PG Courses at the

Department of Materials Science & Engineering

IIT Kanpur

This document contains following information

1. Details of the compulsory courses for the M.Tech. Programme
2. Details of the courses for each of the three streams
    a. **Structure-Characterization-Property**
    b. **Metals Processing**
    c. **Functional Materials**
3. Details of the courses other than the above three streams

Updated on 23rd July 2013

1. Details of the compulsory courses for the M.Tech. Programme

Department of Materials Science and Engineering
Indian Institute of Technology Kanpur

Course Name: ***Structure and Characterization of Materials***
Credits: 3-0-0-0-4
Course No: MSE 615

Prerequisite: None
Category: Compulsory course for all M.Tech. students of MSE Department, to be offered in odd semester

Course Contents:

Basic crystallography and crystal structures (8 Lectures hours)	**Lecture Hours**
Periodic patterns, Lattices, Motif, Unit cells, Crystal structure, Primitive and Non-primitive cells	1
Symmetry elements and point group notations	1
Crystal systems and Bravais lattices	1
Crystallographic directions and planes, Miller indices and Weiss zone law	1
Streographic projections	1
Bonding in materials and atomic packing in metals, co-ordination number concepts	1
Covalent bonding, glasses and polymers	2
Crystal defects and their significance (12 Lectures hours)	**Lecture Hours**
Point defects and their role in materials Processing, performance and failure	1
Ionically bonded structures: Pauling’s rules and some examples	2
Point defects: thermodynamics, schottkey and Frenkel defect, Kroger-Vink notation, defect interactions	2
Dislocations, burgers vector, types of dislocations	1
Dislocation movement, slip systems, energetics of dislocations and their interactions	2
Planar defects: stacking faults, grain boundaries (low angle and high angle), anti-phase domain boundaries, Twinning	2
Surface defects with relevance to thin films	1
Non-equilibrium structures such as metallic glasses	1
Diffraction and Imaging (14 Lectures hours)	**Lecture Hours**
Phenomena of diffraction	1
Radiation-matter Interactions and response signals	1
X-ray diffraction: powder diffraction, phase identification, Scherrer formula, strain and grain size determination	2
Fundamentals of Imaging: magnification, resolution, depth of field and depth of focus, aberration and astigmatism	1
Optical microscopy, stereology basics and quantitative analysis	2
Fundamentals of SEM: imaging modes, image contrast, illustrative applications	2
Imaging with TEM: Contrast mechanisms, BF, DF, Weak beam DF images	1
TEM application in crystal defect analysis	1

Electron diffraction in TEM and applications	1
STM, AFM and nanoindentation	2
Spectroscopic Techniques (4 Lectures hours)	**Lecture Hours**
Fundamental basis of Spectroscopic analysis	1
EDS and WDS, EPMA applications	1
X ray Photon Spectroscopy and Auger electron spectroscopy	1
SIMS and EELS	1
Thermal Analysis Techniques (2 Lectures hours)	**Lecture Hours**
DSC/DTA/TGA/Dilatometry	2
TOTAL LECTURE HOURS	**40**

References:

1. Crystals and Crystal structures, R.J.D. Tilley, John Wiley and Sons, 2006
2. Materials Science and Engineering – W.D. Callister, Jr.Wiley India(P) Ltd., 2007
3. Materials Science and Engineering, G.S. Upadhyaya and Anish Upadhyaya, Viva books, 2010
4. Fundamentals of Materials Science-the microstructure-property relationship using metals as model systems, E.J. Mittemeijer, Springer, 2010
5. Microstructural Characterization of Materials – D. Brandon and W.D. Kaplan, John Wiley and Sons, 2008
6. Science of Microscopy, P.W. Hawkes and J.C.H. Spence, Springer, 2007
7. Scanning Electron Microscopy & X-Ray Microanalysis, J.Goldstein et.al, Springer, 2003
8. Transmission Electron Microscopy – B.D.Williams & C.B.Carter, Springer, 2009
9. Surface Analysis methods in materials science, Editors: D.J.O'Connor, B.A. Sextton, R.St. C. Smart, Springer, 2003.
10. Materials Characterisation Techniques, S. Zhang, Lin Li and Ashok Kumar, CRC Press, 2009

Department of Materials Science and Engineering
Indian Institute of Technology Kanpur

Course Name: **Transport Phenomena**
Credits: 3-0-0-0-4
Course No: MSE 626

Prerequisite: None
Category: Compulsory course for all M.Tech. students of MSE Department, to be offered in odd semester

Course Contents:

1. Fluid dynamics (7 Lectures)

Introduction to Transport phenomena in materials processing	1L
Newton's law of viscosity , equation of continuity, Navier Stokes equations	2L
Macroscopic mass and energy balance ;	1.5
Characteristics of industrial flows	0.5L
Numerical problems on above topics of interest to metals and materials processing	2L

2. Heat transfer (16 lectures)

Fundamentals of conduction heat transfer; Laws and equations; Steady and unsteady heat conduction	2L
Numerical problems on conductive heat transfer	3L
Fundamentals of convective heat transfer; free and forced convective heat transfer, Convective heat transfer rate laws and heat transfer coefficient	1L
Problems on Convective heat transfer	2L
Fundamentals of Radiation heat transfer and rate laws; view factors	3L
Problems on Radiation heat transfer	1L
Application of heat transfer in: Heat treatment, solidification, cooling of slabs, heat flow through refractory walls etc.	3L

3. Mass Transfer (16 lectures)

Fundamentals of diffusion; rate laws, Uphill diffusion and Kirkendal's effect, steady and unsteady diffusion	4L
Numerical problems on diffusion mass transfer	2L
Fundamentals of convective mass transfer; free and forced convective mass transfer transfer, Convective mass transfer, rate laws and mass transfer coefficient	2L
Problems on Convective mass transport	2L
Application of mass transfer in: case hardening, doping of semi conductors, homogenization, oxidation, absorption/desorption of gases in liquid metals.	6L

Recommended Text books:

1. Transport phenomena: D. R. Geiger and G. H. Poirier
2. Transport phenomena: D. R. Gaskel
3. Engineering in process metallurgy: R.Guthrie
4. Mass transport in solids and fluids: D. S. Wilkinson

Recommended Reference books:

1. Diffusion in solids: P. G. Shewman
2. Atom movements - diffusion and mass transport in solids: J. Philibert
3. Diffusion in solids: field theory, solid-state principles, and applications: M. E. Glicksman

Department of Materials Science and Engineering
Indian Institute of Technology Kanpur

Course Name: ***Thermodynamics of Materials***
Credits: 3-0-0-0-4
Course No: MSE 616

Prerequisite: None
Category: Compulsory course for all M.Tech. students of MSE Department, to be offered in odd semester

Course Content

Topics	No of Lectures
Thermodynamic systems and variables.	1
First, second and third laws of thermodynamics.	7
Statistical interpretation of entropy.	2
Free energy functions and criteria for equilibrium.	2
Thermodynamics of solutions. Ideal and non-ideal solutions, Partial and molar quantities	2
Quasi-chemical model and regular solutions,	2
Polynomial expressions for excess Gibbs energy of mixing for binary and higher order solutions. Multi-component dilute solutions and interaction parameters.	2
Chemical reaction equilibrium, equilibrium constant; applications to materials and metallurgical systems.	4
Electrochemical systems, cell reactions and EMF, Formation and concentrations cells.	3
Phase rule and binary phase diagrams	2
Free energy composition diagrams	3
Phase equilibrium calculations	5
Introduction to ternary phase diagrams.	1
Thermodynamics of interfaces; Surface tension and surface energy	2
Absorption and adsorption; Gibbs Thompson effect	2
TOTAL LECTURE HOURS:	**40**

Suggested Books:

1. Chemical Thermodynamics of Materials by C.H.P. Lupis
2. Introduction of Metallurgical Thermodynamics by D.R. Gaskell
3. Thermodynamics of Solid by R.A. Swalin
4. Physical Chemistry of Metals by L.S. Darken and R.W. Gurry

Department of Materials Science and Engineering
Indian Institute of Technology Kanpur

Course Name: *Mathematics and Computational Methods*
Credits: 3-0-0-0-4
Course No: MSE 617

Prerequisite: None
Category: Compulsory course for all M.Tech. students of MSE Department, to be offered in odd semester

Course Content

S. No	Topics	# of Lectures
1	Introduction of functions, vectors, matrices	**1**
2	Partial Differentiation (Total differentiation, Maximum and minimum: method of Lagrange multipliers, Change of variables: Legendre transformation, Differentiation of integral; Leibniz rule)	**2**
3	Multiple Integration (Change of variable: Jacobian, Surface and volume integrals)	**2**
4	Vectors (Geometry: Lines and planes, Directional derivative, gradients (fields, equipotential, grad, normal to surface, curl, div), Line integration (conservative fields, potential, exact differentiation), Green, Stokes, Div and Curl theorems	**4**
5	Coordinate Transformation (Linear transform, Orthogonal transform, Eigen values: diagonalization of matrix)	**3**
6	Ordinary differential equations (Linear first order, Second order: constant coefficient and zero right hand side, Second order: constant coefficient and non zero right hand side)	**4**
7	Statistics a. Introduction to random experiment, computing probability of an event, conditional probability and independence of events b. Optimum design of experiments; smoothening and reconciliation of data c. Concept of distribution, parameters of distributions; moment generating functions d. Regression analysis (linear and non linear) e. Confidence intervals, Hypothesis testing f. Error analysis	**12**

8	Numerical Techniques a. Roots of a equation (Bisection, Newton raphson) (1L) b. Integration (1L) c. Solution of linear equations (one exact, one iterative method) (3L) d. Interpolation and extrapolation (1L) e. Solution of a differential equation by finite difference method (4L)	**12**
Total		**40**

Suggested Books:

1. Mathematical Methods in Physical Sciences, Mary L. Boas
2. Numerical Methods in Engineering, S. K. Gupta

2. Details of the courses for each of the three streams

Stream: **Structure-Characterization-Property**

Sl. No.	**Course Title**
1	**MSE638** Symmetry and Properties of Crystals
2	**MSE 694N** Nanostructures and Nanomaterials: Characterization and Properties
3	**MSE 639** Interfaces and Materials Properties
4	**MSE 676** Materials Failure: Analysis and Prevention
5	**MSE 642** Microscopy and Microanalysis of Materials
6	**MSE 658** Dislocations and Plasticity

MSE638
Symmetry and Properties of Crystals

Course structure and credits : 3-0-0-4
Prerequisite **:** Consent of Instructor

Objectives

At the end of the course the student should be able to attain the following objectives.

