*MATERIALS SCIENCE & ENGINEERING*

# 27-750
# Texture, Microstructure & Anisotropy

formerly known as
Advanced Characterization and Microstructural Analysis

*Fall Semester 2009*
*Last revised: 13th Dec. 2009*

**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). The specific objectives are to develop skills and understanding in the following areas:
(1) The mathematical basis for crystallographic orientation and grain boundary distributions, along with the anisotropy associated with elastic and plastic properties;
(2) Crystallographic preferred orientation (texture) and its representation by pole figures, inverse pole figures and orientation distributions;
(3) Texture of interfaces and its representation by misorientation distributions and Grain Boundary Character Distributions (or Interface Character Distributions in the case of poly-phase materials);
(4) Methods of measuring texture such as X-ray diffraction and Electron Back Scatter Diffraction (EBSD) with reference to orientation mapping (OIM);
(5) The effect of texture on elastic and plastic anisotropy in polycrystals;
(6) Image analysis and extraction of 3D information using stereology.

Emphasis is placed on the use and understanding of 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. Note that the current title of this course is “Texture, Microstructure & Anisotropy” because of the emphasis on these aspects of anisotropic microstructure-property relationships.

4 hours lecture per week (12 units in the CMU system).

**Class Schedule.** This is a 12 unit class for graduates Fall, 2009, and meets twice a week for a total of 4 hours, 11:30-1:20, Tuesday and Thursday. The lectures will be given by Prof. Anthony Rollett (CMU); Prof. Peter Kalu (FSU and FAMU) is not available this year. Since a videolink is used to connect classrooms at CMU, FAMU/FSU, Drexel, Lehigh, EPMA and other participating institutions, each lecture will be made available as a Powerpoint file at the following website shortly before the class begins: neon.materials.cmu.edu/rollett/27750/27750.html.

**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.

**Textbook:** Kocks, U. F., C. Tomé, and H.-R. Wenk, Eds. (1998). *Texture and Anisotropy*, Cambridge University Press, Cambridge, UK, ISBN 0-521-79420-X. This is now available as a paperback. An additional book that is very useful because of its coverage of electron back scatter diffraction is *Texture Analysis: Macrotexture, Microtexture & Orientation Mapping*, by Val Randle and Olaf Engler (2000), Gordon & Breach, Amsterdam, Holland, ISBN 90-5699-224-4. A book with considerable mathematical detail on texture is Adam Morawiec's *Orientations and Rotations* (2003), Springer, ISBN 3-540-40734-0.

**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. Interfaces
    - Characteristics and properties of grain boundaries √ (energy, mainly)

- Coincident Lattice Site theory √
- Calculation of Misorientation Distributions (MDs) from EBSD data √
- Analysis of MD data √
- Texture derived MD (TMD); normalization of measured MDs by TMDs √

6. 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 √.
7. Microstructural Evolution
   - Grain growth
   - Recrystallization
   - Texture development via plastic deformation √

**Course Objectives and Relationship to Program Objectives (Target Skills)**
The motivation for this course is that many practical problems in materials science (and solid state physics) have to do with polycrystals and the fact that they behave differently depending on what direction is tested; this is known as *anisotropy*. Whether it is the mechanical strength, the magnetizability or the electrical properties, the methods used to quantify the anisotropy are the same. Although the field of texture & anisotropy has grown up as a separate subdiscipline, it is actually part of the broader topic of microstructure-property relationships. There is also a close relationship to materials processing because the texture of a material is dependent on its history.

The formal goal of the course therefore is to instruct students to advanced concepts of microstructural characterization. These include stereology, topology, and texture and methods of measuring microstructure including crystallographic orientation. In addition, the impact of microstructure on the directionality of materials behavior is discussed with respect to mechanical behavior. For MSE undergraduates (at CMU) taking the course, it has the most impact on Outcome A, development of a knowledge of mathematics, physics, chemistry, materials and statistics to identify, formulate and solve the problems encountered in the production or application of a material. The discussion of anisotropy addresses Outcome G, development of an ability to employ the techniques, skills and tools of modern engineering practice in materials engineering. Through classroom interaction and presentation of projects and/or homeworks, communication skills are developed (Outcome C). The examples of application of quantitative microstructural techniques addresses both the design of systems (Outcome E) and the application of core concepts in materials science (Outcome B).

