Matter, Molecules, and their Environments, Condensed Matter Track
Univ Lille, France
2024-2025

Document 27 May 2024, Sébastien Merkel

Courses overview

- Dynamical properties of matter (6 ECTS)
- Imperfections in solids (6 ECTS)
- Thermodynamics and phase transitions (6 ECTS)
- Molecular spectroscopy (3 ECTS)
- Atomic scale modeling (6 ECTS)
- Advanced characterization methods (6 ECTS)
- Scientific writing & communication (3 ECTS)
- English or French (3 ECTS)
- Laboratory internship (21 ECTS)

Course details

Dynamical properties of matter (6 ECTS)

- Amorphous materials (3 ECTS)
  - Structural organizations of materials (crystals, mesophases, glasses)
  - Study of molecular mobility: different scales of dynamics, fluctuation/dissipation theorem, measurement techniques
  - Dynamics of glass-forming liquids: non-Arrhenian and non-Arrhenian character - exponential of the main relaxation, secondary relaxations, evolution over time, other relaxations
  - Case of mesophases: semi-crystalline materials, liquid crystals, plastic crystals.
- Crystals (3 ECTS)
  - Vibrational dynamics of three-dimensional crystals: dispersion curves, density of states, quantification of normal and phonon modes
  - Connection to continuous media and elastic constants
  - Thermal properties of crystals and specific heat - Debye-Waller factor - anharmonic effect (thermal expansion and Grüneisen constant).
  - Equations for elastic continuous media.
  - Dispersion and transmission curves, natural modes.
  - Application to phononic crystals and acoustic metamaterials: foundation and applications.
  - Phonon/photon coupling.
  - Introduction to new physical properties: negative refraction, invisibility to acoustic waves, hyperfocusing, revisiting the laws of Snell Descartes, phonon-photon coupling (optomechanics), etc

Imperfections in solids (6 ECTS)

- Fundamentals
  - Plasticity in amorphous materials
  - Defects
  - Introduction to dislocations
  - Elastic theory of dislocations
  - From dislocation to plasticity
  - Lattice friction and dislocation mobility
  - Interactions dislocations – dislocations, dislocations – point defects, dislocations – precipitates
- Grain boundaries:
  - Grain boundary geometry
  - Mechanics of grain boundaries, disconnections and disclinations
- Microstructures and polycrystals:

    - Description of orientations in a polycrystal: Euler angles, matrix form, orientation distribution function
    - Experimental measurement techniques: EBSD and X-ray diffraction
    - Average elasticity and properties of polycrystals
    - Microscopic origins of texture
    - Introduction to modeling methods

Thermodynamics and phase transitions (6 ECTS)

- Phase transitions (3 ECTS)
    - Basics of thermodynamics and usual phase diagrams
    - Thermodynamic classification of phase transitions
    - Stability, metastability and instability
    - Physical states: crystalline polymorphs, mesophases, amorphous
    - Dynamics of phase transitions: Nucleation/Growth – Interfaces – Avrami model – Vitrification
    - Connection between microscopic and macroscopic properties
    - Experimental methods for studying phase transformations.
- Binary systems (3 ECTS)
    - Phase transformation in binary systems
    - Calculation of a Gibbs energy curve
    - Solution models (ideal, regular and real)
    - Introduction to chemical potentials
    - Common tangent rule
    - Variance rule
    - Raoult's laws and of Henry
    - Precipitation of a solid phase into another in a binary system
    - Nature of a heterophase interface (coherent, semi-coherent and incoherent)
    - Calculation of the elastic energy associated with precipitation
    - Loss of coherence
    - Driving force of germination
    - Euler model for growth

Molecular spectroscopy (3 ECTS)

- Molecular symmetry. Symmetry groups
- Molecular Energy Levels
- Rotation-vibration interactions
- Molecular spectra
- Spectroscopy of diatomic radicals

Atomic scale modeling (6 ECTS)

- Calculation of gas electronic structures: Hartree-Fock and density functional theory (DFT)
- Molecular mechanics and classical dynamics (force fields, determination of macroscopic quantities, ensembles, thermostats, stress, Ewald summations, etc)
- Monte Carlo methods
- Introduction to ab-initio molecular dynamics or DFT

Advanced characterization methods (6 ECTS)

- Spectroscopies (3 ECTS)
    - Introduction to spectroscopy characterization techniques
    - High-resolution terahertz spectroscopy and molecular structure (class and practicals)
    - Raman spectroscopy (class and practicals)
    - Fourier transform infrared spectroscopy (class and practicals)
    - Dielectric spectroscopy (class and practicals)
- Diffraction and electron microscopy (3 ECTS)
    - Course
        - Radiation – Matter interactions
        - Diffraction techniques
        - Specificity of powder diffractions and Rietveld refinement

        - Electron microscopy
    - Practicals
        - Rietveld refinement
        - Electron microscopy

Scientific writing & communication (3 ECTS)

English or French (3 ECTS)