

# Physics of amorph materials and nanostructures

## List of topics for the complex exam

### **1. Ultrafine-grained (UFG) and nanocrystalline materials**

Classification of the processing of UFG and nanocrystalline materials. Bottom-up and top-down approaches. Grain-refinement by plastic deformation. Unique mechanical properties of ultrafine-grained and nanocrystalline materials (yield strength, ductility, superplastic deformation).

### **2. Processing of UFG metals and alloys by powder metallurgy**

The main steps of powder metallurgy. Methods for production of nanodisperse powders. Inert gas condensation. Laser ablation. RF plasma synthesis. Cryogenic melting. Electro-explosion of wire. Liquid Atomization. Milling. Changes in microstructure during milling. Mechanical alloying. Formation of non-equilibrium crystalline phases. Mechanical amorphization. Powder consolidation methods. Shock wave consolidation. Transformation assisted consolidation Sintering. Hot pressing. Sinter forging. Hot Isostatic Pressing. Spark Plasma Sintering. Plasma spraying. Effect of oxide phase on the mechanical performance of sintered UFG materials. Application of sintered UFG materials. Special effects during sintering of blends of coarse-grained and nanocrystalline powders.

### **3. Processing of bulk UFG materials by severe plastic deformation (SPD)**

Severe plastic deformation methods. Equal-Channel Angular Pressing (ECAP). Dissimilar-Channel Angular Pressing. High-Pressure Torsion (HPT). Multi-directional forging. Cyclic extrusion and compression. Twist extrusion. Accumulative Roll Bonding. Repetitive Corrugation and Straightening. Evolution of the microstructure during ECAP. Effect of alloying on the microstructure evolution during SPD. Application of UFG metals processed by SPD.

### **4. Preparation and nanocrystallization of amorphous alloys (metallic glasses)**

Processing of amorphous alloys by quenching. Production methods of metallic glasses. Splat Cooling. Melt spinning. Copper-mould casting. Formation of bulk metallic glasses (BMG). Mechanical properties of metallic glasses. Partial or full crystallization of amorphous alloys by heat treatment. Crystallization of metallic glasses by SPD. Processing of bulk nanomaterials from BMGs. Influence of nano-quasicrystalline particles on viscosity of BMGs. Effect of partial crystallization on room-temperature mechanical properties. Magnetic properties of amorphous-nanocrystalline composites.

### **5. Nanocomposites**

Classification of composites: ex-situ and in-situ composites. Classification according to the types of component materials, matrix material, disperse phase morphology. Effect of fibers on the mechanical properties. Processing methods of ex-situ composites. Polymer-matrix nanocomposites. The influence of disperse phase morphology on the percolation threshold. Carbon nanotube reinforced composites. Types of carbon nanotubes. Chiral vector. Single and multi-wall carbon nanotubes. Nanotube junctions. Processing methods of carbon nanotubes. Arc-discharge. Laser ablation. Catalytic Chemical Vapor Deposition. Unique properties of carbon nanotubes. Metal- and ceramic-matrix nanocomposites. In-situ composites. Exothermic dispersion (XD). Gas-assisted process. Direct metal oxidation (DIMOX). Eutectic solidification. Al-Al<sub>2</sub>O<sub>3</sub> nanocomposite formed during sintering of Al nanopowders. Nanocomposites in nature.

### **6. Nanoporous materials**

Classification of porous materials according to the size of pores: microporous, mesoporous and nanoporous materials. Classification of nanoporous materials according to the type of material. Processing of nanoporous materials. Zeolites. Application of nanoporous zeolites. Mesoporous silicates. Nanoporous polymers. MOF (metal organic framework). Application of MOFs. Porous Si as antireflection coating and biosensor.

# Crystal defects in metals and insulators

## List of topics

### **1. Point defects, diffusion**

Types of point defects. Vacancy concentration in thermal equilibrium. Measurement of vacancy concentration (differential dilatometry, electric resistance measurement, positron annihilation spectroscopy). Point defect pairs. Diffusion mechanisms. Fick I. law. Kirkendall effect. Diffusion in the presence of lattice defects. Fick II. law.

