

Lecture Outline and Schedule

Year	Module	Lecturer
Year 4 (2023) Introduction of the material classes and modeling techniques	Introduction to lead-free perovskite ferroelectrics for electro-mechanical systems <ul style="list-style-type: none"> • Mechanical Properties of Ferroelectrics <p>Syllabus: This lecture is an introduction to dielectric, piezoelectric, and ferroelectric properties of ferroelectrics. In the first section, background on dielectric and piezoelectric properties will be discussed with a focus on the influence of material phenomena at multiple length scales, such as domain wall and phase boundary motion, as well as the influence of external thermal, mechanical, and electric fields. Various measurement techniques, such as Rayleigh behavior and impedance spectroscopy, will be introduced. In the second section, the large field response of ferroelectrics, namely ferroelectricity and ferroelasticity will be discussed with a particular focus on the effect of crystal structure and compositional phase boundaries, the role of domain wall motion and defects, and the influence of stress-induced structural phase transformations. Measurement techniques for characterizing large field behavior, such as the Sawyer-Tower circuit, will also be introduced. Following this lecture it is expected that the participant is familiar with the dielectric, piezoelectric, and ferroelectric properties of normal ferroelectrics and has an understanding of the crystallographic origins of the electromechanical properties.</p> • Piezoelectric Properties of Lead-Free Ferroelectrics <p>Syllabus: This course provides basic and latest information on the functional properties of ferroelectric materials, in which the orientation of spontaneous polarization changes with electric field, stress or temperature. In the first section, an introduction of their commercial applications available at present or projected in future is given to participants in order to adopt a backcasting way of learning. Then, the second section of this course deals with the crystal chemistry of ferroelectric materials and differences in history and characteristics among lead-free based materials including (Na,K)NbO₃, (Ba,Ca)(Ti,Zr)O₃, (Na,Bi)TiO₃, BiFeO₃ perovskites and their relative compounds. In the third and fourth sections, the lecture is extended to cover the topics of important ferroelectric families including piezoelectrics which are polarized by stress, and pyroelectrics which hold spontaneous polarization without an external signal. In particular, participants can learn various synthesis and structure control techniques to engineer high-performance materials. The purpose and goal of this course is to understand the characteristics of ferroelectric materials as well as the ways of new material design, through lecture and group discussion.</p> <p>Block Periods: June 12-15 at NITech, June 20-22 at FAU</p> 	Webber Kakimoto
	Materials and devices for opto-electric and energy technologies <ul style="list-style-type: none"> • NGSE5 Seminar <p>Syllabus:</p> <ul style="list-style-type: none"> - 10 Tutorials (each 1h) will be given to acquire theoretical foundations, followed by a debriefing for questions of students. - Supplementary 15 keynote speeches (each 15min) on highly topical issues will be held: 6 presentations on a timely OPV topic, 6 on a timely perovskite topic and 3 on a timely emerging PV topic. • Electronic Materials Analysis <p>Syllabus: This lecture introduces theory and practice of electronic materials characterization and analysis based on the case of semiconductors. Characterization and analysis techniques for semiconductors can easily be applied to other electronic materials, and the techniques are powerful tools to know properties of the electronic materials.</p> <p>A textbook of the lecture will be "Semiconductor Material and Device Characterization" by Schroder, D. Wiley-IEEE Press, c2006</p> <p>Block Periods: July 10-14 at NITech, November 13-17 at FAU</p> 	Brabec Kato
	Introduction to atomistic and mesoscale modeling <ul style="list-style-type: none"> • Electro-Mechanical-Modeling(EMM) <p>Syllabus: This course will cover the following topics:</p> <ul style="list-style-type: none"> - Tensor Calculus - Continuum Mechanics - Electro-Magneto-Dynamics - Electro-Statics - Electro-Mechano-Statics - Electro-Mechano-FEM • Simulation for Nano-Technology <p>Syllabus: This course will cover the following topics related to the molecular dynamics simulation:</p> <ul style="list-style-type: none"> - Empirical Inter-atomic Potentials - Time-evolution Algorithms - Long-ranged Coulomb Interaction - Essential Techniques - Recent Results <p>Block Periods: TBD at NITech, November 6-10,2023 at FAU</p> 	Steinmann Ogata

Year 5 (2024)
Processing and
synthesis
techniques

Processing of functional ceramics and ceramic structures

- Additive Manufacturing of 3D Cellular Ceramic Structures

Syllabus:

- Introduction in Ceramic Processing
- Additive manufacturing methods- an overview
- Advantages in ceramic additive manufacturing
- Characterization and simulation methods for additive manufacturing

- Processing of Lead-Free Polycrystalline and Single Crystal Ferroelectrics

Syllabus: This course provides basic and latest knowledge on the synthesis of ferroelectric materials and their characterization techniques. Various properties of polycrystalline ferroelectric and the related functional materials are brought from the interdependent hierarchies of crystal structure, domain structure, grain structure and boundary/interface structure. The principal and application of instrumental analyses to characterize single- and poly-crystalline materials, thin/thick films and composites are to be explained, followed by understanding the stages of microstructure development in the materials synthesized through various processing routes. The lecture also covers the topics of environmentally benign processing technology targeted for SDGs, as well as important traditional techniques.

