COURSE ID SHEET

Course No.	**5291**		**NTUA**				
Semester:	**8,10**	Core		Elective		Specialization	**X**

Title: **STRUCTURE-PROPERTY RELATIONS IN MATERIALS**

Aim: Study and quantitative interpretation of the macroscopic properties (mechanical, thermal, electrical, magnetic, optical, transport) of solid phases (mainly crystalline solids) with reference to their fundamental microscopic structure.

Content:

- **INTRODUCTION.** Importance and recent achievements of Materials Science and Engineering. The tetrahedron "Structure-Properties-Processing-Performance". Categories of materials and properties. Crystalline and amorphous solids. Composite materials.
- **CRYSTAL STRUCTURE.** Introduction to crystallography and to descriptive crystal chemistry: Point group and space group symmetry, lattices and unit cells, close packing, isomorphism and polymorphism. Miller indices and direction indices. Calculation of distances between crystal planes. Calculations of density from the crystalline structure for metallic, ceramic, and polymer crystals. Theory and applications of X-ray diffraction. The reciprocal lattice.
- **CRYSTAL LATTICE ENERGY.** Atomic-level structure and bonding in molecules and in solids. Cohesive energy and its calculation from experimental measurements via thermodynamic cycles. Calculation of cohesive energy from the lattice geometry and the interaction potential between molecules in crystals held together by dispersion forces. Cohesive energy of ionic crystals: Madelung constant. Calculation of the bulk modulus from the lattice energy. Cohesive energy of covalently bonded crystals (e.g., diamond) and of crystals held together by hydrogen bonds. Cohesive energy of metallic crystals.
- **DIFFUSION IN THE SOLID STATE**. Atom migration and diffusion coefficients. Self-diffusion. Microscopic mechanisms of diffusion: diffusion via vacant sites and via interstitial sites. Elementary jumps involved in the diffusive process. Transition state theory for the calculation of jump rate constants. The diffusion path as a random walk. Connection with the macroscopic diffusion equation. Calculation of the diffusivity and its temperature dependence from atomic-level information. Solution of the diffusion equation under various initial and boundary conditions. Order of chemical reactions in solids: solid-gas and solid-solid reactions. Simple diffusion model for solid-solid reactions.
- **CRYSTAL VIBRATIONS.** Determination of the normal modes from the potential energy function of a crystal and the atomic masses. Vibrations of a simple cubic crystal. Propagation of elastic waves in a linear chain: dispersion relation, Brillouin zones. Vibrations of crystals with more than one atom per unit cell. Optical and acoustic branches.

- **THERMAL PROPERTIES OF CRYSTALLINE SOLIDS.** Statistical mechanics of the harmonic oscillator. Phonons. Einstein model. Debye model: derivation of the density of vibrational states, Debye temperature, calculation of the internal energy and the heat capacity. Law of the third power of temperature at low temperatures. Ideal Fermi gas model for the free electrons in a metal. Density of electronic states. Fermi energy and Fermi temperature. Calculation of the contribution of free electrons to the heat capacity of metals. Anharmonic interactions in crystals and coefficient of thermal expansion. Lindemann criterion for melting of solids. Debye equation of state for solids, Grüneisen parameter. Thermal conductivity of non-metallic solids: Umklapp processes, dependence of the thermal conductivity on temperature. Thermal conductivity of metals: contribution of the free electrons.
- **ELECTRICAL PROPERTIES OF CRYSTALLINE SOLIDS.** Derivation of the electrical conductivity of a metal from the simple ideal Fermi gas model for the free electrons. Mobility of electrons. Relation between electrical and thermal conductivity in a pure metal: Wiedemann-Franz law. Dependence of the electrical conductivity of metals on temperature. Role of impurities and of plastic deformation. Scattering of free electrons by the ion cores in a metal lattice. Nearly free electron model. Energy bands and energy gaps. Electronic properties of metals, insulators, and semiconductors. Intrinsic and extrinsic semiconductors – calculation of the conductivity and its dependence on temperature. Motion of carriers in a magnetic field – the Hall effect. Photovoltaic effect. Organic semiconductors**.**
- **DIELECTRIC PROPERTIES.** Dielectric materials. Polarization: electronic, ionic, dipole contributions. Dielectric constant and dielectric susceptibility. Clausius-Mossotti relation. Frequency dependence of the polarizability. Dielectric spectroscopy. Piezoelectric crystals**.**
- **MECHANICAL PROPERTIES.** Stress-strain, elastic behavior, anisotropy, plastic behavior, strength, ductility. Hardness, fatigue (resistance to fatigue), creep, ageing, damping of vibrations, fracture (brittle fracture, elementary fracture mechanics, morphology of fracture surfaces). Mathematical approach and mechanisms. Mechanical behavior of various categories of materials: polymers, metals, ceramics, advanced materials (graded structure, superalloys, composite materials). Common and advanced techniques for measuring mechanical properties.

LABORATORY EXERCISES OFFERED:

- Analysis of crystal structures by X-ray diffraction
- Calculation of dipole moment from electric permittivity measurements and index of refraction.
- Determination of the mobility of electrons by use of the Hall effect.
- Photovoltaic effect
- Self-assembling multilayered nanomaterials: electrochemical synthesis of multilayered Cu / Cu_2O through potential oscillations under galvanostatic conditions.
- Synthesis, structure and properties of carbon nanotubes and graphene via the thermal vapor deposition technique.

Hours per semester:	LECTURES	**36**	EXERCISES	**4**	LABORA-TORY	**5**	HOME-WORK	**45**	**TOTAL HOURS: 90**

Student performance/ evaluation:	The evaluation of students' performance will be based: • on a final written examination (FE), which will include solution of quantitative problems with open books and other aids. • on an evaluation of performance in the laboratory exercises. The laboratory grade, L, is calculated as an average of the grades given in each laboratory exercise. The grade in each laboratory exercise is based on the written report submitted by the student and on the degree of preparation and participation of the student during the execution of the laboratory exercise. **The final grade for the class is calculated as follows: Final Grade = (FE)*0.6 + (L)*0.4**