**Contribution to meeting the professional component (undergraduates).** 27-550 is primarily intended to introduce students to the concepts required to quantify microstructure, including texture (crystallographic preferred orientation) and to connect microstructure to the elastic and plastic behavior of engineering materials. Practical examples of the impact of anisotropy based on microstructure are introduced to motivate the discussion, e.g. earring in beverage cans, directionality in the electrical properties of superconductors.

**Course Assistants.** The course assistant for grading of homeworks etc. is Ms. Lin Hu, linhu@andrew.cmu.edu.

**Prepared by:** Prof. Anthony D. Rollett, August 2009. The instructor can be reached in his office, Roberts 148, by phone, 8-3177, or by email, rollett@andrew.cmu.edu.

# Desired Outcomes for Students* in the MSE Program

| **MSE Program Outcomes** | **27-750** |
|---|---|
| A. The ability to apply a knowledge of mathematics, physics, chemistry, materials and statistics to identify, formulate and solve the problems encountered in the production or application of a material. | *H* |
| B. An ability to apply core concepts in materials science (structure, properties, processing and performance) to materials engineering problems. | *I* |
| C. An ability to communicate effectively. | *I* |
| D. An ability to design and conduct experiments with an emphasis on relating properties and processing to structure. | *L* |
| E. An ability to relate materials selection and performance to design of engineered systems and components. | *I* |
| F. An ability to function responsibly and ethically in a professional, multidisciplinary environment and as an individual or as a member of a team. | *I* |
| G. An ability to employ the techniques, skills and tools of modern engineering practice in materials engineering. | *H* |
| H. Recognition of the need for lifelong scholarship. | *I* |
| I. A knowledge of contemporary issues. | *L* |
| J. The broad education necessary to understand the impact of engineering solutions in a global and societal context | *L* |

*H indicates that the course is expected to strongly support the outcome; I indicates intermediate support; L indicates that the course is expected to have a lesser impact on the outcome.*

* This table is directed to undergraduate students but may also be of interest to graduate students.

# Lecture Schedule

Lecturers: A.D. (Tony) Rollett *[ADR]* at CMU

Timetable of Lectures

Lectures take place on Tuesdays and Thursdays and run from 11:30am to 1:20.

CMU Semester starts Aug. 24th. First class on Aug. 25th.

Week 1

| | | |
|---|---|---|
| Aug. 25th | *[ADR]* | L1 - Introduction to Microstructure, including texture (crystallographic orientation): examples of engineering problems involving texture; What is a Texture Component? Miller indices and Euler angles; orientation as rotation; stereographic projections; Pole Figures; |
| Aug. 27th | *[ADR]* | L2 Texture Components and Euler Angles: part 1. Show how to convert from a description of a crystal orientation based on Miller indices to matrices to Euler angles. Give examples of standard named components and their associated Euler angles. The overall aim is to be able to describe a texture component by a single point (in some set of coordinates such as Euler angles) instead of needing to draw the crystal embedded in a reference frame. Part 1 provides a mainly qualitative, pictorial approach to illustrate the physical meaning of Euler angles and "orientations".- L3 - Texture Components and Euler Angles: part 2 provides more mathematical detail, e.g. mathematics of conversion from Miller indices to a rotation matrix to Euler angles. |

Homework 1: exercises on locating components, conversion from one representation to another.

*Week 2*

| | | |
|---|---|---|
| Sep. 1st | *[SRW]* | Different representations of rotations and orientations, especially matrices, axis-angle pairs, Rodrigues vectors, quaternions, axis transformations, active (vector) rotations, relationships between them. Misorientations; Rodrigues vectors, space |
| Sep. 3rd | *[Jason Wolf]* | X-ray diffraction, pole figures. |

Homework 2:

*Week 3*

| | | |
|---|---|---|
| Sep. 8th | *[ADR]* | L4 – Pole Figures, Stereographic Projection, Equal Area Projection. |
| Sep. 10th | *[ADR]* | L5 - Tour of popLA. Example of analysis of a set of pole figure data measured for a sample of low carbon steel to obtain an orientation distribution (function), using the popLA software package. This will be a hands-on demonstration with opportunities for students to demonstrate their own use of the package. The accompanying homework will require students to use the package to generate a "standard set" of plots and other analyses. Students will be required to refine the defocusing and background corrections in order to optimize the solution. |

Homework: application of popLA to a data set provided by the instructors; practice with popLA to analyze a data set with iteration on the defocusing correction; maps of components in various spaces; analysis of students' samples' pole figure data with popLA; conversions of sets of discrete data to intensities in orientation space; calculation of locations in pole figures from texture component locations in orientation space.