Block Period: In or after August at NITech, Late November or December at FAU

Fey
Kakimoto

Electrochemistry and growth of single crystal wide band gap semi-conductors

- Growth and Characterization of Single Crystal Semi-Conductors

Syllabus:

1. Fundamentals of Crystal Growth
2. Crystal Growth and Epitaxy of the wide bandgap semiconductors SiC, GaN/AlN, Diamond, ZnSe and Ga2O3
3. Semiconductor Wafer Characterization (optical microscopy // birefringence // defect etching // wafer mapping by photoluminescence, Raman and optical absorption)

- Advanced Industrial Electrochemistry

Syllabus: Students will learn the fundamentals of electrochemistry. They will also learn the basic principles and present problems of several kinds of electrochemical energy devices such as Li ion batteries, Fuel cells, Solar cells, and others. This course also provides the students with the opportunity to discuss the challenges and potential solutions related to environmental problems. This course consists of the following content: Fundamentals of electrochemistry, Electric Double Layer Capacitors, Lithium Ion Batteries, Nano-carbon Electrodes, Fuel Cells, Solar Cells, Photo-catalysts.

Block Periods: May 27-30 at NITech, July 17-21 at FAU

Wellmann
Kawasaki

Synthesis and optical properties of solution processed semiconductive perovskites

- Metal halide perovskite single crystal growth and applications

Syllabus: Some fundamentals of single crystal growth from solutions Metal halide perovskite materials Why metal halide perovskites – unique properties Bulk single crystals and their applications Sheet growth of perovskite single crystals Thin film growth of perovskite single crystals Microcrystal growth of perovskite single crystals Nanocrystals of perovskite single crystals Epitaxial growth of perovskites

- Advanced photonic nanomaterials

Syllabus: This course gives fundamental knowledge on electrical and optical properties of nano-sized semiconductive and ceramic materials as well as their possible applications in fields of illuminations and photovoltaics. The lecture will start with a basic of bulk semiconductors, and explain on recent artificial illuminations based on blue-LEDs. To let participants well to understand photonic properties of the nano-sized materials, a confinement of electrons and holes in nano-space will be lectured. The goal is to acquire skills to perform material designs using nanosized semiconductors and knowledge on characterizations of their electrical and optical properties.

1. Fundamentals of semiconductors
2. Bandgap estimation: Tauc analysis
3. Electron confinements: what happens for electrons and holes in nano-spaces
4. Quantum size effects
5. Applications of nano-sized semiconductors
6. Design of nanosized semiconductors and characterizations of the electrical and optical properties

Block Period: October 1-4 at NITech, July 23-26 at FAU

Heiss
Hayakawa

Nanostructured surfaces

- Modeling of Surface Phenomena

Syllabus: The lecture starts with a brief introduction into quantum-chemical methods for surface science studies. Important practical issues when performing calculations are addressed. In the next section, the basic nomenclature of how to describe the atomic and electronic structure of surfaces is introduced. Basic concepts on how to understand the electronic properties of metal, semiconductor and insulator surfaces, such as surface states, dangling bonds, passivation, charge neutralization with respect to polar and nonpolar surfaces will be explained. This will be combined with a thermodynamic analysis of the stability of surface structures, which will allow to derive surface phase diagrams. These concepts will be used to understand adsorption properties and surface chemical reactions. Finally, methods for calculating STM and AFM data to support the analysis of experimental data from local probe measurements are discussed.

Meyer
Haneda

- Ceramics Interface Chemistry

Syllabus: Ceramics materials, which are representative of the oxide, are complexed with other oxides or metals to improve the surface/interface properties. This lecture provides the physico-chemical properties and their characterization techniques of ceramics interface at which various physical and chemical phenomena such as molecular adsorption, catalysis, electron transfer etc. take place. Students will learn the foundation and application of surface/interface chemistry occurred on advanced ceramics materials, mainly focusing on catalyst.

Block Periods: November 27-December 1, 2023 at NITech, TBD at FAU.

Advanced structural characterization techniques

- **Vibrational Spectroscopy of Amorphous To Nucleated To Fully Crystallized Materials**

Syllabus: This lecture introduces theory and practice of Vibrational Spectroscopy techniques. Students will learn the fundamentals, the instrumentation, and the challenges in data acquisition/interpretation. Therefore, Hands-on training sessions are planned.

- Basic theory and fundamentals;
- Raman and FTIR spectrometers;
- Applications & Complementary techniques
- PRACTICE: Sample preparation & measurements (if allowed)
- PRACTICE: Data handling: from calibration to data presentation
- PRACTICE: Interpretation: quantitative vs qualitative

Cicconi
Hayashi

- **Synchrotron Radiation Techniques for Materials Science**

Syllabus: This lecture introduces materials characterization techniques using synchrotron radiation, which produce strong and energy tunable X-rays. Unlike ordinary X-ray analyses, students will learn how powerful synchrotron-based X-ray techniques for element-selective structural analyses.

