TIE CODE: LECT
GRADING: Letter
SEMESTER OFFERED: Alternate even years in Fall Semester. Dept. in charge will also
alternate starting with CEE in 2010, ME in 2012, etc.
COURSES THAT WILL RESTRICT CREDIT: None
INSTRUCTOR(S): Professors P. Papadopoulos and S. Govindee
DURATION OF COURSE: 15 weeks
EST. TOTAL NUMBER OF REQUIRED HRS OF STUDENT WORK PER WEEK: 9
IS COURSE REPEATABLE FOR CREDIT? No
CROSSLIST: Civil Engineering C235

CATALOG DESCRIPTION

Introduction to statistical mechanics for engineers interested in the constitutive behavior of
matter with a particular interest in continua. Systems of interest will be polymers and crystalline
solids. Coverage includes introduction to statistical mechanics, ensembles, phase spaces,
partitions functions, free energy, polymer chain statistics, polymer networks, harmonic and
quasi-harmonic crystalline solids, limitations of classical methods and quantum mechanical
influences.

EXPANDED DESCRIPTION

The theories of continuum mechanics form a foundation for the description of the deformation of
many engineering materials from gases, to liquids, to solids. At the heart of the application of
such frameworks is a description of the makeup of the material – the constitutive model. In this
regard, one can approach the specification from a phenomenological viewpoint, a mathematical
viewpoint, and/or a physical viewpoint. Of great appeal is the notion of using information from
detailed molecular and atomistic characterizations of materials to construct the constitutive
relations. Statistical mechanics provides an interesting and powerful tool to effect such a
procedure. This course is intended for students with a background in continuum mechanics that
desire a firmer understanding of the atomistic aspects of the subject. The course will first cover a
basic presentation of thermo-elasticty from a continuum viewpoint. Then fundamental concepts
of classical statistical mechanics will be introduced such as Boltzmann’s entropy, phase space
averages and canonical distributions. In this regard, use will be made of Hamilton’s formulation
of mechanics. The special cases of isolated and weakly interacting systems will be defined and
discussed thoroughly along with definitions of equilibrium. These two presentations, continuum
mechanics and statistical mechanics, will next be combined and corresponding notions from both descriptions will be identified and discussed. Particular emphasis will be placed on the statistical basis for continuum state functions and quantities derived from them. Applications of this framework will be made to the development of constitutive relations based on microscale information for a variety of systems: ideal and van der Walls gases, single polymer chains, elastomeric solids, and crystalline solids.

**COURSE PREREQUISITES**

CE C231 or MSE C211 or ME 185 or consent of instructor.

**TEXTBOOK(S) AND/OR OTHER REQUIRED MATERIAL**


**DESIRED COURSE OUTCOMES**

To provide a modern introduction to the application of statistical mechanics for engineering with a particular emphasis on mechanical response.

**TOPICS COVERED**

Week-by-week lecture topics:

1. Overview of thermo-elasticity from a continuum viewpoint
2. Concepts of state functions in thermo-mechanics
3. Introduction to Hamiltonian mechanics
4. Statistics in statistical mechanics, Phase functions and time averages
5. Phase space dynamics of isolated systems, weakly interacting systems
6. Canonical distributions
7. Concepts of temperature, local equilibrium processes, phase functions for generalized forces
8. First and second laws of thermodynamics
9. Partition function relations, continuum formulations of nonuniform processes
10. Equipartition and alternative definitions of entropy, applications to gases
11. Crystal elasticity, Bravais lattices, harmonic and quasi-harmonic approximations to crystals
12. Constitutive laws for crystalline solids
13. Rubber elasticity of single chains
14. Rubber elasticity of networks
15. Quantum mechanical influences on elasticity

CLASS/LABORATORY SCHEDULE

3 Hours of lecture per week.

EXAMS

One midterm examination and a final project.

HOMEWORK

Weekly assignments: both analytical and computational.

GRADING

30% homework, 30% midterm, 40% final project.

PERSON(S) WHO PREPARED THIS DESCRIPTION

Panayiotis Papadopoulos
September 10, 2009