课程详述

COURSE SPECIFICATION

以下课程信息可能根据实际授课需要或在课程检讨之后产生变动。如对课程有任何疑问，请联系授课教师。

The course information as follows may be subject to change, either during the session because of unforeseen circumstances, or following review of the course at the end of the session. Queries about the course should be directed to the course instructor.

1.	**课程名称 Course Title**	氧化物信息功能材料导论 Introduction to Functional Oxides for Information Technology
2.	**授课院系 Originating Department**	材料科学与工程系 Department of Materials Science and Engineering
3.	**课程编号 Course Code**	MSES106
4.	**课程学分 Credit Value**	2
5.	**课程类别 Course Type**	专业选修课 Major Elective Course
6.	**授课学期 Semester**	夏季 Summer
7.	**授课语言 Teaching Language**	中英双语 English & Chinese
8.	**授课教师、所属学系、联系方式（如属团队授课，请列明其他授课教师） Instructor(s), Affiliation& Contact （For team teaching, please list all instructors）**	（授课老师姓名、职称、联系方式、所属单位） 沈洋，教授，shyang_mse@tsinghua.edu.cn，清华大学材料学院 高鹏，研究员，pengg@pku.edu.cn，北京大学 罗震林，副研究员，zlluo@ustc.edu.cn，中国科学技术大学 王杰，教授，jw@zju.edu.cn，浙江大学 谭丛兵，讲师，cbtan@xtu.edu.cn，湖南科技大学 Prof. Shen, shyang_mse@tsinghua.edu.cn, School of Materials Science, Tsinghua University Dr. Gao, pengg@pku.edu.cn, Peking University Dr. Luo, zlluo@ustc.edu.cn, University of Science and Technology of China Prof. Wang, jw@zju.edu.cn, Zhejiang University Dr. Tan, cbtan@xtu.edu.cn, Hunan University of Science and Technology
9.	**实验员/助教、所属学系、联系方式 Tutor/TA(s), Contact**	待公布 To be announced
10.	**选课人数限额(可不填) Maximum Enrolment**	

（Optional）					
11. 授课方式 Delivery Method	讲授 Lectures	习题/辅导/讨论 Tutorials	实验/实习 Lab/Practical	其它(请具体注明) Other（Please specify）	总学时 Total
学时数 Credit Hours	32				32
12. 先修课程、其它学习要求 Pre-requisites or Other Academic Requirements	无 NA				
13. 后续课程、其它学习规划 Courses for which this course is a pre-requisite					
14. 其它要求修读本课程的学系 Cross-listing Dept.					

教学大纲及教学日历 SYLLABUS

15. 教学目标 Course Objectives

1. 掌握功能氧化物材料的基本结构特征，了解其功能特性与结构关联规律，了解功能氧化物材料的重要作用及其发展趋势；
2. 掌握材料对电子散射的主要特征、电子显微镜的工作原理及主要工作模式，了解电子显微学和谱学方法在氧化物薄膜材料体系中的常见应用；
3.掌握 X 射线衍射基础知识、了解其在薄膜材料结构表征方面的应用；
4. 了解基于密度泛函理论的第一性原理计算方法及其在氧化物信息功能材料的电子、结构和能量特性计算与模拟中的应用，掌握氧化物信息功能材料的热力学理论，利用相场动力学理论模拟铁电和铁磁材料畴结构演化；
5. 掌握压电力显微镜的工作原理及其在氧化物铁电和铁磁薄膜材料辅助生长和性能表征中的应用，了解氧化物信息功能材料在信息存储器件中的应用。

1. Master the basic structural characteristics of functional oxide materials, understand structure-function relationship of functional oxides, understand the important role and development trend of functional oxide materials;
2. Master the main characteristics of electron scattering, the operating principles and main operating modes of electron microscopy, and understand the common applications of electron microscopy and spectroscopy methods in oxide thin films;
3. Master the basic concepts of X-ray diffraction and understand its application in the structure characterization of thin film materials;
4. Understand first-principles calculation methods based on density functional theory and their applications in the calculation and simulation of electronic, structural and energy properties of functional oxide materials, master the thermodynamic theory of functional oxide materials, and the simulation of the ferroelectric and ferromagnetic domain evolution using the phase field theory;
5. Master the principle of piezoresponse force microscopy and its application in the assisting growth and performance characterization of the ferroelectric and ferromagnetic oxide thin film materials, and understand the application of functional oxide materials in information storage devices.