1. A thorough understanding of crystallographic symmetry in 2-D, which will include the 2D lattices, point groups and plane groups
2. An understanding of the basis of Bravais Lattices, 3D point groups and space groups.
3. An overview of tensors and their use in the representation of the physical properties of crystals.
4. Applications to pyroelectricity, dielectric constant, piezoelectricity, elasticity and other symmetry dependent properties, such as, optical properties, conductivity, ferroelectricity.

Suggested books (Complete references)

1. M.J. Buerger, Elementary Crystallography.
2. International Tables of Crystallography A, International Union of Crystallography
3. J. F. Nye, Physical Properties of Crystals (1995), Oxford Science Publications
4. D.R. Lovett, Tensor Properties of Crystals (1999), Institute of Physics Publishing
5. Robert E. Newnham, “Properties of Materials: Anisotropy, Symmetry, Structure”, Oxford Pr.

Lecture Outline

TOPICS	No. of Lectures
Introduction - Symmetries in 1D, 2D and 3D - Examples of patterns showing various symmetries	**1**
Symmetries and Lattices in 2D space - Operations of Translation, Rotation and Reflection, standard symbols - Lattices and Unit Cells - Permissible rotational symmetries - Derivation of lattices: oblique, rectangular, centred rectangular, square, hexagonal	**2**
Point Groups in 2D - Set of symmetry operations - Group Theory Essentials - Evolution of 2D crystallographic point groups	**4**
2D Space Groups (Plane Groups) - Glide Planes: combination of lattice translation and reflection - Derivation of all the 17 plane groups - Understanding the Plane Group entries in the International Tables of Crystallography	**6**
3D Point Groups - Combination of rotation axes in 3D - Development of the 32 point groups - Laue Groups	**4**
3D Bravais Lattices - Addition of a third translation to the plane groups - Derivation of Bravais Lattices	**2**
3D Space Groups - Screw Axes: combination of lattice translation and rotation - Development of the 230 space groups - Understanding the Space Groups entries in the International Tables of Crystallography	**4**
Quasi-crystals	**1**
Tensors and Physical Properties - Definition of a tensor, rank of tensor - Transformation laws for tensors Why Transformation? Axis transformations, Orthoganlity conditions, Eulerian angles, Transofrmation operators for the crysllographic symmetry elements followed by 32 crystal classes - Tensor description of physical properties of crystals - Polar Tensor and Axial Tensor properties - Effect of symmetry on crystal properties - Neumann's Principal - Analytical form of Neumann's principle	**3**

Pyroelectricity (First rank property tensors) - Pyroelectric Tensors - Symmetry Limitations Derivation of the symmetry point groups showing pyroelectricity - Polar Axes and Geometric representation	**2**
Dielectric Constant (Second rank property tensors) - Origin of Dielectric constant - Dielectric tensor - Effect of symmetry Neumann's law - Geometric representation	**2**
Stress and strain (Second rank tensors) - Mechanical Stress - Stress transformation - Strain tensor - Matrix transformation for strain	**1**
Piezoelectricity (Third rank property tensors) - Direct and Converse Piezoelectric Effect - Piezoelectric Modulus Tensor: a third rank tensor - Tensor and Matrix formulations - Matrix transformation and Neumann's Law - Reduction in the number of independent modulii: effect of crystal symmetry - Example: piezoelectric properties of quartz	**3**
Elasticity (Fourth rank property tensors) - Thermal expansion of crystals - Generalized Hooke's Law - Stiffness and Compliance Tensors (fourth rank): inherent symmetry - Tensor and Matrix coefficients - Tensor and Matrix transformations - Effect of crystal symmetry	**3**
Generalized approach to other symmetry dependent tensor properties - Optical properties, conductivity, ferroelectricity, etc.	**2**
Total Lectures	**40**

MSE 694N
Nanostructures and Nanomaterials: Characterization and Properties

Course structure and credits : 3-0-0-4

Prerequisite : Consent of Instructor

Objectives

At the end of the course the student should be able to:

- Have an overview of Nanomaterials, their structure and characterization techniques.
- Have an understanding of the properties of nanomaterials arising from size effect.
- Relating the biological-, ionic/electronic-, optical-, magnetic-, and mechanical- properties of nanomaterials with their structure and performance

References

1. Nanomaterials, Nanotechnologies and Design: an Introduction to Engineers and Architects, D. Michael Ashby, Paulo Ferreira, Daniel L. Schodek, Butterworth-Heinemann, 2009.

2. Handbook of Nanophase and Nanostructured Materials (in four volumes), Eds: Z.L. Wang, Y. Liu, Z. Zhang, Kluwer Academic/Plenum Publishers, 2003.

3. Encyclopedia of Nanoscience and Nanotechnology, Ed.: Hari Singh Nalwa, American Scientific Publishers, 2004.

4. Handbook of Nanoceramics and their Based Nanodevices (Vol. 2) Edited by Tseung-Yuen Tseng and Hari Singh Nalwa**,** American Scientific Publishers.

5. Introduction to Nanoscience, G.L. Hornyak, J. Dutta, H.F. Tibbals, A.K. Rao, CRC Press (2008).

Lecture Outline for MSE 694 N: Nanostructures and Nanomaterials: Characterization and Properties

Topic	Lectures
Overview of Nanostructures and Nanomaterials: classification (Dimensionality, Morphology/ shape/structure of nano-entities, New Effect/ Phenomena). Crystalline nanomaterials and defects therein. Hybrid nanomaterials. Effect of size, structure, mechanism, and property on material performance	5
Multiscale hierarchical structures built out of nanosized building blocks (nano to macro). Eucledian, Hyperbolic and Spherical space structures. Nanostructures: Carbon Nanotubes, Fullerenes, Nanowires, Graphene, Quantum Dots.	3
Thermodynamics of Nanomaterials. Configurational entropy and Gibbs free energy of nanocrystals. Wulff reconstruction. Surface reconstruction and reconfiguration. Adsorption and Absorption.	5
Surfaces and interfaces in nanostructures. Solid/Liquid/Vapour interfaces. Grain boundaries in Nanocrystalline materials, Defects associated with interfaces. Overview of characterization of nanostructures and nanomaterials.	4
Nano-biomaterials: Self assembly of nanomaterials, DNA construct, hydrophobic surfaces, biomimicking, Case studies: Lotus leaf, Gecko feet, Nacre/Bone. Application of nanocomposite biomaterials: artificial biomaterials, antidrag coatings, self-cleaning surfaces, sensors, RNA molecules: Riboswitches	6
Nano-ionics/electronics and nanophotonics: Size quantization effect: Electronic state transition from bulk metal/ semiconductor to small cluster to single molecule. Quantum transport of electrons, Electrical conductance through a single atom, nanowire, nanotubes, Molecular scale electronics: Single molecule transistor. Surface plasmons, Transparent ceramics, transparent conducting oxides. Catalytic activity of nanomaterials: Electro-catalysis in fuel cell	8
Nanomagnetic: Magnetic properties of small magnetic clusters, nanoparticles, Ferrofluid Magnetoelectronics, Spintronics: Tunneling magnetoresistance, Giant magnetoresistance. Superparamagnetism: Magnetism relaxation, Effect of interparticle interaction, surface effects.	4
Nanomechanical: Inverse Hall Petch, Nanoindentation/ Nanoscratching, Deformation Behaviour of Nanomaterials, Effect of length scale, Grain boundary and thermal creep, Tribology	6
TOTAL	**41**

MSE 639
Interfaces and Materials Properties

Course structure and Credits : 3-0-0-4

Prerequisite : Consent of Instructor

Course Outline:

Surfaces and interfaces play extremely important role in determining the physical properties of materials. These become of critical important especially when materials approach nanoscale dimensions such as in the form of thin films and nanostructures. The objective of this course is to provide the UG/PG students of MSE department a background on the nature of various interfaces (Solid-Vapour, Solid- Liquid and Solid-Solid), their thermodynamics, their interactions, nature of defect surfaces and domains. Special emphasis will be paid towards understanding of the homophase (e.g. grain boundaries) and heterophase systems (e.g. epitaxial films). As part of case studies, the contents will elucidate a few metal and ceramic interface systems vis-à-vis their impact on the functional properties. Finally, the students will be exposed to the surface modification techniques that affect these interfaces and their functionality.