### **2. Dislocations and plastic deformation**

General definition of dislocation (cut surface). Burgers vector. Edge and screw dislocations. Stress field of edge and screw dislocations. Energy of dislocation. Burgers vectors in cubic crystals. The force acting on a dislocation. Interaction between dislocations. Frank-Read source. Dislocation reactions. Lomer-Cottrell lock. Cross-slip of screw dislocation, climb of edge dislocation. Slip systems in hexagonal close packed structure. Uniaxial tensile test. Schmid factor. Thompson tetrahedron. Single slip, multiple slip. Stages of deformation in single- and polycrystals. Yield strength, ultimate tensile strength, fracture strength, uniform and total elongations. Taylor equation. Hall-Petch equation.

### **3. Stacking and twin faults in face-centered and body-centered cubic crystals**

Intrinsic and extrinsic stacking faults in fcc lattice. Coherent twin boundary. Partial dislocations in fcc lattice: Shockley partial, negative and positive Frank partial dislocations. Dissociated dislocations. Equilibrium splitting distance between partials in dissociated dislocations. The effect of stress on dissociated dislocations. Deformation twinning. The effect of grain size on the splitting distance between partials in dissociated dislocations. Twinning in bcc crystals.

### **4. Twinning in hexagonal crystals**

General description of twinning: invariant plane of shear, shear direction, conjugate plane, conjugate shear direction. Extension and contraction twinning in magnesium. Schmid factors for extension twinning. The orientation change of crystallographic c-axis due to extension twinning in Mg during tension and compression. „Double” twinning. The dislocation model of extension twinning in Mg. Monitoring of extension twinning activity by neutron diffraction and acoustic emission. Effect of grain size and deformation temperature on twinning activity in hcp crystals

### **5. Solid solution hardening**

Interaction between dislocations and solute atoms: size effect, modulus effect. The effect of solute concentration on yield strength. The influence of temperature and difference in atomic sizes on yield strength increment.

### **6. Interaction between dislocations and secondary phase particles**

Processing of microstructures with secondary phase particles. Coherent, semi-coherent and incoherent phase boundaries. Dispersion strengthening. Orowan mechanism. Dipole criterion. Effect of size and spacing between precipitates on yield strength. Cutting mechanism. Dependence of yield strength on precipitate radius for Orowan and cutting mechanisms.

## **7. Grain boundaries**

Characterization of misorientation. Macroscopic and microscopic degrees of freedom for grain boundaries. Coincidence site lattice (CSL). Twist and tilt boundaries. Symmetrical tilt boundary. Displacement shift complete lattice (DSCL). Bollmann-type zero lattice (OL). Correlation between CSL, DSCL and OL. Grain boundary engineering. Brandon and Palumbo-Aust criteria. Marcinkowski-type grain boundary model. Dislocation model of low-angle grain boundaries (GBs). Dependence of GB energy on misorientation. Liquid model of GBs. Temperature dependence of GB energy at high temperatures. Determination of impurity excess concentration segregated at GBs using the Gibbs equation. Langmuir-McLean adsorption theory for grain boundary segregation. Grain boundary coverage as a function of impurity concentration.

## **8. Vacancy condensation**

Formation of vacancy clusters. Dislocation loops formed by vacancy condensation: Frank-type sessile loops, prismatic loops. Transformation of Frank-type loop to prismatic loop. Stacking fault tetrahedron. „Stair-rod” dislocation. Formation of stacking fault tetrahedron from Frank-type loop. Variation of the size of stacking fault tetrahedron as a function of the distance from the free surface.

## **9. Recovery and recrystallization**

Driving force of recovery and recrystallization. Annihilation processes of lattice defects as a function of temperature: reduction of point defect concentration, dislocation annihilation, polygonization, primary and secondary recrystallization. Change of physical properties. Kinetics of recovery and recrystallization.

## **10. Crack propagation and fracture**

Brittle and ductile fracture. Theoretical fracture strength. Griffith theory of brittle fracture. Stress intensity theory. Stress intensity factor. Fracture toughness: definition, measurement. Charpy-type impact test. Dependence of fracture toughness on temperature and strain rate. Brittle-ductile transition.