16. 预达学习成果 Learning Outcomes

1. 掌握功能氧化物材料的基本概念，结构-性能关联分析方法；

2. 掌握利用电子衍射来标定局域晶体结构，能够解释分析常见的电镜图像衬度，学会常见谱学方法的应用；

3. 掌握 X 射线衍射原理及其在氧化物信息功能材料结构表征方面的应用；

4. 掌握利用第一性原理计算方法计算常见氧化物信息功能材料的基本电子、结构和能量特性，能够从热力学自由能得到铁电和铁磁材料的本征多场耦合特性；掌握运用相场动力学模型模拟简单的铁电和铁磁材料畴结构；

5.掌握压电力显微镜辅助氧化物铁电薄膜生长和表征方法，初步认识氧化物信息功能薄膜在信息存储器件中的应用。

1. Master the basic concepts of functional oxide materials, structure-function relationship and analysis methods;

2. Master the use of electron diffraction to calibrate the local crystal structure, be able to interpret and analyze the contrast of common electron microscope images, and learn the application of common spectroscopic methods;

3. Master the principle of X-ray diffraction and its application in the characterization of the structure of functional oxide materials;

4. Master the basic electronic, structural and energy characteristics of common functional oxide materials using first-principles calculation methods, and be able to obtain the intrinsic multi-field coupling characteristics of the ferroelectric and ferromagnetic materials from the thermodynamic free energy; Mastering the simulation of the domain structure of the ferroelectric and ferromagnetic materials using the phase field dynamics model;

5. Grasp the growth and characterization methods of oxide ferroelectric thin films assisted by piezoresponse force microscopy, and understanding of the basic application of functional oxide materials in information storage devices.

17. 课程内容及教学日历（如授课语言以英文为主，则课程内容介绍可以用英文；如团队教学或模块教学，教学日历须注明主讲人）
Course Contents (in Parts/Chapters/Sections/Weeks. Please notify name of instructor for course section(s), if this is a team teaching or module course.)

1. 功能氧化物材料基本概念及构效关系（共 4 学时）

1）功能氧化物材料基本概念及其应用（2 学时）：晶体结构、信息能源领域的重要意义；

2）构效关系及举例（2 学时）：结构-性能关联、热/电/磁性能调控举例。

2. 电子散射（TEM）基础（共 8 学时）

1）电子散射与显微学导论（1 学时）：弹性与非弹性散射；空间分辨率；像差矫正技术；单色仪技术

2）电镜的结构与样品制备（1 学时）：电子枪；磁棱镜；电子探测器；原位技术；纳米结构样品；截面样品；平面样品；FIB 制样；

3）电子衍射与成像（4 学时）：选区电子衍射；会聚电子衍射；菊池线；明场像；暗场像；高分辨像；扫描透射像；原子像；

4）非弹性电子散射 （2 学时）：能谱；电子能量能损谱；芯电子跃迁；晶格振动

3. X 射线衍射基础（共 8 学时）

1）晶体结构基础知识（2 学时）：晶体、晶格（正格子）、基元、晶胞、晶系、倒格子

2）X 射线简介（2 学时）：X 射线源、X 射线与物质的相互作用、X 射线弹性散射；波粒二象性；光的波动性；双缝衍射、光栅；劳厄衍射、布拉格衍射、Ewald 作图法

3）X 射线散射（2 学时）：单电子散射、单原子散射（原子散射因子）、晶胞的散射（结构因子）、晶体的散射、结构消光

4）薄膜衍射(表面衍射)的一些例子及前沿（2 学时）

4. 氧化物信息功能材料多尺度模拟（共 8 学时）

1）密度泛函理论及第一原理计算（3 个学时）：多粒子系统的哈密尔顿量、薛定谔方程、密度泛函理论、多电子波函数、赝势、平面波展开法、交换关联泛函、局域密度近似(Local Density Approximation)、广义梯度近似（Generalized Gradient Approximation）、杂化泛函 （Hybrid Functionals）；采用 VASP 软件计算常见氧化物信息功能材料的电子、

结构和能量特性。

2）氧化物铁电和铁磁材料的热力学理论（2 学时）：铁电性和磁性的微观起源、铁电材料的一级和二级相变、Landau-Devenshire 理论、铁磁相变、铁电和铁磁相变的热力学描述、微磁理论、电致伸缩、磁致伸缩、磁晶各向异性能

3）氧化物铁电和铁磁材料微结构演化的相场建模与模拟（3 学时）：Time-dependent Ginsburg-Landau 方程、应力平衡方程、Maxwell 方程、铁电和铁磁材料的相场模型、 相场方程的数值求解、磁电畴结构、拓扑磁电畴结构，磁电畴结构在外场作用下演化的相场模拟

5. 氧化物信息功能材料与器件（共 4 学时）

1）氧化物信息功能薄膜及制备方法（1 学时）：氧化物薄膜的物理化学制备原理与方法，激光脉冲沉积方法；

2）氧化物外延薄膜生长与原子力显微镜辅助制备（1 学时）：薄膜外延生长动力学、原子力显微镜辅助生长、氧化物外延薄膜结构调控；

3）压电力显微镜测试（1 学时）：铁电性及其物性、铁电畴和畴翻转、铁电体的特性、压电力显微镜工作原理及其在铁电和磁电薄膜中的表征

4）信息功能器件（1 学时）：铁电随机存储、铁电场效应存储、极性拓扑结构信息存储。

1. Basic concepts and structure-function relationship of functional oxide materials (4 Credit hours in total)

1) Basic concepts of functional oxide materials and their applications: Crystal structure, important significance in the field of information and energy; (2 hours)

2) Structure-function relationship and examples; Thermal-, electrical-, and magnetic-properties manipulation and examples. (2 hours):