*Week 4*

| | | |
|---|---|---|
| Sep. 15th | *[ADR]* | Tour of popLA, contd.; Electromigration resistance in Interconnects. |

Sep. 17th *[ADR]* (L7) Concept of Orientation Distribution; Orientation space; OD maps; Euler angles; discrete vs. functional ODs; Texture Components (review).

*Week 5*

Sep. 22nd *[ADR]* (L8) Symmetry; Sample vs. Crystal Symmetry; Effect of symmetry on Representation of Texture; square, polar plots; invariant measure; examples of fiber textures in thin film, Cu, HTSC.

Sep. 24th *[ADR]* Volume fractions (L9); Misorientation calculation

*Week 6*

Sep. 29th *[ADR]* Elastic anisotropy (L10).

Oct. 1st *[ADR]* Single Crystal Plastic Anisotropy: Schmid's Law; Tour of LApp code and how to run the code.

Week 7

Oct. 6th *[ADR]* Rate Sensitive Yield. Introduction to the Taylor model;

Oct. 8th *[ADR]* The Bishop-Hill model.

Week 8

Oct. 13th *[ADR]* Yield Surfaces.

Oct. 15th *[ADR]* In-class test

Homework:

Week 9

Oct. 20th *[ADR]* Application of Taylor Model for anisotropy: Plastic Anisotropy: r-value, polycrystal yield surfaces.

Oct. 22nd *[ADR away]* (possible guest lecture; also, make up lecture time via tutorials)

Homework:

Week 10 *MS&T Week in Pittsburgh*

Oct. 27th *[ADR]* Key aspects of EBSD data acquisition. Short presentations (10 mins.) on any topic relevant to 27-750 by students; topics related to research project(s) are preferred. For 27-Oct-09, Li, Neyer, Anglin, Teevan

Oct. 29th *[ADR]* Analysis of EBSD data; Short presentations (10 mins.) on any topic relevant to 27-750 by students; topics related to research project(s) are preferred. For 29-Oct-09, Pathak, Zhu, Humphrey, Budruk

Week 11

Nov. 3rd *[ADR]* Grain Boundaries, Misorientation Distributions, Fundamental Zone for MD, plotting of MD; lecture delivered remotely (instructor in OR).

Nov. 5th *[ADR]* What is a Coincident Site Lattice? CSL boundaries; Short presentations (10 mins.) on any topic relevant to 27-750 by students; topics related to research project(s) are preferred. Short presentations (10 mins.) on any topic relevant to 27-750 by students; topics related to research project(s) are preferred. For 5-Nov-09, Newby, Nakano-Baker, Li, Zhu, Teevan, Wu.

Week 12

Nov. 10th *[ADR]* Final section of CSL exposition; Stereological approach to 5-parameter grain boundary character distributions.

Nov. 12th *[ADR]* Stereological approach to 5-parameter grain boundary character distributions, contd.

Week 13

Nov. 17th *[ADR]* Grain boundary properties; GB Energy.
Nov. 19th *[ADR]* Grain boundary properties; GB Energy, contd..

Week 14
Nov. 24th *[ADR]* Introduction to Percolation theory; application to materials problems
Nov. 26th *[ADR]* (Thanksgiving Holiday)

Homework:

Week 15 Last Week of Classes at CMU:
Dec. 1st *[ADR]* Project presentations, day 1
Dec. 3rd *[ADR]* Project presentations, day 2
Since these presentations will be graded, only students taking the class for credit will be required to give presentations.
The written report that is the complement to the presentation is due Saturday, Dec. 12th.

Exam: Take-home, due Saturday, Dec. 12th.

*Unassigned lectures:*

Homework: Microscopy exercises (PK)
Homework: literature search; stereology, topology questions
Homework: calculation of OD's from measured textures; calculation of volume fractions
Homework5: Stereology, image analysis, use of ImageJ
Homework 6: texture development in thermomechanical processing
Homework: calculation of percolation of a network; pair correlation function.
Homework: solution of Bishop-Hill equations for single crystals (use of matlab or mathematica advised)
Triple Junctions, equilibrium at junctions, networks of boundaries.
Conversions between different grain boundary descriptions.
Stereology
Topology of Microstructures
Grain Growth

*Unassigned homeworks:*

Calculation of volume fractions along the beta fiber in rolled Cu (Hwk 3 from Spg 2000).