- Basics of Synchrotron Radiation;
- Introductions of Various Synchrotron-Based X-ray Techniques;
- X-ray Absorption Fine Structure (XAFS)
- X-ray Fluorescence Holography (XFH)

Block Periods: TBD

Year 6 (2025)
Device
development
and advanced
characterization
techniques

Communications systems design and bio-safety assessment

- **Electronics Design for Energy Harvesting System**

Syllabus: This lecture will focus on the circuit topologies used with energy harvesters and pay special attention to power and energy budgets. It will consist of several parts:

- 1) Imperfections of passive and active components used with harvester circuits, component modelling including parasitics
- 2) Simple rectifier/harvester circuits, loss mechanisms present in these circuits, realistic views on achievable power and efficiency figures
- 3) Advanced rectifier/harvester circuits, differences between harvesting schemes for stationary processes (e.g. vibration) versus instationary processes (e.g. stepping, shock actuation) optimization of circuitry and minimization of losses, Advanced harvester topologies making use of resonant phenomena, discussion on timings and I/U transient behavior
- 4) System architectures including battery management and voltage conversion, State of Charge SoC derivation, power and energy budget calculations
- 5) Application examples of power needs by circuitry in wearables and medical electronics with wireless interfaces, schemes for energy management, benefits from duty cycles in wireless communication.

Fischer
Anzai

- **Body Area Communications**

Syllabus: This lecture will introduce basic knowledge and application examples using body area communication. It mainly consists of five parts. (1) On-body transmission mechanism and characteristic, (2) In-body transmission mechanism and characteristics, (3) Transceiver design example, (4) Application to wireless robot control, and (5) Related electromagnetic compatibility (EMC) issues.

- **Multiphysical Simulation Technique and Bio-safety Assessment**

Syllabus: This lecture explains computational techniques for human exposure to electromagnetic field, including resultant temperature rise. The relationship between exposure and product safety standards is discussed including the rationale from engineering viewpoint from extremely low frequencies to millimeter waves. Recent standardization related to emerging wireless communications system is also summarized.

Periods: TBD

Advanced modeling techniques for mechano-electrical systems

- **Modeling and Simulation of Piezo-Electric Energy Harvesters**

Syllabus: The course provides an overview of modeling and simulation approaches for piezoelectric energy harvesters. In the first part of the course, there is a short introduction about the applications of piezoelectric energy harvesters. Then, the basic equations of electro-mechanical models are derived, both for linear and nonlinear material behavior. Building on these continuous equations, the simulation of piezoelectric structures using the finite element method is shown. This is followed by a discussion of the simulation of electric circuits and their coupling with electromechanical structures. Examples of linear energy harvesters and their dynamic simulation using harmonic response analysis follow. In the last part of the course, the coupled simulation of nonlinear energy harvesters with nonlinear circuits is discussed.

Mergheim
Kosaka

- **Advanced Lecture on Motor Drives**

Syllabus: In recent years, an electric and a fuel cell vehicle have been put to practical use in the market for a demand of CO₂ emission reduction for protecting global warming. These kinds of vehicles employ electric motor drives for their propulsion. This lecture provides explanations about various types of the electric motors and their working principles, drive methods based on power electronics and aspects from a viewpoint of the vibration that is a dominant source of noise to be suppressed by piezo-actuated shape-adaptive structures as well as gives us an opportunity of developing piezo-actuated energy harvesting system.

Block Periods: TBD

Crystal growth and material processing - experimental and numerical approaches

- **Introduction to the phase-field method for crystal growth, processing and multiferroics**

Syllabus: This lecture introduces the key ingredients to understand and implement the phase-field method (PFM), which has established as an important simulation tool to understand mesoscopic structure evolution in alloys, ceramics and soft matter. In the course the focus lies on applications in crystal growth, solidification and thin film growth of multi-component systems (alloys and minerals), but we will also touch domain or variant evolution in multiferroic systems, such as ferroelectrics, shape memory alloys (SMAs) and ferromagnetic SMAs.

The basic idea of introducing diffuse interfaces that simplify the numerical treatment of this kind of free boundary value problems is explained, and the mathematical and physical background including thermodynamics is developed. A lecture of its own will be dedicated to implementation of this method, including feasible and flexible software packages that can be used without long-standing experience in numerics.

From elementary description of interfacial phenomena to the kinetics of crystalline interfaces, increasingly complex models including single phase-field to multiple phase-field methods are exploited. Important transport processes containing diffusion, fluid flow and mechanical deformation are coupled. The goal is to convey a tool to study intricate pattern formation during solidification (dendrites), eutectic lamellae growth, precipitate growth and solutal crystal growth. Additional chapters on the relationship of PFM to atomistic simulation techniques (MD, DFT) will be presented, allowing for a length scales bridging in computational modeling.

Wendler
Miyagawa

- **Crystal growth of semiconductor and material processing using ultrashort laser pulses**

Syllabus: This course provides basic and latest knowledge on the crystal growth of semiconductor materials, especially about epitaxial growth. This course also provides the latest fine processing technique using ultrashort pulse lasers.

Block Periods: TBD
