.Town (TBD)

## Course content

- Reading: Google Drive shared folder, articles / e-books through [library.illinois.edu](http://library.illinois.edu)
- Additional webnotes: Prof. Helmut Foll's webnotes and frameless webnotes, hosted locally
- Assignment upload: [my.matse.illinois.edu/courses/upload](http://my.matse.illinois.edu/courses/upload), select MSE 584
- Course website: [courses.engr.illinois.edu/mse584](http://courses.engr.illinois.edu/mse584); PDF syllabus
- Recorded lectures: [mediaspace.illinois.edu/channel/MSE+584](http://mediaspace.illinois.edu/channel/MSE+584); subscribe here

## Scope

- Point and line defects in crystalline materials: metals, semiconductors, insulators, and ionic materials.
- Quantification and measurement of defect properties: thermodynamic, structural, electronic, characterization.
- Defect interactions.
- Influence of defect properties on macroscale transport (including diffusion), mechanical, and electronic material properties.

## Objectives

Students will be able to

- (a) critically review the scientific literature;
- (b) apply your knowledge to answer scientific questions related to defects;
- (c) apply thermodynamics, mechanics, and quantum theory to the properties of defects;
- (d) connect defect properties to macroscale material properties;
- (e) explain their reasoning to their colleagues in small and large settings;
- (f) work together with their colleagues in a professional, scientific manner.

## Prerequisites

- Thermodynamics
  - MSE 401/500, CHEM 484, PHYS 427, ME 404 or equivalent
- Electronic Properties of Materials/Condensed Matter Physics
  - MSE 304, PHYS 460/560, or equivalent.
- Introductory Solid Mechanics
  - TAM 251, or equivalent

## Instructor

Dallas R. Trinkle (dtrinkle@illinois.edu; 308 MSEB in the west stairwell).

- Professor in Materials Science and Engineering (joined Univ. Illinois in 2006)
- Computational materials science
  - Crystalline defects (dislocations, point defects, interfaces) from density functional theory
  - Development of new algorithms, computational tools
  - Solid solution softening / strengthening, pipe diffusion, general theory of diffusion

## Teaching approach: Team-based learning

An “active learning” approach where we focus on the course objectives: *applying knowledge to answer scientific questions about defects and critically engaging with the scientific literature*. You will:

- **Prepare** individually for class (reading papers, background literature, working out conceptual questions);
- **Evaluate** your team readiness in class with conceptual questions;
- **Discuss** your questions and deeper points with me and your colleagues;
- **Assess** the literature, develop consensus with your team, and discuss with other teams.

## Team-based learning: Team basics<sup>1</sup>

### First off: Teams are not easy.

As you will find out, group work is not always easy. Team members sometimes cannot prepare for or attend group sessions because of other responsibilities, and conflicts often result from differing skill levels and work ethics. When teams work and communicate well, however, the benefits more than compensate for the difficulties. Chances of success are greatly improved if there is an agreement beforehand on what everyone on team expects from everyone else: *Team expectations*.

In addition, the real world, for the most part, requires people to work together and interface skills, etc. Teamwork is a highly valued skill, but like all skills, requires practice.

## Team-based learning: Team construction and expectations

- Teams are created for you using CATME by balancing your different skills, viewpoints, etc.
- **Team Expectations.** First meeting of teams will require mutual agreement of team expectations: rules and expectations for everyone in their dealings together as a team. These expectations are for your use and benefit; I will not grade them or even comment on them unless you ask. Be thorough without being unrealistic, as this will give the team the best chance of success:

*Realistic:* “We will have read the assigned papers and attempt all prelecture problems before class.” or “We will make sure any who misses meeting for good cause gets caught up on work.” *Unrealistic:* “We will give 110% on every assignment.” Or, “We

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<sup>1</sup>Adapted from Prof. Richard Felder, NCSU.

will read 20 papers in addition to the assigned papers before meeting.” Or, “We will never miss a meeting upon penalty of DEATH.”