References:

1) Interfaces in Materials: Atomic Structure, Thermodynamics and Kinetics of Solid-Vapor, Solid-Liquid and Solid-Solid Interfaces, James M. Howe, Wiley-Interscience
2) Physics and chemistry of interfaces By Hans-Jürgen Butt, Karlheinz Graf, Michael Kappl, Wiley-VCH
3) Physics of surfaces and interfaces, H. Ibach, Springer.
4) Solid surfaces, interfaces and thin films, Hans Lüth, Springer.
5) Physical Chemistry of Surfaces, Arthur W. Adamson, Wiley-Interscience

Lecture Outline

Topic	**#Lec**
1) **Introduction to the interfaces: basic classification and definitions**	1
2) Basics of Energetics • Definitions and relations to physical properties • Broken bond model • Gamma plot • Wulff plot and construction	4
3) Solid-Vapour interfaces • Surface structure (Terraces, ledges and kinks) and defects • Surface relaxation and reconstruction • Phase transformations • Crystal growth from vapour (Nucleation and Growth, Vicinal surfaces) • Surface films	6
4) Solid-Liquid Interfaces • Structure and properties of liquids • Interfacial structure and energy • Crystal growth • Solute partitioning and morphological stability • Electrical aspects of surfaces and surface chemistry such as electrical double layer, zeta potential	6
5) Solid-Solid Interfaces **a) Types of solid-solid interfaces and basics** **b) Home-phase Interfaces** • Grain boundary structure and energy • Types of grain boundaries and dislocation models • Stacking Fault and Twin Boundaries • Grain Boundary Segregation • Grain boundary and twin boundary equilibria • Domains in ferroelectric and ferromagnetic systems: energetic **c) Hetero-phase Interfaces** • Interphase boundaries	10

• Coherent and semcoherent interphase boundaries and their energetic • Roughening and Phase transformations on interphase boundaries • Antiphase Boundaries • Interfaces between differences materials and structures • Terrace-ledge and kink models • Growth, morphology and segregation at the heterophase interfaces	
6) Interfaces and Functional Behaviour: Case Studies • Effect of interfaces in mechanical properties o Effect on the strength of materials o High temperature behaviour: Creep o Grain boundary engineering, sliding and migration o Fracture of metals and alloys: surface embrittlement, grain boundary embrittlement, failure of ceramics and interface strengthening o Friction and adhesion • Electrical Properties o Role of interfaces in conduction in metals and ceramics o Interfaces effects in dielectrics, ferroelectrics and piezoelectrics and their thin films and heterostructures, domains and grainboundaries o Heterostructures, strain and epitaxy and their effects on functional behavior • Interface effects on the magnetic properties of bulk magnetic materials and thin film devices • Interfaces in optical devices with emphasis on the solar cells and displays	10
7) **Surface modification and impact on properties**	3
Total	**40**

MSE676
Materials Failure: Analysis and Prevention

Course structure and credits **:** 3-0-0-4
Prerequisite **:** Consent of Instructor

Course Objective: Materials failure has to be understood through a systematic analysis so that the weak link in the design-fabrication-performance chain can be identified and efforts in control/prevention of failures can be implemented. Failure analysis has grown over the year by trying to answer basic questions like: Why materials failure occurs? Can we predict failures? How best one can prevent common failures? etc.

Failure analysis is a fascinating subject as probing failures calls for application of a wide range of ideas and techniques in 'Materials Science and Engineering'. This course intends to be a 'Primer' to an highly applied field involving many technical concept and sophisticated experimental techniques. Many illustrative and interesting cases studies will be considered to give a comprehensive feel about the topic.

Lecture Outline

TOPICS	Lectures
Engineering Aspects of Failure and Failure Analysis General Practice in failure Analysis: Categories of failure, Importance of failure prevention -	**2**
Tools and techniques in failure analysis: General Practices, Photography, X-rays techniques, Mechnical property evaluations, Metallographic techniques, Fractography, Non-destructuive testing technique	**6**
Failure mechanisms and modes: Fracture modes, Ductile fracture of metallic materials and their interpretations, factors affecting ductile-brittle relationships. (2 Lectures) Brittle fracture in normally ductile metallic alloy, microstructural aspects of brittle fracture (1 Lectures) Failure characteristics of Ceramics and Plastics (2 Lectures) Fatigue fracture, macroscopic and microscopic characteristics, statistical aspects of fatigue, Fatigue failure prediction and life assessments (2 Lectures) Wear Failures and Prevention. (2 Lectures) Corrosion related failures, Stress corrosion cracking, Hydrogen damage and embrittlement, Biological corrosion failures. (2 L) Elevated temperature failures, creep and stress rupture, metallurgical instabilities (2 L) Distortion failures and deformations (1 Lectures) -	**12**
Examples of engineering failure Improper processing practice: Casting, metal working, welding, etc., Improper heat treatment: Gears, locomotive axle, shafts, etc. Improper design:Tools and dies, integrated circuits etc. Unanticipated service conditions: lifting equipment, reactors, etc. Improper material selection: Orthopedic implants, pressure vessels etc. Improper service condition: Pipelines, mechanical fasteners etc.	12
Comprehensive failure analysis illustration At least two cases based on aircraft crash, ship sinking, boiler blast, space mission failure, industrial catastrophe etc. (6 hours)	**6**
Total Lectures	**40**

Reference books:

1. Source book in failure analysis, American Society of Metals, Metals Park, Ohio, 1974.
2. Understanding how components fail, D.J Wulpi, ASM International, The Materials Information Society, 1999.
3. A.J. McEvily, Metal Failures: Mechanisms, Analysis, Prevention, John Wiley and Sons, 2002.
4. Practical engineering failure analysis, H.M. Tawancy, A. Ul-Hamid and N.M. Abbas, Marcel Dekker, New York, 2004.
5. Failure analysis and prevention, Volume 11, ASM Handbook, The Materials Information Society, 2002.
6. Failure analysis of engineering structures: Methodology and case histories, V. Ramachandran, A.C. Raghuram, R.V. Krishnan and S.K. Bhaumik , ASM International, 2005.
7. Failure analysis of Engineering Materials, Charles R. Brooks and Ashok Choudhury.

MSE642
Microscopy and Microanalysis of Materials

Course structure and Credits **:** 3-0-0-4
Prerequisite of the course **:** Consent of Instructor

Objectives

At the end of the course the student should be able to attain the following objectives.

1. An exposure to a range of the basic characterisation techniques in the study of materials.
2. Good appreciation of the experimental data acquisition, interpretation, documentation and presentation.
3. An over all idea of the appropriate technique to adopt for a characterisation problem on hand.
4. One should a able to easy appreciate and understand research publication and presentation related to the techniques discussed.

Suggested Text/reference books:

1. Fundamental of light microscopy and electronic imaging, D.B. Murphy, Wiley-Liss, 2001
2. Microstructural Characterization of Materials – D. Brandon and W.D. Kaplan, John Wiley and Sons, 2008
3. Scanning Electron Microscopy & X-Ray Microanalysis, J.Goldstein et.al, Springer, 2003
4. Transmission Electron Microscopy – B.D.Williams & C.B.Carter, Springer, 2009
5. Science of Microscopy, P.W. Hawkes and J.C.H. Spence, Springer, 2007
6. Surface Analysis methods in materials science, Editors: D.J.O'Connor, B.A. Sextton, R.St. C. Smart, Springer, 2003.
7. Materials Characterisation Techniques, S. Zhang, Lin Li and Ashok Kumar, CRC Press, 2009
8. Fundamentals of Materials Science-the microstructure-property relationship using metals as model systems, E.J. Mittemeijer, Springer, 2010

Lecture Outline

1	**Advanced Optical microscopy** • Special microscopy techniques and applications: Bright field and dark field imaging; confocal microscopy; interference microscopy; polarized light microscopy; phase contrast microscopy. • Scanning near field laser microscopy • Image processing and quantification	4
2	**Scanning electron microscope** • Basis of image contrast and various operating modes in SEM SE and BSE, X-ray, EBIC, cathodoluminescence, voltage contrast mode, Magnetic contras tmode. (2) • Environmental SEM, Low voltage SEM, and applications (1) • Electron back scattered diffraction /OIM: Basic principles, the micro-textural data acquisition and analysis, applications (3) • Fractography and failure analysis (2)	8
3	**Transmission electron microscope** • Wave properties of electrons, lens defects, aberration corrected TEM and sub-Angstrom resolution (2L) • Origin of contrast: mass-thickness contrast, diffraction contrast and crystal defect analysis. Dynamic diffraction and anomalous absorption effects, image artifacts (3L) • BF, DF, Weak beam DF images and applications (1L) • Electron Diffraction: SADP, Micro-diffraction, CBED. Diffuse scattering and fine-structure in Diffraction pattern. (2L) • Phase contrast and HRTEM: Contrast transfer function and lattice imaging , Computer simulation of lattice and structural images, Interpretation of images and illustrative examples(2L) • STEM-HAADF imaging, information limit (1L) • Lorentz microscopy and holography (1) • Specimen preparation: Mechanical thinning, electrochemical thinning, ion milling, sputter coating and carbon coating, replica methods (2L)	14
4	**Microanalysis in SEM and TEM** • X-ray microanalysis: EDS and WDS: Basic principles and analysis modes (1L) Quantitative analysis and elemental mapping (1L) • Comparisons: EDS vs WDS, quantification in SEM/EPMA vs AEM (1L) • Electron Energy Loss spectroscopy: Limits of detection and resolution (1L) Typical applications in materials analysis (1)	5
5	**Surface Imaging and microanalysis**	10

	• Rutherford back scattering(RBS): principles and applications (1L) • Scanning Tunneling Microscopy (1L) • Atom Force Microscopy (AFM) and different operational mode and typical applications (2) • Focus ion beams (FIB) and TEM sample preparation (1) • X-ray Photoelectron Spectroscopy(XPS): Basic principles and typical application (2) • Auger Electron Spectroscopy (AES): Principle, instrumentation and applications (2) • Dynamic SIMS and static SIMS, principles and applications (2)	
	Total	**40**

MSE 658
Dislocations and Plasticity

Course structure and credits : 3-0-0 -4
Prerequisite: Consent of Instructor

Objectives

At the end of the course the student should be able to:

- Have a broad understanding of defects in materials and their role in determining properties of materials.
- Have an overview of plastic deformation mechanisms and the role of dislocations in plasticity, fracture, fatigue and creep.
- Have a thorough understanding of the structure of dislocations in various crystals and their elastic fields.

