MATERIALS SCIENCE & ENGINEERING

27-731

SPECIAL TOPICS: Texture, Microstructure & Anisotropy

Spring Semester 2022

Course Description:

The purpose of Texture, Microstructure, & Anisotropy is to acquaint the student with a selected set of characterization tools relevant to the quantification of microstructure (including crystallographic orientation, i.e. texture) and anisotropic properties. The motivation for the course is problem solving in the areas of property measurement (e.g. grain boundary energy), prediction of microstructural evolution (e.g., in grain growth and recrystallization), and prediction of properties based on measured microstructure (e.g., anisotropy of work hardening and ductility). In this 6-unit mini version of the course, the specific objectives are to develop skills and understanding in the following areas:

(1) The mathematical basis for crystallographic orientation distributions (aka ODFs), with explanations of the many representations of rotations/orientations
(2) Crystallographic preferred orientation (texture) and its representation by pole figures, inverse pole figures and orientation distributions, with a particular emphasis on the effects of symmetry in representations
(3) Methods of measuring texture such as X-ray (diffraction) Pole Figures and Electron Back Scatter Diffraction (EBSD) with reference to orientation mapping
(4) The effect of texture on elastic and plastic anisotropy in polycrystals; the uniform stress model (Sachs), the Taylor-Bishop Hill model, the Eshelby analysis

The goal of the course is for students to use and understand quantitative tools for texture data acquisition analysis (e.g., orientation distribution determination from pole figure data, and automated electron back-scatter diffraction/EBSD/OIM), the effect of crystal and sample symmetry on distributions and their representation, and the prediction of anisotropy (e.g., calculation of yield surfaces for plastic deformation). Since the datasets are often large, such as from EBSD scans, computer programs are essential.

The relevance of the course is that essentially all materials are anisotropic, i.e., their properties are directional, which means that methods for quantifying this variation are useful across much of engineering and science.

Class Schedule:

This is a 6-unit class for graduates and meets twice weekly, from 8:00 PM – 9:50 PM on Mondays and Wednesdays in Doherty Hall 1112. The lectures will be given by Prof. A.D. (Tony) Rollett, along with other potential guest lecturers. Previous versions of the lecture materials are available as a Powerpoint files at the following website: pajarito.materials.cmu.edu/rollett/27750/27750.html. See the end of this document for a schedule, with adjustments for absence of the instructor or the insertion of a guest lecturer. A weekly time slot for a recitation regarding the lecture material will be chosen by the instructor at a later date.

Recommended Pre-requisites:
27-201 (Structure of Materials), 27-202 (Defects in Materials), 27-301(Microstructure and Properties I). The course requires students to be comfortable with (or develop skills in) basic aspects of crystallography, crystal plasticity and the mathematics associated with geometry, vectors, tensors and rotations.

Textbooks:

U. Fred Kocks, Carlos Tomé, and H.-Rudy Wenk, Eds. (1998). *Texture and Anisotropy*, Cambridge University Press, Cambridge, UK, ISBN 0-521-79420-X. This is now available as a paperback.

Satyam Suwas and Ranjit K. Ray (2014), *Crystallographic texture of materials*, Springer

Olaf Engler, Stefan Zaefferer, and Valerie Randle *Texture Analysis: Macrotexture, Microtexture & Orientation Mapping* (2023, expected), 3rd Edition, CRC Press, ISBN 978-1032189420. This is very useful because of its coverage of electron back scatter diffraction (EBSD).

J.F. Nye, *Physical Properties of Crystals*, Clarendon Press (1957) (reprinted more recently).

Robert E. Newnham, *Properties of Materials: Anisotropy, Symmetry, Structure* (2005), Oxford Univ. Press, ISBN 9780198520764.

Adam Morawiec, *Orientations and Rotations* (2003), Springer, ISBN 3-540-40734-0. This provides considerable mathematical detail on texture.

A.I. Borisenko & I.E. Tarapov, *Vector & Tensor Analysis, with Applications* (1968), Dover; translated by R. Silverman. This provides a more complete mathematical basis for axis transformations.

B.D. Cullity, *Elements of X-ray Diffraction* (1978).

H.-J. Bunge, *Texture Analysis in Materials Science* (1982). Excellent reference work but challenging to learn from.

