

Statistical Mechanics of Elasticity (revised)

Level: Masters

Short Description: Introduction to statistical mechanics for engineers interested in the constitutive behavior of elastic continua. The primary systems of interest will be polymers and crystalline solids. Coverage will include an introduction to statistical mechanics, notions of ensembles, phase spaces, partitions functions, derivation of constitutive relations, polymer chain statistics, polymer networks, harmonic and quasi-harmonic crystalline solids, limitations of classical methods and quantum mechanical influences.

Description The theories of continuum mechanics form a solid foundation for the description of the deformation of many engineering systems. At the heart of the application of such frameworks is a description of the make up 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-elasticity 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. Use will be made of Hamilton's formulation of mechanics in this regard. The special cases of isolated and weakly interacting systems will be defined and discussed thoroughly. 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 Waals gases, single polymer chains, elastomeric solids, and crystalline solids.

Contents:

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

Course Format/Time: 2 hours lecture and 1 hour discussion/problem section

Exam: (Sessionsprüfung) Oral 30 minutes

Testatbedingung: Completion of 80% of homework assignments

Primary Goal: To provide a modern introduction to the application of statistical mechanics to the determination of constitutive relations for elastic solids.

Reading Material: Required: Statistical Mechanics of Elasticity, J.H. Weiner, Dover Press, 2002 (or Wiley Press 1983). Recommended: Crystals, Defects and Microstructures, Rob Phillips, Cambridge University Press, 2001. Elementary Principles in Statistical Mechanics, J.W. Gibbs, Dover Press, 1981 reprint of 1902 original. Mathematical Foundations of Statistical Mechanics, A.I. Khinchin, Dover Press, 1949.