### **Team-based learning: Logistics**

The course will cover 8 subtopics in point and line defects. Each week:

- **Monday:** Prelecture questions are due **by midnight**. Done individually, and based on papers and concepts from the papers.
- **Tuesday.** Initial preparation for discussion in class.
  - In-class concept questions that you answer *as a group*.
  - Full class discussion to clear up misconceptions and questions.
  - Team discussions of literature assessment.
- **Wednesday.** Team summary assessment with supporting slides are due **by midnight**.
- **Thursday.** Full class discussion in class.
  - Initial summary of team findings.
  - Full class discussion of papers and team assessments.
  - End of class summary, minute papers
- **End of week:** peer evaluation of team.

### **Prelecture questions**

- Each Monday (starting **Sept. 7**) a few (1-3) prelecture questions will be due at midnight.
- Will be posted on the course website, along with the papers, and suggested background reading.
- Designed to help you check your understanding of concepts in the papers, or used in the papers.
- Will guide opening discussion in Tuesday’s class.
- All assignments are to be submitted electronically as portrait PDF files. Upload information will be available shortly. If you choose to turn in handwritten homeworks, you will need to scan them and create a PDF (either through a dedicated scanner, or using a free app like JOTNOT).

### **Concept quizzes**

- Each Tuesday (starting **Sept. 8**, with practice on Sept. 3) several conceptual questions to check your team understanding.
- Will guide opening discussion in class.
- Multiple choice questions, with partial credit (retry after first attempt).
- Team chooses a weekly “team captain” to lead discussion, arbitrate and manage time. Should rotate weekly.
- Open notes (including prelecture questions).
- Available in-lecture on PrairieLearn.

## Literature assessment<sup>2</sup>

The primary driver for our class is *engaging actively with scientific literature*. This is a primary activity for scientists, and is a skill. It requires

- Reading primary papers, and the papers' bibliography.
- Working through background reading to build understanding.
- Discussing with others to test your understanding.
- Come to a judgment about:
  - What has been done well/poorly;
  - What experiments might be done to test theories;
  - What modeling might be done to make predictions;
  - What are the outstanding questions?
- In class, your team will **summarize and support** your assessment in a few Google slides that will drive Thursday discussion.

## Minute paper

In the final minutes of Thursday's class, we will conclude with a **minute paper** which helps to synthesize your understanding of the lecture, think about your questions, and prime discussion for the next class period. This will be done electronically using the link: [illinois.edu/fb/sec/806118](https://illinois.edu/fb/sec/806118). There, you will have three questions:

1. What are the two (or more) most significant (central, useful, meaningful, surprising) things you have learned during this lecture?
2. What main question(s) remain for you?
3. Is there anything that you did not understand?

Following class, I will compile the questions, organize them, and answer some of them online (on the course website). Your responses also help me to adjust the course as needed.

## One-on-one meetings

We will meet multiple times (at least twice, possibly three) for 20-30 minutes one-on-one during the semester to discuss your understanding of the topics we've discussed in class. There will be one at the culmination of the point defect topics, and one at the culmination of the line defect topics. These meetings can be considered exams, and your grade will depend on the level of understanding you demonstrate in these meetings. After each one-on-one meeting, you will be provided a written report discussing your performance. This is unusual, but it has been successful in many high level courses. Do not hesitate to ask questions.

## Grading

Breakdown to be determined by majority vote in class:

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<sup>2</sup>This is what your advisor and future employers (academic, labs, industry) will expect you to be able to do after you graduate.

- **0–10%** Individual prelecture problems (drop lowest)
- **10–30%** Team in-class concept questions (drop lowest)
- **30–60%** Team assessment and discussion of papers (drop lowest)
- **10%** Minute papers (drop lowest)
- **20%** One-on-one meetings

All participating team members receive the same grade on team assignments; however, this will be adjusted based on peer evaluation of member contributions over the course of the semester.

### **Formal and Informal Accommodations**

I am committed to assisting students requiring special accommodations for circumstances that are registered with the DRES Student Services Department. These formal accommodations should be discussed with me as early as possible in the semester or as soon after DRES approval as possible.

