**Engineering Spectroscopy ME 498**

**MWF 9-9:50 glumac.mechse.illinois.edu/ME498/**

Overview

This course aims to provide the theory and practical experience in making measurements of thermodynamic parameters by using the spectral distribution of light. We will present the theoretical foundations for spectroscopic measurements of temperature, pressure, and concentration, including structure of matter, nature of light, statistical mechanics, and matter/light interactions. After these foundational topics, basic applications of emission spectroscopy, absorption spectroscopy, and fluorescence will be covered. A basic review of practical optics will be conducted, followed by a more detailed coverage of instrumentation for spectroscopic measurements, with a hands-on component. Scattering theory and non-linear optics will be reviewed, followed by a discussion of Rayleigh scattering and Raman scattering.

Topics Covered:

**Fundamental Physics**

1) *Nature of matter.* Basic quantum mechanics, energy storage mechanisms (translation, rotation, vibration, electrical excitation), quantization of energy. Energy levels and degeneracies. Simple model for solids. Phonons, and phonon energy distribution. Atomic and molecular structure and terminology.

2) *Nature of light.* Classical theory of dipole oscillation. Maxwell's equations. Oscillator strength. Quantum theory of light. Photon energy, linear momentum, angular momentum. Diffraction and refraction.

3) *Light/matter interaction.* Spontaneous emission, stimulated emission, absorption. Einstein coefficients. Rate equations. Thermal distribution of light emission from a blackbody. Relations among Einstein coefficients. Line broadening – natural, pressure, Doppler. Dieke narrowing. Emission/absorption/transmission in condensed matter. Emissivity variation with temperature and wavelength.

4) *Statistical mechanics.* Boltzmann distribution. Speed distribution. Rotational, vibrational, electronic state distributions. Non-equilibrium distributions. Definition of temperature. Specific heat of solids.

5) *Radiation Transport Equation.* State populations. Radiosity, radiance, irradiance. Solid angles. Limiting forms for emission and absorption. Optical depth.

## Measurement of Light

6) *Basic practical optics.* Refraction. Snell's law. Index of refraction. Lens equation. Lens and mirror types; spherical vs aspheres, compound lenses. Diffraction. Diffraction gratings. . Collimation, f-number. Fiber optics. Prisms, beamsplitters, interference filters, notch filters. Spectrometer equations with focus on Czerny-Turner systems. Overview of aberrations. Formulas for Czerny-Turner.

7) *Optical Instrumentation:* Detector types for different wavelength ranges. Optical materials. Photon statistics, NEP, signal to noise considerations, array detectors: CCD, CMOS, InGaAs, MCT, microbolometer, etc. Aligning a monochromator. Converting images to spectra. Wavelength and intensity calibration.

8) Light Sources: incandescent, arcs, sparks, LEDs, infrared sources, argon candle. Laser theory. Laser types: solid state, semiconductor, gas. Nd:YAG, dye, HeNe, excimer, diode, QCL, Ti:sapphire, etc.

## Spectroscopic Measurements

9) *Emission and absorption theory and practice.* Line of sight averaging. Extraction of temperature and concentration. Boltzmann plots. Optical depth effects. Curve of growth. Multicolor pyrometry. Elemental analysis in discharges (LIBS, spark, flame). Determination of temperature in atomic plasmas. Atmospheric measurements of trace gases. Flame temperature measurement. Astrophysical spectroscopy. Pyrometric measurements.

10) *Fluorescence measurement.* Fluorescence theory. Linear and saturated limits. Collisional quenching. Planar methods (PLIF). Challenges and opportunities.

11) *Basic scattering theory.* Classical Rayleigh theory. Polarizability. Gases and particles. Aerosols. Cross-sections. Raman theory. Rotational and vibrational Raman Scattering. Raman scattering from surfaces. Wavelength dependences. Stokes and anti-stokes. Stimulated and spontaneous Raman.

12) *Spectroscopic scattering diagnostics*. Raman spectroscopy, Rayleigh scattering, filtered Rayleigh scattering, CARS. Practical Raman spectroscopy: fast spectrometers, notch filters, time-gating, signal augmentation techniques.

<u>Conduct of the Course:</u>

3 hours lecture ($4^{th}$ hour for graduate students available as special project). Weekly homework. Mid-term exam. Final exam. Laboratory projects.

Grade Distribution:

Homework 20%, Mid-term Exam: 25%   Final Exam: 30%  Project 25%

**Some Helpful Texts (you don't need them, but I'll draw a lot from them):**

Two most relevant:

Laurendeau, N.M., 2005. *Statistical thermodynamics: fundamentals and applications*. Cambridge University Press.

> Probably the text that I'll draw most material from for the class.  Laurendeau was an optical diagnostics pioneer, and his text is less stat thermos, and more preparation for diagnostics. Covers quantum, stat mech, light interactions, and a decent coverage of laser diagnostics.

Linne, M.A., 2002. *Spectroscopic measurement: an introduction to the fundamentals*. Academic Press.

> Another very good self contained book that doesn't get a lot of love in the field, but I like it. Fills in some detail to supplement Laurendeau.  Table of contents reads a lot like the class syllabus,

Good Supplemental Sources:

Thorne, A., Litzén, U. and Johansson, S., 1999. *Spectrophysics: principles and applications*. Springer Science & Business Media.

> Great text that covers almost everything in the course.  Out of print, and expensive if you find a copy.  But a spectacular work.

Bernath, P.F., 2020. *Spectra of atoms and molecules*. Oxford university press.

> On the spectroscopy side, there's probably no better text than this small work by Piotr Bernath who is a king in the field.

Demtröder, W., 2014. *Laser spectroscopy 1: basic principles*. Springer.

> A classic on laser spectroscopy.  Heavily cited.

Kohse-Hoinghaus, K. and Jefferies, J.B., 2002. *Applied combustion diagnostics*. CRC Press.

> Another pretty good work on laser diagnostics for combustion.  Modern.