Measurement of a set of PF data (each student will provide their own specimen)

## Presentation Schedule, 1st and 3rd Dec.:

| Tuesday, 1st | | |
|---|---|---|
| Time | Topic | Name |
| 11:30 | | Stephen Newby |
| 11:45 | | Oliver Nakano-Baker |
| 12:00 | | Abhijeet Budruk |
| 12:15 | | Ben Anglin |
| 12:30 | | Dan Satko |
| 12:45 | | Emma Humphreys |
| 13:00 | | Sarah Neyer |
| 13:15 | | |
| | | |

| | | |
|---|---|---|
| **Thursday, 3rd** | | **Name** |
| 11:30 | | Jiangxi Zhu |
| 11:45 | | Jia Li |
| 12:00 | | Clayton Stein |
| 12:15 | | Reeju Pokharel |
| 12:30 | | Kevin Wu |
| 12:45 | | James Teevan |
| 13:00 | | |
| 13:15 | | |
| | | |
| | | |

# Test, Exams, Grading Policy

| | |
|---|---|
| Homeworks: approx. 1 per week | 100 points |

Exams: one in-class test at mid-term; one take-home final - 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 | 30 |
| | Mid-term Exam | 15 |
| | Final Exam | 30 |
| | Project (Written and Oral) | 25 |

Notes:

1. The final is comprehensive.
2. The presentation must be accompanied by a written report. The format of the written report will depend on whether it is a report primarily on analysis of data, or a literature review. The length should be between 4 and 12 pages, 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 25 points for the Project are divided up as 12 points for the Oral report and 13 points for the Written report.

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.

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: Wiley-Interscience; ISBN 0471310433.

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

Morawiec, A., *Orientations and Rotations* (2003), Springer (Europe), ISBN 3-540-40734-0.

Newnham, R. E. (2005). *Properties of Materials*. Oxford, Oxford University Press.

Nye, J. F. (1957). *Physical Properties of Crystals*. Oxford, Clarendon Press.

Ohser, J. and F. Mücklich (2000), *Statistical Analysis of Microstructures in Materials Science*., Chichester, England: Wiley, 381pp, ISBN 0-471-97486-2.

Randle, V. and O. Engler (2000). *Texture Analysis: Macrotexture, Microtexture & Orientation Mapping*, Gordon & Breach, Amsterdam, Holland, ISBN 90-5699-224-4.

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.

Underwood, E. E., *Quantitative Stereology*, (1970), Addison Wesley Longman, ISBN: 0201076500.

Links: a sampling from a recent search in Google with "crystallographic texture".

Texture (crystalline) - Wikipedia, the free encyclopedia
In materials science, texture is the distribution of crystallographic ... The full 3-dimensional representation of crystallographic texture is given by the ...
en.wikipedia.org/wiki/Texture_(crystalline) - 27k -
Cached - Similar pages

Texture and Anisotropy of Crystalline Materials
Since nearly 20 years I am dealing with crystallographic textures. This are not the pictures of covered bodies, which are used as background in web-pages ...
www.texture.de/index_e.htm - 7k -
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File Format: PDF/Adobe Acrobat - View as HTML
crystallographic texture on Si substrates (courtesy of. Ramtron Corporation International) ... Bingert, A Method for Crystallographic Texture Investigations ...
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Crystallographic Texture of Stress-Affected Bainite
MAP_STEEL_TEXTURE, PROGRAM: Calculation of the crystallographic texture obtained when austenite transforms into martensite. The austenite itself can be ...
www.msm.cam.ac.uk/phase-trans/2007/texture_bainite.html - 10k

Crystallographic Texture
Crystallographic Texture of Stress-Affected Bainite; Crystallographic Texture and Intervening Transformations; Transformation Texture, Stainless Steel ...
www.msm.cam.ac.uk/phase-trans/texture.html - 9k -
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(IUCr-Crystallographic Education Online) Educational Resources
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Similar pages

CCP14 Homepage - Single Crystal and Powder Diffraction - Methods ...
QTA Internet Course (Learn how to Quantitatively Determine the Crystallographic Texture of materials using x-ray and neutron diffraction): ...
www.ccp14.ac.uk/solution/pole_figure/index.html - 18k -
Cached - Similar pages

An Analysis of the Influence of Crystallographic Texture on ...
Scientific.Net: An Analysis of the Influence of Crystallographic Texture on Residual Stress Estimation for Metallic Films and Coatings.
www.scientific.net/An+Analysis+of+the+Influence+of+Crystallographic+Texture+on+Residual+Stress+Estimation