Topics Covered:
1. Microstructural Characterization Techniques with Orientation
   - Average texture by X-ray diffraction pole figures
   - Electron diffraction in the SEM (EBSD, OIM); analysis of EBSD data acquisition
   - Serial sectioning for 3D mapping
   - 3D Orientation mapping with synchrotron radiation
2. Analysis of Characterization data
   - Basics of Image Analysis
   - Stereology (selected examples)
   - Interface networks, dihedral angles
   - Serial sectioning (e.g. alignment of parallel sections)
   - Percolation Analysis (e.g. for electrical conductivity)
   - Shape and Cluster Analysis (e.g. of particles)
   - Reconstruction techniques 3D for digital microstructures
   - Boundary tangent analysis to obtain 5-parameter distributions
3. Representation of Texture
   - Mathematical Representations of Orientation
   - Crystal, Sample Symmetry

- Graphical Representations of Texture
- Orientation Distributions
- Interface texture – misorientation (3-parameter) vs. boundary normals (5-parameter)
- Lattice Curvatures (geometrically necessary dislocations)

4. Analysis of Orientation Distributions (OD)
   - OD calculation from projections (pole figures)
   - Analysis of OD data for volume fractions
5. Structure-Property Relationships
   - Anisotropy of second rank tensor properties, e.g. conductivity
   - Anisotropy of fourth rank tensor properties, e.g. linear elasticity
   - Anisotropy of non-linear tensor properties, e.g. plasticity
   - Taylor-Bishop-Hill theory for crystal plasticity
   - Yield surfaces
   - Eshelby analysis (inclusions, effective medium theory)
6. Microstructural Evolution
   - Texture development via plastic deformation
   - Simulation of anisotropy with the Visco-plastic Self-Consistent (VPSC) code

Assessment:
Student performance will be assessed through a mix of quizzes, homeworks, tests, a term paper or independent study and a final exam.

Computational Alternate to Term Paper:
As an alternative to the term paper, you may instead perform a computational exercise. Unless you have access to some other code, the obvious choice is VPSC. If you have your own texture data, e.g., from EBSD, you could compute the anisotropy of your measured material and write your report on how you used VPSC, what you understand about the way that it works and how you interpret the results that you obtained. You will need to find some comparable work in the literature, preferably on the same material, that you can cite and include in your Discussion section.

Term Paper:
The length of your term paper should be between 11 and 15 pages, *not* including the reference list. It must include a Summary or Abstract, an Introduction, Conclusions, and a list of References cited. The main part of the report may follow the pattern of Methods-Results-Discussion, or, for a review, it may be divided into whatever sections make sense for the chosen topic. The due date for the Term Paper is given in the schedule (below). This will be configured as a "Turnitin" assignment (to check for plagiarism). No presentation is required. The criteria for grading the term paper include the following: quality of the technical & scientific content, choice of topic (e.g., how relevant to texture and anisotropy), use of advanced analytical methods (e.g., orientation analysis, correlation analysis), quality of the writing, referencing of relevant literature, and organization of the paper (logical flow etc.).

Titles from previous years:
Anisotropy of AA 5754
Anisotropic mechanical behavior in AlSi10Mg parts produced by selective laser melting
Understanding Stress Hotspots in Materials
Texture Evolution in Additively Manufactured Ti
Review of Monte Carlo Simulation of Grain Growth
Dihedral Angle Distribution in an Austenitic and Ferritic Steel
Modeling Work Hardening in AA 5754

Analysis of Orientation Gradients between 3D Printed SS316 and Annealed 2% Strained Copper at Varying Thresholds
Orientation Dependence in the Growth of Short Cracks in Single Crystals, Bicrystals and Textured Polycrystals
Calculation of Stress Zone and Plastic Zone with a Fast Fourier Transform Model
Potts Model Simulation of 2D Anisotropic Grain Growth with Pinning Particles
A study of the relationship between misfit, precipitate-size, elastic anisotropy and precipitate morphology in Ni-based superalloys

Course Assistants: The course assistant for grading of homeworks etc. is TBD.

Prepared by: ADR. ADR can be reached in his office, DH A309, by phone, 412-268-3177, or by email, rollett@andrew.cmu.edu. ADR, an open-door policy applies but feel free to email in order to obtain a definite time to meet.

Class Schedule Spring 2022

Date (Day)	Topic	Lecturer	Assignment (Due date)	Topic/ Comment
19th Jan. (Weds.)	Introduction: anisotropy and symmetry	ADR		Introduction; Components_EulerAngles
24th Jan. (Mon.)	Euler Angles and Texture Components			
26th Jan. (Weds.)	Effect of symmetry on Orientation Distribution	ADR	HW 1	OD_symmetry
31st Jan. (Mon.)	Orientation Distributions	ADR		Orient_Dist
2nd Feb. (Weds.)	X-ray Pole figures	ADR	HW 2	Xray_PFs
7th Feb. (Mon.)	Volume fractions of texture components	ADR		Volume_Fractions
9th Feb. (Weds.)	Orientation analysis using EBSD data	ADR	HW 3	EBSD-acquisition, EBSD-analysis
Weekend of 12/13 Feb	Take-home test	ADR		
14th Feb. (Mon.)	Anisotropic Elasticity	ADR		Elastic_Aniso
16th Feb. (Weds.)	Plastic deformation of single crystals	ADR	HW 4	Single_Xtal_Aniso1
21st Feb. (Mon.)	Plastic deformation of polycrystals	ADR		Polycrystal_plasticity-Aniso3
23rd Feb. (Weds.)	Eshelby analysis (Elastic inclusion)	ADR		Polycrystal_plasticity-Aniso4-SelfConsistent-Model
28th Feb. (Mon.)	Self-consistent modeling of heterogeneous plasticity	ADR		1st half lecture, 2nd half demo VPSC
2nd Mar. (Weds.)	VPSC-based modeling of heterogeneous plasticity	ADR	HW 5: Written HW + Bishop-Hill code	Lecture on use of VPSC code
28th Feb. (Mon.)	VPSC -based crystal plasticity modeling, pt. 2	ADR		
1st Mar. (Weds.)	Term paper due	ADR		Literature review, or, computational exercise (e.g., use of MASSIF)
Date TBD	Final Exam Review	ADR		