If you are not formally registered with DRES and have anxiety, depression, learning disabilities, or other issues that affect your ability to fully participate and learn in this class, you are encouraged to check-in with me so we can determine together the kind of support you need to thrive in this class. Please set up a meeting with me via email.

### **Inclusion and Diversity**

I value all students regardless of their background, race, religion (creed), ethnicity, gender, gender expression, age, country of origin, disability status, marital status, sexual orientation, or military status, etc., and am committed to providing a climate of excellence and inclusiveness within all aspects of the course. If there are aspects of your culture or identity that you would like to share with me as they relate to your success in this class, I am happy to meet to discuss. Likewise, if you have any concerns in this area of facing any special issues or challenges, you are encouraged to discuss the matter with me (set up a meeting via email) with an assurance of full confidentiality (only exception being mandatory reporting of academic integrity / code violation and sexual harassment).

**Harassment or discrimination of any kind will not be tolerated.**

### **Anti-Racism and Inclusivity Statement**

The intent is to raise student and instructor awareness of the ongoing threat of bias and racism and of the need to take personal responsibility in creating an inclusive learning environment.

The Grainger College of Engineering is committed to the creation of an anti-racist, inclusive community that welcomes diversity along a number of dimensions, including, but not limited to, race, ethnicity and national origins, gender and gender identity, sexuality, disability status, class, age, or religious beliefs. The College recognizes that we are learning together in the midst of the Black Lives Matter movement, that Black, Hispanic, and Indigenous voices and contributions have largely either been excluded from, or not recognized in, science and engineering, and that both overt racism and micro-aggressions threaten the well-being of our students and our university community.

## **Learning Environment**

The effectiveness of this course is dependent upon each of us to create a safe and encouraging learning environment that allows for the open exchange of ideas while also ensuring equitable opportunities and respect for all of us. Everyone is expected to help establish and maintain an environment where students, staff, and faculty can contribute without fear of personal ridicule, or intolerant or offensive language. If you witness or experience racism, discrimination, micro-aggressions, or other offensive behavior, you are encouraged to bring this to the attention of the course director if you feel comfortable. You can also report these behaviors to the Bias Assessment and Response Team (BART) [bart.illinois.edu](http://bart.illinois.edu). Based on your report, BART members will follow up and reach out to students to make sure they have the support they need to be healthy and safe. If the reported behavior also violates university policy, staff in the Office for Student Conflict Resolution may respond as well and will take appropriate action.

## **Religious Observances**

Illinois law requires the University to reasonably accommodate its students' religious beliefs, observances, and practices in regard to admissions, class attendance, and the scheduling of examinations and work requirements. You should examine this syllabus at the beginning of the semester for potential conflicts between course deadlines and any of your religious observances. If a conflict exists, you should notify your instructor of the conflict and follow the procedure at ODOS to request appropriate accommodations. This should be done in the first two weeks of classes.

## **Sexual Misconduct Reporting Obligation**

The University of Illinois is committed to combating sexual misconduct. Faculty and staff members are required to report any instances of sexual misconduct to the University's Title IX Office. In turn, an individual with the Title IX Office will provide information about rights and options, including accommodations, support services, the campus disciplinary process, and law enforcement options.

A list of the designated University employees who, as counselors, confidential advisors, and medical professionals, do not have this reporting responsibility and can maintain confidentiality, can be found here: [wecare.illinois.edu/confidentiality](http://wecare.illinois.edu/confidentiality).

Other information about resources and reporting is available here: [wecare.illinois.edu](http://wecare.illinois.edu).

## **Family Educational Rights and Privacy Act (FERPA)**

Any student who has suppressed their directory information pursuant to Family Educational Rights and Privacy Act (FERPA) should self-identify to the instructor to ensure protection of the privacy of their attendance in this course. See FERPA info for more information on FERPA.

## **Academic Integrity**

You are bound by the University Honor Code in this course. Any violation of the Honor Code will result in disciplinary action.