References

6. *Introduction to Dislocations*, D. Hull and D.J. Bacon, Pergamon Press, Oxford, 1984.

7. *Theory of Dislocations*, J. P. Hirth and J. Lothe*,* McGraw–Hill, New York, 1968.

8. *Crystal Defects and Crystalline Interfaces*, W. Bollmann, Springer-Verlag, Berlin, 1970

9. *Elementary Dislocation Theory*, J. Weertman and J. Weertman, The MacMillian Company, New York, 1964.

10. *http://www.tf.uni-kiel.de/matwis/amat/def_en/*

Lecture Outline

Topic	Lectures
Overview of defects in Materials - (point, line, planar and volume defects) and their classification. - Overview of plastic deformation mechanisms	**1**
Point defects: - interaction and distributions - statistical thermodynamics - role in diffusion and deformation.	**4**
Basic understanding of dislocations using physical and computer models: - the Volterra cut - Burgers vector and the Burgers circuit - the line vector - edge, screw and mixed dislocations - Role of dislocations in weakening the crystal and in plasticity.	**4**
Elasticity theory of dislocations: - Stress, strain and displacement fields and energy of a dislocation - Forces on dislocations (including image force) - Interaction between dislocations - Core of a dislocation.	**3**
Motion of dislocations: - The Peierls stress - role of the core structure - interaction of dislocations with other defects (including yield point phenomenon); - kinks; jogs; cross-slip; climb - Temperature and strain-rate dependence of flow stress - Dislocation dynamics and the tensile stress-strain curve.	**5**
Dislocations in FCC Metals: - Partial dislocations (Shockley and Frank partials) - stacking faults - Thompson's tetrahedron	**4**

- Lomer-Cotrell sessile dislocation	
Overview of dislocations in other crystal structures: - HCP metals - BCC metals - ionic crystals - superlattices - covalent crystals.	**2**
Origin and multiplication of dislocations: - dislocations in freshly grown crystals - nucleation of dislocations - multiplication of dislocations (by Frank-Read sources, cross slip and climb) - Grain boundary sources - Recovery and recrystallization.	**4**
Geometrically/structurally necessary dislocations: - low-angle & general grain boundaries - indentation - interfacial dislocations - Twinning including incoherent twins.	**5**
Specific examples of role of dislocations and case studies: - Dislocations in nanocrystals - The Hall-Petch relation and the Inverse Hall-Petch Effect (IHPE) - Dislocations in epitaxial systems - Severe Plastic deformation - Role of dislocations in Creep, Fatigue and Fracture	**8**
TOTAL	**40**

Stream: **Metals Processing**

Sl. No.	Course Title
1	**MSE421** Iron and Steel Making
2	**MSE 422** Selection and Design of Engineering Materials
3	**MSE 670 N** Solidification Processing and Joining
4	**MSE 657** Deformation Processing
5	**MSE 659** Powder Metallurgy
6	**MSE 671** Heat-Treatment and Surface Hardening

For these two UG courses details are not given in this document

MSE 670N
Solidification Processing and Joining

Course structure and credits : 3-0-0-0 [9 credits]
Prerequisite : None

Course Content:
Thermodynamics of solidification, Nucleation and growth, Pure metal solidification, Gibbs-Thomson effect, Alloy Solidification: Mathematical Analysis of redistribution of solute during solidification, Constitutional undercooling, Mullins-Sekerka instability, Dendritic growth, Multiphase solidification: eutectic and peritectic, Structure of casting and ingots, Types of casting, Heat transfer, Design of riser and gating, Joining, different joining processes, Fusion welding, Solidification, heat transfer, fluid flow during
fusion welding, Modelling of solidification under different conditions

Books Recommended:

1. Solidification Processing; Fleming, M.C., McGraw-Hill, N.Y., 1974
2. Solidification of Casting; Ruddle, R.W., Institute of Metals, 1957
3. Solidification and Casting, Davies, G.J., John Wiley and Sons, 1973
4. Science and Engineering of Casting Solidification; Stefanescu, D.M., Kluwar Publications, 2002
5. Fundamentals of Solidification by Kurz, W. and Fisher, D.J., Trans-Tech Publications, Switzerland, 1989
6. Applied Welding Engineering: Process, Codes and Standard; R.Singh,. Elsevier Inc.,2012

Lecture wise distribution of various topics:

Sl.No	Topic	No of lectures
1	Introduction to the course: Relevance of solidification natural and industrial processes and welding	1
2	Thermodynamics of solidification: -Thermodynamics of undercooled melts, Driving force for solidification - Free energy formulation for metastable phase formation	2
3	Nucleation and Growth: -Theory of homogeneous nucleation, -Concept of solid-liquid interfacial energy, Theory of heterogeneous nucleation; -Interface kinetics, growth mechanisms: continuous growth, step wise growth	6
4	Pure metal solidification: -Undercoolings, -Gibbs-Thomson effect	2
5	Alloy solidification: - Solutal undercooling -Mathematical analysis of redistribution of solutes, - Constitutional undercooling, - Mullins-Sekerka instability	6
6	Single alloy phase solidification: -Cellular and Dendritic growth: Cell formation; cell to dendrite transition; -Free dendritic growth, instability of a growing spherical nucleus, -Propagation of dendrite main stem, marginal stability, -Marginal stability	6
7	Multiphase solidification: - Eutectic growth, classification, eutectic range -Peritectic growth: aligned peritectic growth	6
8	Structure of casting and ingots: -Types of casting, Heat transfer - Ingot structure: chill zone, columnar zone, equiaxed zone, continuous casting	3
9	Design of riser and gating: -Gating, Fluidity, Risering pure materials	2
10	Welding -solidification during welding, different types of fusion welding processes, -solid state welding : friction welding, friction stir welding	4
11	Nucleation and growth of phases during welding	1
12	Heat transfer, fluid flow, and solute distribution during welding	2
13	Mathematical modeling of solidification - Phase field modeling - Solidification during welding	2

Total lectures planned=41

INDIAN INSTITUTE OF TECHNOLOGY KANPUR
DEPARTMENT OF MATERIALS SCIENCE AND ENGINEERING

MSE657
Deformation Processing

Course structure and Credits **:** 3-0-0-0 [9 credits]
Prerequisite: None

Course Content:
Slip planes and systems in various crystal systems; Elasticity and Plasticity; Deformation processes including Rolling ;Forging, Extrusion; Drawing and deep drawing etc.; Deformation of plastics and polymers; superplasticity; Formability; Failures;Friction wear and lubrication

Recommended text books:

1. Hosford, W. F., and Cadell, R. M., 2007, *Metal Forming: Mechanics and Metallurgy*, Cambride University Press, Cambridge.
2. George Dieter, 1986, Mechanical Metallurgy, Mc-Graw Hill

Other Sources:

1. http://www.doitpoms.ac.uk/tlplib/metal-forming-2/index.php

Lecture wise distribution of various topics:

Sl.No.	TOPICS		Number of Lectures
1	Introduction	Importance of deformation processes to Industrial Manufacturing	1
2	Fundamentals	Slip planes and systems in various crystal systems	1
		Elasticity and Plasticity	2
		Texture and its effect	2
		Effect of Temperature (Grain Refinement and Growth)	2
3	Processes	Rolling	3
		Forging	2
		Extrusion	3
		Drawing (Wire, Rods, Tube)	3
		Sheet Metal Forming	3
		Deep Drawing	2
		Machining	3
		Deep Drawing and Stamping	1
4	Deformation of Plastics	Deformation processes for plastics and polymers	2
5	Superplasticity	Introduction	1
		Theory of superplasticity and Material Design	2
		Applications	2
6	Failure, Formability, Friction, Lubrication and Wear	Failures, Formability and the Formability Limit Diagrams	3
		Friction, Wear and Lubrication	2

Total lectures planned:40

Powder Metallurgy
MSE 659

Course structure and credits : 3-0-0-0 [9 credits]
Prerequisite : TA201 (MSE)

Course Content:
Powder Production (Chemical Methods, Electrolytic Methods, Atomization, Mechanical Methods), Powder Characterization (Chemical Composition and Structure, Particle Size and Surface Topography, Pyrophorocity and Toxicity), Powder Compaction, Phenomenological Aspects of Sintering, Solid-State Sintering, Analytical Approach to Sintering, Non-Isothermal Sintering, Microstructural Evolution, Liquid Phase Sintering, Stages of Liquid Phase Sintering, Supersolidus Sintering, Activated Sintering, Pressure- Assisted Sintering, Microwave Sintering, Select Case Studies.

