**Irreversible thermodynamics and transport of charge, heat, and spin (ME8603)**

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**Syllabus**

**Brief Catalog Description**

Ohm’s, Fourier and Fick’s laws, which relate linearly the transport of electrical charge, heat and matter to voltages, temperatures and concentrations gradients, are generalized in the framework of irreversible thermodynamics. The microscopic mechanisms of transport of heat, electrical charge and magnetization by elemental excitations (electrons, phonons and magnons) are explained.

**Goals:**

1. Learn the basics of irreversible thermodynamics: how to treat thermodynamic systems that are slightly out of thermodynamic equilibrium, using linear perturbation theory.

2. Learn the concept of fluxes and flow of matter, heat, electrical charge, and magnetization or spin. Learn about thermodynamic driving forces, pressure differences, temperature differences, voltage (differences in electrical potential), magnetization differences. The Onsager relations, a form of generalized Ohm’s law (the linear relation between current and voltage) relate the fluxes linearly to the thermodynamic forces: pressure differences drive flow of matter, temperature differences flow of heat, and related phenomena.

3. The Onsager relations also relate fluxes to forces that are not directly related: a voltage can drive flow of matter (electrophoresis), a temperature difference a flow of electricity (thermoelectrics) or of matter (thermal diffusion) or of magnetization (spin caloritronics). These cross-terms drive devices that can convert energy from one type (thermal, mechanical, electrical, magnetic) to another.

4. Review of the properties of the three types of elemental excitations that carry electricity, heat, and magnetization are electrons, phonons (lattice waves) and magnons (spin waves) in solids.

5. The microscopic theory of the transport of charge (electrical conductivity, thermoelectric effects) in solids

6. The microscopic theory of the transport of heat (phonon, electron and magnon thermal conductivity) in solids

7. The microscopic theory of the transport of spin (magnons, electrons and also phonons) in solids

8. Interactions between electrons, phonons and magnons, and corrections to the transport theory due to these interactions, such as phonon-drag, magnon-drag and the spin-Seebeck effect.

**Text:** Powerpoint lectures and notes from the instructor

**Prerequisites:** Statistical thermodynamics (ME 8503) or statistical mechanics. Engineering knowledge of condensed matter physics, or permission of the instructor.

**Reference books/articles:**

* H. Callen, Thermodynamics, John Wiley & Sons, New York, 1960
* J. M. Ziman, Electrons and Phonons, Clarendon, Oxford (1960), reprint 1972
* Heikes et Ure, Thermoelectricity: Science and Engineering, Interscience, New York 1961
* S.R. Boona and J. P. Heremans: Spin Caloritronics, Energy and Environmental Science (2014)

**Evaluation:** graded (conventional A-E scale) take-home homework problems, to be solved individually. All external sources of material are allowed. Approximately one problem per chapter (7 problems total).

**Detailed content of the course:**

Chapter 1: Review of classical thermodynamics and introduction to transport

 1.1 Irreversible versus reversible thermodynamics

 1.2 Review of reversible thermodynamics:

* extensive vs intensive parameters
* the free energies, Legendre transforms
* relations: heat; mechanical, chemical, electrical, magnetic work

 1.3 Electrical transport, current/voltage relations

* Linear: Ohm’s law
* Types of transport: diffusive, ballistic, quantized
* Boltzmann versus Landauer-Büttiker formalisms
* Non-linear: drift/diffusion equations

Chapter 2: The Onsager relations

 2.1 Ohm’s, Fourier’s and Fick’s laws: linear relations between flux and force

 2.2 The Onsager formalism: generalized linear transport law, generalized fluxes and forces

 2.3 Dissipation, reversible and irreversible heat production

 2.4 Cross effects at zero external magnetic field

 2.5 The effects of an applied external magnetic field

Magnetoresistance, Magnetothermal resistance.

Electrical cross effects: Hall, Maggi-Righi-Leduc effects.