2. Fundamentals of electron scattering (8 Credit hours in total)

1) Introduction to electron scattering and transmission electron microscopy (TEM): Elastic and inelastic scattering; Spatial resolution; Aberration correction technology; Monochromator technology; (1 Credit hour)

2) Electron microscope structure and sample preparation: Electron gun; Magnetic prism; Electronic detector; In-situ technology; Nanostructured samples; Cross-sectional TEM sample; Plan-view TEM sample; FIB sample preparation; (1 Credit hour)

3) Electron diffraction and imaging: Selected area electron diffraction; Convergent electron diffraction; Kikuchi lines; Light field image; Dark field image; High resolution image; Scanning transmission image; Atomic resolution image; (4 Credit hours)

4) Inelastic electron scattering: Energy spectrum; Electron energy loss spectrum; Core electron transition; Lattice vibration;(2 Credit hours)

3. Fundamentals of X-ray Diffraction (8 Credit **hours in total)**

1) Basic concepts of crystal structure: lattice and basis; unit cell; the seven primitive crystal systems; reciprocal lattice; (2 Credit hours)

2) Introduction to X-ray: X-ray source; Interaction with matter, X-ray elastic scattering; Wave-particle duality; wave of light; Double-slit and multi-slit interference; grating; Bragg's Law diffraction; Laue condition; Ewald sphere; (2 Credit hours)

3) X-ray scattering: Single electron scattering; Single atom scattering (atomic scattering factor); unit cell scattering (structure factor); Crystal scattering; extinction; (2 Credit hours)

4) Some examples and frontiers of thin film diffraction (surface diffraction). (2 Credit hours)

4. Multi-scale simulation of functional oxide materials (8 Credit hours in total)

1) Density functional theory and First-Principle calculation: Hamilton; Schrodinger equation; Density functional theory; Multi-electron wave function; Pseudopotential; Plane-wave expansion method; Exchange correlation function; Local density approximation; Generalized gradient approximation; Hybrid function; Calculations of the electronic, structural

and energy characteristics of functional oxide materials using VASP software; (3 Credit hours)
2) Thermodynamic theory of oxides ferroelectric and ferromagnetic materials: Microscopic origin of ferroelectric and magnetic properties, First- and second-order phase transitions in ferroelectric materials; Landau-Devenshire theory; Thermodynamic description of ferroelectric and ferromagnetic phase transitions; Micromagnetic theory; Electrostriction; Magnetostriction; Magneto-crystalline anisotropic energy; (2 Credit hours)
3) Phase field modeling and simulation of microstructure evolution of oxide ferroelectric and ferromagnetic materials: Time-dependent Ginsburg-Landau equation; Stress balance equation, Maxwell equation; Phase field model of ferroelectric and ferromagnetic materials; Numerical solution of phase field equation; Magneto-electric domain structure; Topological magneto-electric domain structure; Phase field simulation of evolution of magneto-electric domain structure under the action of external field. (3 Credit hours)
5. Oxide information functional materials and devices (4 Credit hours in total)
1) Oxide information functional thin films and preparation methods: Principles and methods of Physical- and chemical-preparation of oxide thin films; Pulsed laser deposition; (1 Credit hour)
2) Growth of oxide epitaxial films and atom force microscopy (AFM)-assisted preparation: Growth kinetics of oxide epitaxial films; AFM-assisted growth; Structural manipulation of oxide epitaxial films; (1 Credit hour)
3) Measurements of piezoresponse force microscopy: Ferroelectricity and its properties; Ferroelectric domain and domain switching; Principle of piezoresponse force microscopy and its applications in ferroelectric and magnetoelectric thin films; (1 Credit hour)
4) Information function device: Ferroelectric random storage, Ferroelectric field effect transistor; Information storage based on polar topological structure. (1 Credit hour)

18. 教材及其它参考资料 Textbook and Supplementary Readings

1. 钟维烈，《铁电体物理学》科学出版社 （2019）
2. 封东来翻译版本：Elements of modern x-ray physics
3. 王杰等，材料微结构演化的相场模拟，固体力学学报 37：1-33（2016）
4. David B. Williams&C. Barry Carter, Transmission Electron Microscopy: A Textbook for Materials Science （或李建奇的中文译本）

课程评估 ASSESSMENT

19. 评估形式 Type of Assessment	评估时间 Time	占考试总成绩百分比 % of final score	违纪处罚 Penalty	备注 Notes
出勤 Attendance		50%		
课堂表现 Class Performance		20%		
小测验 Quiz		0		
课程项目 Projects		0		
平时作业 Assignments		0		
期中考试 Mid-Term Test		0		
期末考试 Final Exam		0		
期末报告 Final Presentation		30%		

其它（可根据需要改写以上评估方式） **Others (The above may be modified as necessary)**		0		

20. 记分方式 **grading system**

☑ A. 十三级等级制 **Letter Grading** ☐ B. 二级记分制（通过/不通过） **Pass/Fail Grading**

课程审批 Review and Approval

21. 本课程设置已经过以下责任人/委员会审议通过
This Course has been approved by the following person or committee of authority