Books Recommended:

1. R.M. German, Powder Metallugy Science, 2nd ed. John Wiley, 1999.
2. A. Upadhyaya, G.S. Upadhyaya, Powder Metallurgy: Science, Technology and Materials, 2011.
3. ASM Handbook, Volume 7: Powder Mtal Technologies & Applications (1998)

Lecture wise distribution of various topics :

Sl.No.	Topics	Lectures
1	Introduction 1.1 Powder Production and Characterization 1.2 Powder Compaction 1.3 Sintering 1.4 Full Density Processing 1.5 Secondary Treatments 1.6 Applications	3
2.	Powder Production 2.1 Chemical Methods *Solid-state reduction; hydrometallurgical reduction; ion Exchange method, direct synthesis.* 2.2. Electrolytic Methods 2.3 Atomization Method 2.3.1. Solidification and Microstructural Evolution 2.3.2. Gas Atomization and Water Atomization 2.4 Evaporation Methods 2.5 Mechanical Methods 2.5.1. Basic Aspects 2.5.2. Particle Size Reduction Equipments	5
3.	Powder Characterization 3.1. Chemical Composition and Stucture 3.2. Particle Size and Surface Topography; 3.3. Pyrophorocity and Toxicity 3.4. Powder Production Methods and Characterization	4
4.	Powder Treatment 4.1. Annealing and Diffusion Alloying Al-Si MMCs 4.2. Granulation 4.3. Coating of Metal Powders	2
5.	Powder Compaction 5.1. Die Compaction *Pressing operation, press selection, factors affecting tooling design, tooling materials* 5.2. Warm Compaction 5.3. CIP and Roll Compaction 5.4. Powder Extrusion 5.5. Injection Molding	5
6.	Pressureless Powder Shaping 6.1. Slurry Molding and Slip Casting 6.2. Tape Casting 6.3. Electrophoretic Deposition 6.4. Spray Deformation 6.5. Solid-Preform Fabrication	4
7.	Sintering Theory 7.1. Solid-State Sintering (Pressureless) 7.1.1. Analytical Approach to Sintering 7.1.2. Non-Isothermal Sintering	8

	7.1.3. Microstructural Evolution 7.1.4. Numerical Simulation of Sintering 7.1.5. Phenomenological Aspects of Sintering 7.1.6. Sintering Maps 7.1.6. Sintering Nano-Powders 7.2. Liquid Phase Sintering 7.2.1. Stages of Liquid Phase Sintering 7.2.2. Microstructural Evolution 7.2.3. Supersolidus Sintering 7.3. Activated Sintering 7.4 Pressure-Assisted Sintering 7.4.1. Plastic Yielding Mechanisms 7.4.2. Creep Mechanisms 7.4.3. Viscous Flow Mechanisms 7.5. Electronic Theory of Sintering *Basics; Liquid Phase Sintering, Activated Sintering* *Case Study: Sintering of Refractory Carbides.*	
8.	Sintering Technology 8.1. Rapid Protyping Process 8.3. Sinter Hardening 8,2. Microwave Sintering	3
9.	Select Case Studies	4

Total lectures planned: 38

MSE 671

Heat Treatment and Surface Hardening

Course structure and Credits **:** 3-0-0-0 [9 credits]
Prerequisite: Phase Transformation for UG and None for PG

Course Content:

Introduction, Theory of Heat Treatment, Heat Treatment Environment, Different Heat Treatment Techniques, Fundamentals and Properties; Annealing, Tempering, Hardening, Thermomechanical treatment, Fundamentals of Surface Hardening Treatment, Carburizing, Carbonitriding, Nitriding, Modern surface hardening techniques; Economy of Heat Treatment Processes

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Books Recommended:

1. Principles of Heat Treatment of Steels by R.C. Sharma
2. The Heat Treating Source Book, ASM, 1986
3. Heat Treatment of Metals by W.S. Owen (1963) (Institute for Metallurgists)
4. Engineering Physical Metallurgy and Heat Treatment by Y. Lakhtein (Mir Publisher)
5. Phase Transformations in Metals and Alloys by D.A. Porter and K.E. Easterling (Taylor and Francis)

Lecturewise distribution of various topics

Sl. No	TOPICS	No. of Lectures
1.	Introduction 1.1 Definition 1.2 Aim 1.3 Trends in Heat Treatment Technology	1
2.	Theory of Heat Treatment 2.1 Structure of Metals and Alloys and Materials 2.2 Phase diagram and phase transformation 2.3 Effect of Alloying 2.4 Fundamentals of TTT and CCT diagram 2.5 Microstructure and Properties as a function of Heat Treatment	12
3	Heat Treatment Environment 3.1 Vacuum 3.2. Furnace 3.2 Atmosphere	2
4	Different Heat Treatment Techniques, Fundamentals and Properties 4.1 Annealing 4.1.1 Full and partial annealing 4.1.2 Spheroidizing Anneal 4.1.3 Isothermal Anneal 4.1.4 Normalizing 4.2 Hardening and Quenching 4.2.1 Hardenability 4.2.2 Use of transformation diagram 4.2.3 Fundamentals of Martensite formation 4.3 Tempering 43.1 Tempering of martensite 4.4 Thermomechanical Treatments 4.4.1 Recrystallization and Grain growth 4.5 Heat Treatment of non-ferrous alloys (Al alloys, Ni-based super alloys) 4.5.1 Stages of precipitation and ageing 4.6 Heat Treatment of PM Products	16
5	Fundamentals of Surface Hardening Treatment 5.1 Carburizing 5.2 Nitriding 5.3 Carbonitriding 5.4 Induction and Flame Hardening 5.5 Laser and Electron Beam Heat Treatment	8
6	Economy of Heat Treatment Processes 6.1 How to design low cost effective and improved heat treatment processes	1

Total Lectures planned=40

Stream: **Functional Materials**

Sl. No.	**Course Title**
1	**MSE604** Science and Technology of Thin Films and Device Fabrication
2	**MSE 624** Energy Materials and Technologies
3	**MSE 628** Electronic Devices and Characterization
4	**MSE 631** Electroceramic Materials and Applications
5	**MSE 693N** Materials Science Technologies for Applications in Life Sciences

MSE604
Science and Technology of Thin Films and Device Fabrication

Course structure and Credits **:** 3-0-0-4
Prerequisite **:** Consent of Instructor

Objectives

To provide the essential basic knowledge related to thin films and device fabrication. Emphasis will be placed on various thin film technologies based on vacuum processes and chemical process followed by detailed discussion on device fabrication including aspects of photolithography, patterning, etching, heat treatment(s), and metallization by considering certain device cases.

Reference Books:

- VLSI Fabrication: S.K. Gandhi
- Si Processing (Volume I and II)
- Lou and Mayer
- Introduction to Microfabrication by Sami Fransilla (Wiley)
- Fundamentals of Microfabrication: The Science of Miniaturization by Marc Madou (CRC Press)
- Thin film deposition by Donald Smith (Mc Graw Hill)
- Materials science of thin films by Milton Ohring (Academic Press)
- Pulsed Laser deposition of thin films by Chrisey and Hubler (Wiley Interscience)

Lecture Outline

Sl. No.	TOPICS	# Lectures
1. Introduction	• Introduction to device processing steps • Examples of various devices (with emphasis on solar cells and MOSFETs) • Need for miniaturization	4
Thin Film Deposition		
2. Basics of thin film growth	• Brief review of kinetic theory • Adsorption and desorption • Film growth: nucleation and growth kinetics • Epitaxy • Thin film growth control	3
3. PVD Processes	• Evaporation (Thermal and e-beam) • Principles of glow discharge and various sputtering processes	5
4. Chemical Growth Processes	• Fundamentals of CVD growth • Modern variants: MOCVD, PECVD and ALD • Spin Coating	4
5. Basic Thin Film Characterization	• Thickness measurement • Phase analysis • Optical analysis • Morphology analysis	1
Device Fabrication		
6. Substrate selection and preparation	• Selection of substrates • Single crystal growth (Silicon) • Role of substrate surface and contaminants • Physical and chemical methods of substrate surface preparation	3
7. Pattern fabrication	• Concepts of lithography • Photoresists (Negative, Positive etc) • Exposure • Development • Masking • Variants of lithography with emphasis on Photo and e-beam • Precautionary steps	5
8. Material Removal	• Wet (Chemical) and dry (Plasma, RIE etc.) etching	5
9. Ion implantation, Doping, oxidation and heat treatment	• Doping and Ion Implantation • Diffusion control of composition in devices • Oxidation and heat treatment	6

10. Metallization and Interconnects	• Adhesion and morphology issues • Introduction to electromigration vis-à-vis metallization: Impact on device performance and methods of prevention •	2
11. Process Integration for a particular case (take the case of a device)	• Example of process integration for a particular kind of device e.g. Si Solar Cell, MOSFET, III-V solar cell devices	4
Total		**42**

MSE 624

Energy Materials and Technologies

Course structure and Credits : 3-0-0 -4

Prerequisite : Consent of Instructor

Objectives

To provide the fundamental knowledge for understanding concepts of different technologies based on electronic devices. Focus in this course will be on manufacturing techniques and materials selection.