Date TBD	Final Exam	ADR		

Test, Exams, Grading Policy

Homeworks: approx. **five (5) planned** ~100 points each

Exams: one test near the end of the course - see weighting below

Grading Policy	A > 90%
	B > 80%
	C > 65%
	D > 55%

The instructor will request an Oral exam in borderline cases.

Weighting:	Homeworks	45 %
	Mid-term test (take-home), Feb. 12/13th	20 %
	Term paper or Independent Study	30 %
	Participation	5%

General Policies

Expectations
The following guidelines will create a comfortable and productive learning environment throughout the semester.

You can expect me:

- To start and end class on time.
- To reply to e-mails within 24 hours on weekdays and 48 hours on weekends.
- To assign homework that adequately covers the material and meets the learning objectives of the course while adhering to the time expectations for a 6-unit course.
- To give exams that reflect accurately the material covered in class and assigned in homework.
- To be reasonable in asking question of students in class.

I expect you as students:

- To seek help when appropriate.
- To be attentive and engaged in class, including answering questions from the instructor.
- To spend an adequate amount of time on the homework each week, making an effort to solve and understand each problem.
- To come to class on time.
- To refrain from using laptops, cell phones and other electronic devices during class.
- To engage with both the abstract and computational sides of the material.

Some of these expectations are based on research on learning that shows that unexpected noises and movement automatically divert and capture people's attention, which means you are affecting everyone's learning experience if your cell phone, pager, laptop, etc. makes noise or is visually distracting during class.

Accommodations for Students with Disabilities
If you have a disability and are registered with the Office of Disability Resources, I encourage you to use their online system to notify me of your accommodations and discuss your needs with me as early in the semester as possible. I will work with you to ensure that accommodations are provided as appropriate. If you suspect that you may have a disability and would benefit from accommodations but are not yet registered with the Office of Disability Resources, I encourage you to contact them at access@andrew.cmu.edu.

Your State of Mind
Take care of yourself. Do your best to maintain a healthy lifestyle this semester by eating well, exercising, avoiding drugs and alcohol, getting enough sleep and taking some time to relax. This will help you achieve your goals and cope with stress.

If you or anyone you know experiences any academic stress, difficult life events, or feelings like anxiety or depression, we strongly encourage you to seek support. Counseling and Psychological Services (CaPS) is here to help: call 412-268-2922 and visit http://www.cmu.edu/counseling/. Consider reaching out to a friend, faculty or family member you trust for help getting connected to the support that can help.
If you or someone you know is feeling suicidal or in danger of self-harm, call someone immediately, day or night:
CaPS: 412-268-2922

Re:solve Crisis Network: 888-796-8226
If the situation is life threatening, call the police
On campus: CMU Police: 412-268-2323
Off campus: 911

Your One and Only Warning: Zero Tolerance of Cheating & Plagiarism

Plagiarism means using words, ideas, or arguments from another person or source without citation. Cite all sources consulted to any extent (including material from the internet), whether or not assigned and whether or not quoted directly. For quotations, four or more words used in sequence must be set off in quotation marks, with the source identified.

Any form of cheating will immediately earn you a failing grade for *the entire course*. By remaining enrolled, you consent to this policy. I will seek the harshest penalties under CMU's policy on "Standards for Academic and Creative Life" and "Ch Plagiarism" in the Student Guidebook (aka The Word, online at http://synergy.as.cmu.edu.edu/Student_Affairs/handbook/).

Read it now.
Here are some examples of acceptable collaboration:

- Clarifying ambiguities or vague points in class handouts, textbooks, or lectures.
- Discussing or explaining the general class material.
- Discussing the assignments to better understand them.
- Getting help from anyone concerning issues which are clearly more general than the specific assignment.

Now for the dark side. As a general rule, if you do not understand what you are handing in, you are probably cheating. If you have given somebody the answer, you are probably cheating. In order to help you draw the line, here are some examples of clear cases of cheating:

Copying (assignment) documents from another person or source, including retyping their files, and copying anything without explicit citation from previously published works (except the textbook), etc.

