Course Tentative Title: Chemistry and Physics in Mechanics

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ELMS Description: Fundamental physics and chemistry underlying theoretical mechanics. Basic principles starting from solid state physics suited for multiscale understanding of material behaviors of potential interest to mechanical engineers.

Recommended Background: 1st or 2nd year graduate students or advanced undergraduates with courses in one or more of the following: Continuum Mechanics, Thermal Conduction & Radiation, Molecular Thermodynamics, or Modeling Material Behavior.

Reference Materials:

- Charles Kittel, *Introduction to Solid State Physics*, 8th ed., New York, NY: John Wiley & Sons., 2004 ISBN: 9780471415268 (**required**)
- Ashcroft, Neil W., and N. David Mermin. *Solid State Physics*. New York, NY: Holt, Rinehart and Winston, 1976. ISBN: 9780030839931 (**optional**)

Course Objective: This is an advanced foundations course, covering fundamentals in the underlying physics and chemistry of mechanics. The course will provide valuable introduction to the physics basis of mechanics, primarily targeting properties and behaviors relevant to contemporary mechanics applications in solid mechanics and solid state heat transfer.

Learning Outcomes:

- Understand the atomic (multiscale) structure of solids and the role of atomic interactions in solid mechanics
- Understand the types of approaches for representing and studying atomic interactions
- Develop theoretical insights for the study of mechanical and thermal transport properties through the atomic and electronic nature of solids
- Understand the role of vibrations and temperature in the physical properties of solids
- Analyze mechanical functionality of materials using physical first principles

Applications: Mastery of course concepts will equip students with foundational knowledge for:

- Design of new materials for device properties or functionality.
- Research in novel material and mechanical mechanisms in contemporary research areas.
- Study of deformability, vibrations, energy transport, and mechanical failure in high performance or novel materials.
- Study of novel material architectures such as metal organic frameworks, low-dimensional materials, and metamaterials.

Topic Schedule:

- **The Structure of Solid Matter**

- Week 1 Structure of Lattices: Periodic lattices, Unit Cells, Supercells, Amorphous materials, Bravais lattice, primitive cell, lattice with a basis, crystal structures, Miller indices, point/line/plane defects
- Week 2 Reciprocal Space: Diffraction, reciprocal lattice, brillouin zones, fourier transforms, reciprocal vectors, Bragg's law, von Laue's formulation
- Week 3 Bonds: Chemical bonding, classical bond models, quantized Hamiltonian, Born-Oppenheimer approximation, bond-breaking
- Week 4 Electrons in solids: Drude theory, Sommerfeld theory, Fermi sphere and surface, single electron approximation and electron density

- **Mechanical Properties of Solid Matter**
  - Week 5 Deformability of solids: deformation gradient, internal energy, virial stress, elastic constants
  - Week 6 Mechanics of defects: defect mobility, Peach-Koehler forces, defect diffusivity
  - Week 7 Vibrational properties: phonons, band structure, specific heat, normal coordinates, spectral energy density, quantum harmonic theory
  - Week 8 Functional materials: Solid-solid phase transition, ionic crystals, polarizability, dielectric properties, Clausius-Mossotti relation, ferroelectricity, piezoelectricity, domain walls
  - Week 9 Statistical thermodynamics of solids: autocorrelation, partition function, statistical distributions
- **Thermal and Transport Properties of Solid Matter**
  - Week 10 Temperature effects in solids: Free energy, quasiharmonic approximation, thermal expansion
  - Week 11 Thermal transport: Thermal conductivity, electron & phonon transport, free gas phonon and electron models, Debye and Einstein models, Allen-Feldman model, Cahill Watson Pohl model
  - Week 12 Quantized carriers: Quantum anharmonic transport, relaxation time, mean free path, perturbation methods, Fermi's Golden Rule, conservation of crystal momentum, conservation of energy
- **Hydrodynamic Properties of Solid Matter (if time permits)**
  - Week 13 Shock physics of solids: Basic shock physics, shock waves, conservation of mass/momentum/energy, equations of state, Rankine-Hugoniot relations, isentropic shock, Chapman-Jouguet condition
- **Other Properties of Solid Matter (if time permits)**
  - Week 14 Optical properties, magnetic properties, semiconductors, Hall effect, spintronics, superconductors, radiation-matter interactions

Grading:

- Quizzes based on reading: 50%
- Literature report: 15%
- Final Project: 35%

Course Format:

Traditional lecture course with a semi-flipped format based on pre-reading of lecture notes and textbook prior to each lecture with a graded Canvas quiz before lecture. Lectures will primarily consist of discussions centered on explaining the differences between different theoretical models and derivation of some of the mathematical formalisms.