Reference Books:

1. Handbook of Photovoltaics Science and Technology, By Antonio Luque and Steven Hegedus
2. Physics of Solar Cells, By Jenny Nelson
3. Physics of solar cells: from basic principles to advanced concepts, By Peter Würfel and Uli Würfel
4. Organic photovoltaics: materials, device physics, and manufacturing technologies, By Christoph J. Brabec, Vladimir Dyakonov, Ullrich Scherf
5. Principles of Solar Cells, LEDs and Diodes: The Role of the PN Junction, By Adrian Kitai
6. Electroceramics: materials, properties, applications by A.J. Moulson and J.M. Herbert
7. Electroceramics-based MEMS: fabrication-technology and applications, By Nava Setter

Lecture Outline

Sl. No.	TOPICS	Number of Lectures
Introduction	Relevance of renewable energy generation, conservation and harvesting vis-à-vis environmental concerns (Energy requirement of society and depleting fossil fuels; Break-up of various renewable energy sources and consumption patterns)	1
Optoelectronic devices	Solar cell device physics LED device physics	4
Generation: Photovoltaic technologies	Solar energy: amount of energy available area wise; Available solar energy technologies (0.5) PV technologies, materials, processes and issues **First generation technologies – Si based (2)** **Thin film (a-Si, CdTe, CIGS): 6** **Solar concentrators (3)** **Third generation (high efficiency and low cost) – Organic and dye solar cells, multi-junction, quantum dots (5)** Present Status and future outlook and Indian Scenario (0.5)	17
Energy Efficient Lighting	a. Introduction, Energy efficient buildings, role of sensors etc (0.5) b. Comparison of LEDs with conventional technologies (0.5) c. Principles of light emission; Optical processes and materials d. Light Emitting Diodes (LEDs): Introduction to p-n junction, hetero-junctions, recombination processes, semiconductor materials (III-V, II-VI, SiC, ternary and quaternary alloys) for LEDs, metallurgical considerations (crystal defects, lattice mismatch, optical losses, degradation), and fabrication technology e. OLED for lighting f. Characterization	10

Energy Conversion Devices	Description of Operation, Configurations, Cell Components, Materials Requirements, Manufacturing Techniques, Losses, Efficiency • Solid Oxide Fuel Cells • Solid Oxide Electrolyzer Cells • Batteries • Capacitors	5
Energy Harvesting Materials and Technologies	Working principles and case studies of with emphasis on materials, their selection vis-à-vis their characteristics: Piezoelectric Sensors, Actuators, Transducers and MEMS (3) Thermoelectrics (1) Applications: Ultrasound Imaging, Pyroelectric Sensors IR imaging (1)	5
Total		42

MSE628
Electronic Devices and Characterization

Course structure and Credits **:** 3-0-0-4
Prerequisite **:** MSE303 or equivalent

Objective:
To develop understanding of two important device structures that is, p-n diode and Metal-oxide- semiconductor field-effect transistor (MOSFET). Also, provide knowledge of various device characterization techniques that determine/control the functioning of devices.

References

(1) Semiconductor Material and Device Characterization, Dieter K. Schroder, January 2006,
Wiley-IEEE Press

(2) Metal-Semiconductor Contacts (Electrical & Electronic Engineering Monographs), E. H. Rhoderick and R. H. Williams, Oxford University Press, USA; 2 edition (September 1, 1988)

(3) Electronic Structure of Metal-Semiconductor Contacts, Winfried Mönch (Nov 30, 1990)Springer; 1 edition (November 30, 1990)

(4) Optical Techniques for Solid-State Materials Characterization, Rohit P. Prasankumar and Antoinette J. Taylor, CRC Press; 1 edition (July 5, 2011)

(5) Semiconductor Device Fundamentals by Robert F. Pierret, Addison Wesley; 2nd edition (April 12, 1996)
(6) Advanced Semiconductor Fundamentals (2nd Edition) by Robert F. Pierret, Prentice Hall; 2 edition (August 19, 2002)

(7) Semiconductor Devices: Physics and Technology, Simon M. Sze, Ming-Kwei Lee, Wiley; 3 edition (May 15, 2012)

Lecture Outline

	Topic	Lec.
1.	Electronic Device related characteristics of a semiconductor material Review: -n and –p type semiconductors, wafers, carrier mobility, conductivity, equilibrium carrier statistics, generation-recombination processes and carrier transport, traps and defect states (2) <u>Characterization</u> (a) Doping density: Secondary Ion Mass Spectroscopy (SIMS) (0.75) (b) Resistivity: Four-point probe (0.75) (c) Charge carrier type, density, mobility: Hall effect (1) (d) Band-gap: UV-Visible spectroscopy (0.75) (e) Absorption coefficient (0.5)	5
2	Semiconductor – semiconductor junction (a) P-N junction in thermal equilibrium, J-V characteristics: qualitative (3) (b) P-N junction's J-V characteristics of an ideal device, origin of non idealities (4) (c) Diode variants: solar cell (J-V with illumination and bias effect and PIN diode, LEDs (2.5) (d) Device measurement of a solar-cell (Light and dark J-V, R_s, R_{sh}, Efficiency) (0.5) (e) BJTs: Principle and device measurement (2)	10
3	Metal – Semiconductor junction (a) Schottky and Ohmic contacts, thermionic-emission, Tunnelling, Schottky diodes (2) (b) Contact resistance: Two terminal; Four terminal technique (0. 5) (c) Barrier height: From I-V, C-V, Photo-current; comparison of three (1) (d) Capacitance – Voltage measurements: Doping-Density and majority carrier density profiling (1) (e) Band-offset for a semiconductor – semiconductor junction using C-V technique (0.5)	5
4	Metal-insulator-semiconductor junctions (a) MOS capacitor, quantitative analysis of a flat band device, C-V characteristics (4.5) (b) MOS capacitor: deviations from flat band conditions (2.5) (c) Oxide charges: fixed, mobile, trapped and interface-trapped charges (1) (d) MOSFET (5) (e) Fin-FET MOSFET: Architecture for creating simple Boolean logic, memory Dopant density profiling using CV (already discussed in section 3 above)	13
5	Defects in Semiconductors a. Defects as recombination-generation centres or traps-levels (0.5) b. Defect density: Capacitance measurements (C-t): Steady and transient measurement	4

	(0.5) Current measurement (I-t) (0.5) Deep Level Transient Spectroscopy (DLTS) (2.5)	
6	Charge Carrier Life time and diffusion length: Why important? Optical methods a. Generation and Recombination life time, Surface generation and recombination velocity (0.5) b. Photoconductance decay (0.5) c. Short circuit current and Open-circuit voltage decay (1) d. Photoluminescence Decay (0.5) e. Surface photovoltage(0.5) f. Electron beam induced current (0.5) Electrical methods a. Diode current-voltage(0.5) b. Open-circuit voltage decay (0.5) c. Pulsed MOS capacitor(0.5)	5
Total lectures		42

MSE631
Electroceramic Materials and Applications

Course structure and Credits **:** 3-0-0-4
Prerequisite**:** MSE303

Course Objective:
The objective of this course is to provide an advanced understanding of electroceramic based materials. It is intended to give the material scientist an understanding of the physics behind the important electroceramic materials. State-of-the-art problems and challenges are discussed to give students a better appreciation of a fast moving field. The course is complemented with a critical assessment of classical papers and review articles to provide an in depth perspective for the student.

Reference Books:

1. L.L. Hench and West, Electroceramics, Wiley
2. D. M. Smyth, "The Defect Chemistry of Metal Oxides", Publisher: Oxford University Press, ISBN10: 0195110145
3. Wei Gao and Nigel M. Sammes, "An Introduction to Electronic and Ionic Materials," Publisher: World Scientific.
4. A.J. Moulson & J. M. Herbert, "Electroceramics: Materials, Properties, Applications", Publisher : Wiley
5. M. W. Barsoum, "Fundamentals of Ceramics", Publisher: Institute of Physics
6. "Impedance Spectroscopy: Theory, Experiment and Applications", Edited by J. Ross Macdonald & Evgenij Barsoukov, Publisher: John Wiley and Sons.
7. Robert Huggins, "Use of defect equilibrium diagrams to understand minority species transport in solid electrolytes", Solid State Ionics, 143 (2001) 3-16.
8. "CRC Handbook of Solid State Electrochemistry", Edited by P. J. Gellings & H. J. M. Bouwmeester, Publisher: CRC Press
9. Jaffe B., Cook W. R. and Jaffe H., "Piezoelectric Ceramics," Academic Press, New York, (1971)
10. Principles and applications of ferroelectrics and related materials, M. Lines & A. Glass, Oxford University Press, New York
11. Properties of Materials: Anisotropy, Symmetry, Structure, Robert E. Newnham
12. Ferroelectric Crystals, Franco Jona & G. Shirane
13. Solid State Physics, A.J. Dekker
14. Physical ceramics: Yet-Ming Chiang, Dunbar P. Birnie, W. David Kingery, Wiley
15. Introduction to Ceramics by WD Kingery, Wiley

Lecture Outline

Sl.No.	TOPICS	Number of Lectures
Structures of common electroceramic oxides	Introduction, FCC packed structures (MgO, CeO_2 etc), HCP packed structures ($LiNbO_3$ etc), Other structures such as Perovskite ($BaTiO_3$ etc) and Rutile structures	**3**
Introduction to Defects and Thermodynamics	Defects in Elemental Solids and Ionic Compounds, Defect Classes, Point Defects, Kröger-Vink Notation, Point Defect Formation & Equilibrium, Law of Mass- Action and electrical neutrality, Thermodynamics of Intrinsic Defects and Defect Reactions.	**10**
Defect Complexes and **Associates**	Complexes Containing an Impurity Center and an Ionic Defect, Intrinsic Ionic Defect Associates and Effect of Impurities on the Concentration of Defect Complexes and Associate.	
Defect Equilibria and **Brouwer Diagrams**	Defect Equilibria in Pure and Stoichiometric Compounds with Schottky Defects, Frenkel Defect Pairs and Intrinsic Ionization of Electrons, Defect Equilibria in Non-stoichiometric Oxides (Cases of oxygen and metal deficiency, oxygen and metal excess), Brouwer Diagrams for selected materials such as YSZ, Undoped and Doped CeO_2, TiO_2 and $BaTiO_3$.	
Ionic and Electronic **Transport**	Basic Concepts of Diffusion, Tracer Diffusion, Self Diffusion, Chemical Diffusion, Ambipolar Diffusion, Ionic Conduction in Crystalline Solid, Intrinsic and Extrinsic Ionic Conduction, Transference Number, Nernst-Einstein Relationship, and Conductivity-Diffusion Relationship, Polaron theory, metal-ceramic interfaces and electronic transport into and through a dielectric material, Conduction mechanism in terms of Mott insulators, semiconductors, Measurement techniques, Examples of ionic transport, in important	**8**