Students are responsible for producing their own work. Collaborative interaction is encouraged, but each student must do their own individual prelecture work, and contribute their own work to the group. **Plagiarism will not be tolerated, and verified incidents will result in all parties receiving a zero and formal academic sanctions.** Students are responsible for familiarizing themselves with the definition of and penalties for plagiarism in Section I-401 of the UIUC Student Code. Note that plagiarism includes “copying another student’s paper or working with another person when both submit similar papers without authorization to satisfy an individual assignment.”

### **Changes to syllabus**

May occur as deemed necessary by the professor; they will be announced and the updated syllabus posted on the course website.

### **Accessing files**

The Univ. Illinois library has access to a huge variety of electronic resources; this plus additional online resources will be our references. Many can be accessed from the library’s website, or via the campus VPN. Alternatively, you can take advantage of the library proxy. This is done by appending `proxy2.library.illinois.edu` to the web address; when reloaded, you will be asked for Univ. Illinois authentication, and then will be able to access the resource as if you were on campus. In general, this authentication is required only once per session. So, the website

`http://journals.aps.org/prl/abstract/10.1103/PhysRevLett.113.025504`  
would become

`http://journals.aps.org.proxy2.library.illinois.edu/prl/abstract/10.1103/Phy`

Alternatively, install the Proxy Bookmarklet which makes it extremely easy to use the proxy. I highly recommend this method.

### **Google Drive / Google Apps @ Illinois**

In addition, we will use Google Drive to share files. You should have an “infinite” amount of free storage on Google Drive, and you can set up Google Drive so that files are automatically synced to your computer. You may want to upload PDFs from the pre-lecture reading there; if you place these PDFs in the shared folder, please name them `FirstAuthorLastName-Journal-Year.pdf` so that they remain organized. The team slides will be made available using Google Apps.

This means that you will need to either:

- Use your personal Google account to access Google Apps. Be aware that this will count towards your Google storage limitations.
- Activate and use your campus Google account. See the FAQ and more information (including how to create your account).

Your campus Google account will be separate from an existing Google account, should you have one.

## Lecture topics and reading calendar

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Tuesday	Thursday	notes
8/25	8/27	intro to MSE584 / concept review
9/1	9/3	concept review / practice concept quiz
9/8	9/10	<b>Topic 1:</b> how many PDs are in a material?, PDF
9/15	9/17	<b>Topic 2:</b> how do PDs change electronic properties?, PDF
9/22	9/24	<b>Topic 3:</b> how do PDs react in an open system?, PDF
9/29	10/1	<b>Topic 4:</b> how do PDs diffuse?, PDF
10/6	10/8	<i>no class</i> (One-on-one meetings)
10/13	10/15	concept review
10/20	10/22	concept review
10/27	10/29	<b>Topic 5:</b> what is the core structure of a $\perp$ ?, PDF
11/3	11/5	<b>Topic 6:</b> how do PDs and $\perp$ s interact?, PDF
11/10	11/12	<b>Topic 7:</b> how do $\perp$ s move in a material?, PDF
11/17	11/19	<b>Topic 8:</b> how do $\perp$ s interact?, PDF
<del>11/24</del>	<del>11/26</del>	<i>Thanksgiving break</i>
12/1	12/3	<i>no class</i> (One-on-one meetings)
12/8	<del>12/10</del>	Review discussion day (Tuesday)

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## Background reading

You may want to review the following references to refresh yourself on particular prerequisite topics:

- Ibach, H. and Lueth, H. *Solid-State Physics*. (Springer Berlin Heidelberg: Berlin, Heidelberg, 2010). doi:10.1007/978-3-540-93804-0. There are multiple useful chapters here:
  - Chapters 2 and 3 cover lattices and crystals
  - Chapters 4 and 5 cover phonons
  - Chapters 6 and 7 cover electrons and band structure
- Thermodynamics: chemical potential and mass action law available in Prof. Helmut Foll's webnotes
  - The chemical potential
  - Mass action law
  - Pitfalls and Extensions of the Mass Action Law
  - Chemical examples for mass action law applications
  - Alternative derivations of the mass action law