Thermal cross effects, Magneto-Seebeck effect, isothermal versus adiabatic effects

Double-cross effects: Nernst, Ettingshausen effects.

 2.6 The Onsager reciprocity relations

 2.7 Onsager vs crystallography, “Umkehr” effects

 2.8 Thermoelectricity

Chapter 3: Diffusive electron transport in crystalline solids

 3.1 The Boltzmann equation: how a temperature gradient becomes a force.

 3.2 Density of states in 1,2,3 dimensions

 3.3 The transport integrals, no magnetic field, one-carrier systems (Bloch-Grüneisen; semiconductors)

 3.4 Galvanomagnetic and Thermomagnetic transport coefficients

 3.5 The “method of the four coefficients”

 3.6 Multicarrier transport

Chapter 4: Corrections to electron transport

 4.1 Landau levels

 4.2 Size-quantization

 4.3 Weak localization

 4.4 The Ioffe-Regel rule; generalized conductivity with the density of states only defined as function of energy

 4.5 The Mott relation and its derivatives, the Heikes formula

Chapter 5: Diffusive phonon transport in crystalline solids

 5.1 Phonons

 5.2 The thermal conductivity integral

 5.3 Intrinsic scattering, phonon-phonon interactions, “Normal” and “Umklapp” processes

 5.4 Extrinsic scattering

 5.5 The Callaway model

 5.6 The spectral thermal conductivity

Chapter 6: Corrections to phonon transport

 6.1 The Slack-Cahill rule (the Ioffe-Regel rule for phonons)

 6.2 “Lattice” thermal conductivity in amorphous solids: Anderson

Chapter 7: Magnons and magnon thermal conductivity

 7.1 Introduction to thermodynamics of magnetism

 7.2 Spin waves

 7.3 Thermal spin pumping

 7.4 Crossing interfaces

 7.5 Spin Onsager relations

Chapter 8: ­Interactions and mixed effects

 8.1 Phonon-electron interactions

 8.2 Phonon-electron drag

 8.3 Phonon-magnon interactions

 8.4 Phonon-magnon drag

 8.5 The spin-Seebeck effect, ferromagnets

 8.6 The spin-Seebeck effect, spin-polarized non-magnetic systems

Chapter 9: Applications

 9.1 Thermoelectric heat engines, the thermoelectric figure of merit zT

 9.2 Thermoelectric materials optimization

 9.3 Prospects for spin-thermal engines

**Schedule of the course:**

Lecture 1: 1.1-1.2

Lecture 2: 1.2-1.3

Lecture 3: 1.3

Lecture 4 : 2.1

Lecture 5: 2.2, 2.3

Lecture 6: 2.3,

Lecture 7: 2.4

Lecture 8: 2.5

Lecture 9: 2.6

Lecture 10: 2.7

Lecture 11 :2.8

Lecture 12: 3.1-3.2

Lecture 13: 3.3

Lecture 14: 3.4

Lecture 15: 3.4, 3.5

Lecture 16: 3.6

Lecture 17 : 4.1

Lecture 18 : 4.2

Lecture 19 : 4.3

Lecture 20: 4.4

Lecture 21: 4.5

Lecture 22: 5.1-5.2

Lecture 23: 5.3

Lecture 24: 5.4

Lecture 25: 5.5

Lecture 26: 5.5-5.6

Lecture 27: 6.1, 6.2

Lecture 28: 6.2

Lecture 29. 7.1

Lecture 30: 7.2

Lecture 31: 7.3

Lecture 32: 7.4

Lecture 33: 7.5

Lecture 34: 8.1

Lecture 35: 8.2

Lecture 36. 8.3

Lecture 37: 8.4

Lecture 38: 8.5

Lecture 39: 8.6

Lecture 40: 9.1

Lecture 41: 9.2

Lecture 42: 9.3

For a total of 3 55-min-hours/week.