	applications	
Theory of Linear Dielectrics	Basics of dielectrics, Clausius-Mossotti Relationship, Polarization mechanisms (Electronic, atomic dipole, space charge polarization) and estimation of polarizabilities:, Frequency Dependence of permittivity and dielectric Loss, Intrinsic and extrinsic contributions to polarization, Relaxation phenomena: Debye equations, Cole-Cole plots, Impedance spectroscopy, Dielectric breakdown and degradation	**7**
Non-linear dielectrics	Polar and nonpolar ceramics: Crystal structure and Noncentrosymetricity, Tensor representation of properties, Piezoelectrics, Pyroelectrics, Ferroelectrics, Antiferroelectrics, Relaxors Phenomenological theory (phase transitions) and soft mode theory, domain switching and domain-dynamics., Measurement methods, **Applications**	**7**
Thermoelectric Oxides	See-back and Peltier effect, materials and applications	**1**
Magnetic Ferrites	Ferrites structure and properties and their applications	**2**
Multiferroics and Magnetoelectrics	Principles, Classification, Magnetoelectric Coupling, Materials, Issues and Possible Applications	**2**
Superconductors	Basic theory, Oxide superconductors such as YBCO, Applications	**1**
Total		**41**

MSE693N
Materials Science Technologies for Applications in Life Sciences

Course structure and Credits **:** 3-0-0-4
Prerequisite **:** Consent of Instructor

Objectives

The basic objective of the course is to expose the participants to the advancement in materials science targeted for life sciences applications. The course will cover proteins and DNA concepts, advancement in materials science and nanotechnology targeted for life sciences application, and integration of life sciences and materials science for applications like bioMEMS, drug delivery, and biomedical devices. After successful completion of the course, the participants will be expected to know about proteins, DNA, lab-on-a-chip concepts, self assembly, drug delivery, biofunctionalisation of nanomaterials, and several characterization techniques used in life sciences.

References:

1. B. Alberts *et al*., *Essential Cell Biology*. (Garland Publishing Inc., New York, ed. Third, 2009).
2. S. S. Saliterman, *Fundamentals of bioMEMS and medical microdevices*. (Wiley-Interscience, Bellingham, 2005).
3. T.J. Kindt *et al.*, *Kyby immunology*. (W.H. Freeman, 6th edition 2007)
4. C. S. S. R. Kumar, *Biofunctionalization of Nanomaterials*. C. S. S. R. Kumar, Ed., Nanotechnologies for the life sciences (Wiley-VCH, Weinheim, 2006), vol. 1, pp. 366.
5. C. S. S. R. Kumar, *Nanomaterials for biosensors*. C. S. S. R. Kumar, Ed., Nanotechnologies for the life sciences (Wiley-VCH, Weinheim, 2006), vol. 8.
6. C. S. S. R. Kumar, *Nanosystem characterization tools in the life sciences*. C. S. S. R. kumar, Ed., Nanotechnologies for the life sciences (Wiley-VCH, Weinheim, 2005), vol. 3.
7. J. M. Anderson, Annu Rev of Matl Res, **31,** 81 (2001)

Lecture Outline

Topic	Lectures
Introduction to integrating nanotechnology and materials science with life sciences • Introduction to various size regimes in life science and materials science • Importance of integration of materials science and engineering with life sciences	3
Proteins and DNA: Structure and properties • Cells organelles and building blocks of important molecules in cell (1) • Protein structure, organization, functions with emphasis on antibodies and enzymes, regulation of enzyme activity, protein phosphorylation • DNA: structure and function of DNA, DNA replication and repair	5
Microfabrication techniques and soft lithography; Fundamentals of bio-MEMS, microfluidic devices and Lab-on-chip devices • Materials for MEMS • Photolithography: (single crystal silicon, mask, oxide formation, resist application, baking, exposure, positive and negative resist, developing, etching. • Etching: Dry Vs wet and isotropic Vs anisotropic, plasma (DC arc and RF), DRIE, wet bulk surface micromachining, 3D structure with sacrificial layer, LIGA • Deposition: physical and chemical vapour deposition • Soft fabrication: application of polymers in bio-MEMS, microcontact printing, microtransfer moling, micromolding in capillaries, injection molding, hot embossing	11
Biocompatibility • Definition of biocompatibility, host response to implanted device, *in vivo* and *in vitro* tests for biocompatibility • Overview of immune system (inntate and adaptive immunity, cell mediated and humoral immunity), B cells, T cells, MHC	5
Self assembly: Structure, Mechanism and Applications • Difference between self assembly and self organization, example (organothiol molecules on gold substrate) • Techniques for assembly: microcontact printing, dip pen nanolithography • Layer by layer self assembly: methods, materials applications • Application of multilayer biofilm and ultrathin coatings on medical implants	5
Biofunctionalization of nano-materials and drug delivery techniques • Introduction to advanced drug delivery system, active Vs passive drug delivery	4

systems • Protein drugs and challenges in delivery • Encapsulation: synthesis and loading of drugs in polyelectrolyte shells, advantages of polyelectrolyte shells	
Overview of characterization techniques: • Fluorescence microscopy • Quantum dot labelling • Single molecule detection techniques • Atomic Force Microscopy • Quartz crystal microbalance,	5
Applications of Materials Science in Life Sciences including sensing, bio-MEMS devices, drug delivery, and biomedical devices using case studies	2
TOTAL	**40**

2. Details of the courses other than the three streams

MSE 634
Fundamentals of Spray Techniques

Course structure and credits : 3-0-0-3
Prerequisite: None

Course Contents:

Topic	Distribution	Lectures
Introduction	• Different Spray Techniques and their need	**2**
Thermal Spraying Techniques: Principle and Working	• Combustion Spraying: o Flame Spraying o D-Gun o High Velocity oxy-fuel • Arc and Plasma Spraying: o Wire/Powder Arc Spraying o Plasma Spraying (Air/ Vacuum) • Cold Spraying	**12**
Spraying Parameters	• In-flight conditions • Plasma/ Primary/ Secondary/ Carrier gases • Power rating • Feed rate • Standoff distance • Substrate preparation	**6**
Powder	• Powder size and distribution • Powder Injection • Reaction of particles • Evaporation/Condensation	**5**
Coating Formation	• Comparison of deposition techniques • Single Splat Formation • Heat transfer and spreading of splat • Splay layering and deposition • Microstructure and densification of deposited coatings	**6**
Diagnostics and Coating Reliability	• Thermal and Kinetic Profiles • Inflight particle sensor • Control of Deposition parameters • Microstructural distribution	**4**
Bulk Nanostructure and Near Net Shape	• Design and control of bulk nanostructure • Mandrel choice • Mandrel removal • Case Studies: Thermal Barrier/ Ultra high temperature ceramics	**5**

Duration: One semester **Total: 40**

Textbook:
Thermal Spray Fundamentals, Joachim Heberlein, Pierre Fauchais, Maher I. Boulos. Springer (2012)

Reference Books:
1. Handbook of thermal spray technology, Joseph R. Davis, ASM International. Thermal Spray Society
   Training Committee (2004).
2. Advanced Structural Ceramics, Bikramjit Basu and Kantesh Balani, Wiley (2011).
3. *Course materials will be supplemented with handouts, and journal publications.*

MSE 658
Dislocations and Plasticity

Course structure and credits : 3-0-0 -4
Prerequisite: Consent of Instructor

Objectives

At the end of the course the student should be able to:

- Have a broad understanding of defects in materials and their role in determining properties of materials.
- Have an overview of plastic deformation mechanisms and the role of dislocations in plasticity, fracture, fatigue and creep.
- Have a thorough understanding of the structure of dislocations in various crystals and their elastic fields.

References

6. *Introduction to Dislocations*, D. Hull and D.J. Bacon, Pergamon Press, Oxford, 1984.
7. *Theory of Dislocations*, J. P. Hirth and J. Lothe, McGraw–Hill, New York, 1968.
8. *Crystal Defects and Crystalline Interfaces*, W. Bollmann, Springer-Verlag, Berlin, 1970
9. *Elementary Dislocation Theory*, J. Weertman and J. Weertman, The MacMillian Company, New York, 1964.
10. *http://www.tf.uni-kiel.de/matwis/amat/def_en/*

Lecture Outline

Topic	Lectures
Overview of defects in Materials - (point, line, planar and volume defects) and their classification. - Overview of plastic deformation mechanisms	**1**
Point defects: - interaction and distributions - statistical thermodynamics - role in diffusion and deformation.	**4**
Basic understanding of dislocations using physical and computer models: - the Volterra cut - Burgers vector and the Burgers circuit - the line vector - edge, screw and mixed dislocations - Role of dislocations in weakening the crystal and in plasticity.	**4**
Elasticity theory of dislocations: - Stress, strain and displacement fields and energy of a dislocation - Forces on dislocations (including image force) - Interaction between dislocations - Core of a dislocation.	**3**
Motion of dislocations: - The Peierls stress - role of the core structure - interaction of dislocations with other defects (including yield point phenomenon); - kinks; jogs; cross-slip; climb - Temperature and strain-rate dependence of flow stress - Dislocation dynamics and the tensile stress-strain curve.	**5**
Dislocations in FCC Metals: - Partial dislocations (Shockley and Frank partials) - stacking faults - Thompson's tetrahedron	**4**