- Allowing someone else to copy your written assignment, either in draft or final form.
- Getting help from someone whom you do not acknowledge on your solution.
- Copying from another student during an exam, quiz, or midterm. This includes receiving exam-related information from a student who has already taken the exam.
- Writing, using, or submitting a program that attempts to alter or erase grading information or otherwise compromise security.
- Inappropriately obtaining course information from instructors and TAs.
- Looking at someone else's files containing draft solutions, even if the file permissions are incorrectly set to allow it.
- Receiving help from students who have taken the course in previous years.
- Lying to course staff.
- Copying on quizzes or exams.
- Reviewing any course materials from previous years.
- Reading the current solution (handed out) if you will be handing in the current assignment late.

Attendance and Participation Policy

Class Presence and Participation. Class presence and participation points are given to encourage your active class participation and discussion. You will be rewarded with a perfect score as long as you frequently come to class and actively contribute to the class discussion during recitations and lectures.

Presence: Although it is not required, most students send their professor a brief e-mail to explain their absence in advance. Students who repeatedly arrive late to recitation will have their Class Participation grade lowered. Please sign the attendance sheet when you come to the class. Any false signatures will result in zero participation grades for all parties involved. Participation: The instructor expects students to follow the development of ideas and derivations. Any student may be asked at any time to complete a statement, answer a question, come up the to board to continue a derivation or explain a concept that has been covered in the class. Active participation by students in the learning process is well-known to enhance and reinforce learning.

How to Use Your Study Time More Efficiently

1. Read your lecture notes over within 24 hours of lecture (or at least once before the next lecture). Highlight or make marginal notes for important words or concepts. This will help fix ideas and will help you to actively learn the material. This review takes about 20-30 minutes and really yields a large return. Re-do examples yourself, step by step, with pencil and paper. Examples often look easy when explained in class, but often turn out to be much harder when you do them yourself. Write down questions about things you do not understand. Bring these questions to lecture, lab, and to office hours and ask them.

2. Lecture notes are provided for each class. Read them - if not before the class for which they are assigned then certainly after that class and before the next. Also, as you read, highlight, re-work examples yourself, and write down questions, as suggested above.

3. **DO HOMEWORK PROBLEMS**. Actively doing problems is the only way to learn the material. Exam questions will be similar to homework problems. Start early. Do not leave assignments until the night before they are due. Try doing the problems yourself before discussing them with other people.

4. Use office visits productively. Ask thoughtful questions about things that you do not understand. In other words, if you do (1)-(3) above, it will be much easier to isolate what is giving you trouble.

5. Review solutions to assignments and exams. Just because you do not lose points on a homework question does not necessarily mean you fully understand the question and answer. Also, the solutions should serve as a model for how to write, using proper sentences and paragraphs, discussions and interpretations of data analyses.

6. We will make every effort to help you learn the course material, but you must also make an effort to utilize the resources that are made available to help you. Please come talk to us – not only when you are having trouble but also when things are going well.

Students' Recording of Classes

Classroom activities may be recorded by a student for the personal, educational use of that student or for all students presently enrolled in the class only, and may not be further copied, distributed, published or otherwise used for any other purpose without the express written consent of the course instructor. All students are advised that classroom activities may be taped by students for this purpose.

BOOKS

Altmann, S. L. (1986). *Rotations, Quaternions and Double Groups*. Oxford, Clarendon Press.

Cullity, B. D. (1978). *Elements of X-ray Diffraction*, Addison-Wesley, Reading, Mass.

Bunge, H. (1982). *Texture Analysis in Materials Science*. London, Butterworths. (located in the reference section)

Gottstein, G. and L. S. Shvindlerman (1999). *Grain Boundary Migration in Metals*, CRC Press, Boca Raton, FL, ISBN 0-8493-8222-X. Note: 2nd edition is available.

Howe, J.M. (2000). *Interfaces in Materials*, Wiley Interscience, New York, NY, ISBN 0- 471-13830-4.

Khan, A.S. and S. Huang, *Continuum Theory of Plasticity*. 1995, New York: WileyInterscience; ISBN 0471310433.

*** Kocks, U. F., C. Tomé, and H.-R. Wenk, Eds. (1998). *Texture and Anisotropy*, Cambridge University Press, Cambridge, UK.**

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Reid, C. N. (1973). *Deformation Geometry for Materials Scientists*. Oxford, UK, Pergamon.

Sutton, A. P. and R. W. Balluffi (1995). *Interfaces in Crystalline Materials*. Clarendon Press, Oxford, UK.

Torquato, S., *Random Heterogeneous Materials: Microstructure and Macroscopic Properties*. 2001, New York: Springer Verlag, ISBN: 0387951679.

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