- Lomer-Cotrell sessile dislocation	
Overview of dislocations in other crystal structures: - HCP metals - BCC metals - ionic crystals - superlattices - covalent crystals.	**2**
Origin and multiplication of dislocations: - dislocations in freshly grown crystals - nucleation of dislocations - multiplication of dislocations (by Frank-Read sources, cross slip and climb) - Grain boundary sources - Recovery and recrystallization.	**4**
Geometrically/structurally necessary dislocations: - low-angle & general grain boundaries - indentation - interfacial dislocations - Twinning including incoherent twins.	**5**
Specific examples of role of dislocations and case studies: - Dislocations in nanocrystals - The Hall-Petch relation and the Inverse Hall-Petch Effect (IHPE) - Dislocations in epitaxial systems - Severe Plastic deformation - Role of dislocations in Creep, Fatigue and Fracture	**8**
TOTAL	**40**

MSE 664
Solid State Ionics

Course structure and credits: 3-0-0-4
Pre-requisite: none

Course Contents: Perfect Structure, Defects in Elemental Solid and Ionic Compound, Defect Classes, Point Defects, Kröger-Vink Notation for Point Defects, Point Defect Formation & Equilibrium, Law of Mass-action, Thermodynamic Related to Intrinsic Defects and Defect Reactions. Complexes Containing an Impurity Center and an Ionic Defect, Intrinsic Ionic Defect Associates and Effect of Impurities on the Concentration of Defect Complexes and Associate. Basic Concepts of Diffusion, Tracer Diffusion, Self Diffusion, Chemical Diffusion, Ambipolar Diffusion, Ionic Conduction in Crystalline Solid, Intrinsic and Extrinsic Ionic Conduction, Transference Number, Nernst-Einstein Relationship, and Conductivity- Diffusion Relationship. Defect Equilibria in Pure and Stoichiometric Compounds with Schottky Defects, Frenkel Defect Pairs and Intrinsic Ionization of Electrons, Defect Equilibria in Non-stoichiometric Oxides such as Oxygen Deficient Oxide, Oxide with excess Metal, Metal Deficient Oxide, Metal Oxide with Excess Oxygen. Brouwer Diagrams for YSZ, Undoped and Doped CeO_2, TiO_2 and $BaTiO_3$. Electrical Characterization Techniques such as AC Electrochemical Impedance Spectroscopy, Four Point Probe D.C. Method, Van Der Pauw Method, I-V Curves, Blocking Electrodes, and Hebb-Wagner Method. Open Circuit Potential, Efficiency, Nernst Equation Analysis, Activation Losses (Tafel Equation), Ohmic Losses, Concentration Losses. Description of Operation, Configurations, Cell Components, Materials Requirements, Manufacturing Techniques, and Performance of the following electrochemical devices such as Solid Oxide Fuel Cells, Gas Sensors and Batteries.

1. Description about Defects and Defect reactions	[4]
2. Defect Complexes and Associates	[3]
3. Ionic Transport	[6]
4. Defect Equilibria and Brouwer Diagrams	[13]
5. Electrical Characterization Techniques	[6]
6. Solid State Electrochemical Devices	[8]

Reference Books

1 D. M. Smyth, "The Defect Chemistry of Metal Oxides", Publisher: Oxford University Press, ISBN10: 0195110145

2 A.J. Moulson & J. M. Herbert, "Electroceramics: Materials, Properties, Applications", Publisher : Springer

3 M. W. Barsoum, "Fundamentals of Ceramics", Publisher: Institute of Physics

4 "Impedance Spectroscopy: Theory, Experiment and Applications", Edited by J. Ross Macdonald & Evgenij Barsoukov, Publisher: John Wiley and Sons.

5 Robert Huggins, "Use of defect equilibrium diagrams to understand minority species transport in solid electrolytes", Solid State Ionics, 143 (2001) 3-16.

6 "CRC Handbook of Solid State Electrochemistry", Edited by P. J. Gellings & H. J. M. Bouwmeester, Publisher: CRC Press

7 "High Temperature Solid Oxide Fuel Cells, Fundamental, Design and Applications ", Edited by Subhash C. Singhal & Kevin Kendall, Publisher: Elsevier

8 "Physical Chemistry of Ionic Materials: Ions and Electrons in Solids", Joachim Maier, Wiley, ISBN: 978-0-470-87076-1

MSE676
Materials Failure: Analysis and Prevention

Course structure and credits **:** 3-0-0-4
Prerequisite **:** Consent of Instructor

Course Objective: Materials failure has to be understood through a systematic analysis so that the weak link in the design-fabrication-performance chain can be identified and efforts in control/prevention of failures can be implemented. Failure analysis has grown over the year by trying to answer basic questions like: Why materials failure occurs? Can we predict failures? How best one can prevent common failures? etc.

Failure analysis is a fascinating subject as probing failures calls for application of a wide range of ideas and techniques in 'Materials Science and Engineering'. This course intends to be a 'Primer' to an highly applied field involving many technical concept and sophisticated experimental techniques. Many illustrative and interesting cases studies will be considered to give a comprehensive feel about the topic.

Lecture Outline

TOPICS	Lectures
Engineering Aspects of Failure and Failure Analysis General Practice in failure Analysis: Categories of failure, Importance of failure prevention -	**2**
Tools and techniques in failure analysis: General Practices, Photography, X-rays techniques, Mechnical property evaluations, Metallographic techniques, Fractography, Non-destructuive testing technique	**6**
Failure mechanisms and modes: Fracture modes, Ductile fracture of metallic materials and their interpretations, factors affecting ductile-brittle relationships. (2 Lectures) Brittle fracture in normally ductile metallic alloy, microstructural aspects of brittle fracture (1 Lectures) Failure characteristics of Ceramics and Plastics (2 Lectures) Fatigue fracture, macroscopic and microscopic characteristics, statistical aspects of fatigue, Fatigue failure prediction and life assessments (2 Lectures) Wear Failures and Prevention. (2 Lectures) Corrosion related failures, Stress corrosion cracking, Hydrogen damage and embrittlement, Biological corrosion failures. (2 L) Elevated temperature failures, creep and stress rupture, metallurgical instabilities (2 L) Distortion failures and deformations (1 Lectures) -	**12**
Examples of engineering failure Improper processing practice: Casting, metal working, welding, etc., Improper heat treatment: Gears, locomotive axle, shafts, etc. Improper design:Tools and dies, integrated circuits etc. Unanticipated service conditions: lifting equipment, reactors, etc. Improper material selection: Orthopedic implants, pressure vessels etc. Improper service condition: Pipelines, mechanical fasteners etc.	12
Comprehensive failure analysis illustration At least two cases based on aircraft crash, ship sinking, boiler blast, space mission failure, industrial catastrophe etc. (6 hours)	**6**
Total Lectures	**40**

Reference books:

1. Source book in failure analysis, American Society of Metals, Metals Park, Ohio, 1974.
2. Understanding how components fail, D.J Wulpi, ASM International, The Materials Information Society, 1999.
3. A.J. McEvily, Metal Failures: Mechanisms, Analysis, Prevention, John Wiley and Sons, 2002.
4. Practical engineering failure analysis, H.M. Tawancy, A. Ul-Hamid and N.M. Abbas, Marcel Dekker, New York, 2004.
5. Failure analysis and prevention, Volume 11, ASM Handbook, The Materials Information Society, 2002.
6. Failure analysis of engineering structures: Methodology and case histories, V. Ramachandran, A.C. Raghuram, R.V. Krishnan and S.K. Bhaumik , ASM International, 2005.
7. Failure analysis of Engineering Materials, Charles R. Brooks and Ashok Choudhury.

MSE682

Computer Simulations in Materials Science

Course structure and Credits : 3-0-0-4
Prerequisite : Consent of the instructor

Course objectives:

Objective of the course is to introduce students to the field of computational materials science. The course commences with a brief discussion of basic physics and numerical methods, essential for the rest of the course. The topics are divided into two major categories, classical and quantum mechanical simulation techniques. The first part focuses primarily on two popularly used methods, molecular dynamics and Monte Carlo; discussing basic theory, applications and examples related to materials science. The second part focuses on density functional based tight binding (DFTB) method. Basic applications, such as simple band structure calculation and geometry optimization and advanced topics such as electron transport calculations will be discussed.

Suggested reading /Text books:

1. Molecular dynamics simulation: Elementary methods, J. M. Haile (Wiley Professional).
2. The art of molecular dynamics simulation, D. C. Rapaport (Cambridge University Press).
3. Computer simulation of liquids, Allen and Tildesley (Oxford).
4. Computational materials science: an introduction, June Gunn Lee (CRC Press).
5. Electronic structure: basic theory and practical mehtods, Richard Martin (Cambridge).

Lectureoutline

Topic	No. of lectures
Introduction to computational materials science, relevance and scope	1
Necessary background	
Brief overview of classical, statistical & quantum mechanics and mathematical methods	5
Molecular dynamics (MD) and Monte Carlo (MC) methods	
• Interaction potentials - pair potential, empirical potential	2
• MD under different constraints like NVE, NVT and NPT	4
• MD simulation of thin film growth and crack propagation	2
• Non-equilibrium molecular dynamics	2
• MD simulation of phonon mean free path and thermal conductivity	2
• Introduction to MC methods	4
• Monte Carlo simulation of surface adsorption	2
• Monte Carlo simulation of grain growth	2
Quantum-Mechanical calculations	
• Tight binding model and simple band structure calculations	2
• Density functional based tight binding (DFTB) method	2
• Applications: band structure of metal, insulator and semiconductor	4
• Applications: geometry optimization	2
• Applications: transport calculation	2
• Density functional theory (DFT)	2
Total no. of lectures	**40**