# **Experimental methods in condensed matter physics**

list of questions

- 1. X-ray diffraction for structure and composition determination**
- 2. X-ray Line Profile Analysis**
- 3. Transmission Electron Microscopy**
- 4. Scanning Electron Microscopy**
- 5. Scanning X-ray Photoelectron Spectroscopy (XPS/ESCA)**
- 5. Electron backscatter diffraction (EBSD)**
- 6. Scanning tunneling microscopy (STM)**
- 7. Atomic force microscopy (AFM)**
- 8. Mechanical testing, hardness measurement, nanoindentation**
- 9. Differential Scanning Calorimetry (DSC), Thermal Gravimetry (TG)**
- 10. Acoustic Emission**
- 11. Positron Annihilation**
- 12. Mössbauer Spectroscopy**
- 13. Nuclear magnetic resonance (NMR)**

## Materials Physics

### List of questions

1. Crystalline structures, experimental determination of crystalline structures (basic structures, symmetry properties, direct and reciprocal lattice, X-ray-, electron-, and neutron-diffraction)
2. Disordered systems ( alloys, amorphous materials, liquid crystals, quasicrystals)
3. Molecular dynamics ( empirical pair potentials, many particle (embedded) potentials, MD by first principle calculation) , MD with thermostat and barostat
4. Thermal properties of crystalline materials (heat capacity of phonon gas, anharmonicity, thermal expansion, heat conductivity).
5. Point defects (equilibrium concentration, mixing and formation entropy and enthalpy, evolution of point defects)
6. Dislocations (topological properties, continuum description, force acting on a dislocation, partial dislocations). Field theory of dislocations (dislocation density tensor, incompatibility tensor, stress calculation, collective dislocation motion)
7. Internal surfaces (grain boundary, phase boundary, energy of the boundaries, nanostructural materials)
8. Diffusion in solid states (macroscopic and microscopic descriptions, concentration dependence of diffusion constant, Kirkendall-effect, Darken equations), Generalized theory of diffusion (Cahn–Hilliard phase field theory, spinodal decomposition)
9. Mechanical properties (plasticity, work hardening, hardening by solid solution and precipitates)
10. Solid solutions (thermodynamic of multicomponent systems, quasi chemical theory, ideal and ordered solid solutions, factors determining the solubility limit)
11. Phase diagram (equilibrium and non equilibrium phase diagrams, calculating the phase diagram from free energy), solidification (homogeneous and heterogeneous nucleation, crystal growing, cleaning by zone melting, non equilibrium solidification)
12. Phase transformations in solid phase (precipitation, phase transformations without diffusion, martensitic transformation)
13. Principle of phase field theories (conserved, nonconserved fields, nucleation, precipitation)
14. Ceramics and composite materials (chemical structure of ceramics, properties, properties of composites, how to select materials for composites)

# Solid state physics

## list of questions

1. Bonding in solid states (van der Waals, ionic, covalent, and metallic bonding)
2. Crystalline structures, experimental determination of crystalline structures (basic structures, symmetry properties, direct and reciprocal lattice, X-ray-, electron-, and neutron-diffraction)
3. Disordered systems (alloys, amorphous materials, liquid crystals)
4. Lattice vibrations (classic and quantum description, acoustic and optic branches, experimental determination of phonon spectra)
5. Thermal properties of crystalline materials (heat capacity of phonon gas, anharmonicity, thermal expansion, heat conductivity by phonons), Superfluidity.
6. Electron states in periodic systems (Bloch and Wannier functions, tight-binding approximation, LCAO, band structure and its relation to the symmetry of the crystal, experimental determination of band structure, metals, semiconductors, insulators)
7. Semiclassical description of the dynamic of electrons. Experimental determination of Fermi surface (motion of electron in electric and magnetic fields, cyclotron resonance, size effects, magneto-acoustic effect)
8. Pure and doped semiconductors, (Fermi energy, donor and acceptor levels, excitons). Schottky barrier, p-n transition, transistor.
9. Nonperiodic systems (fullerene, molecular crystals, quasicrystals)
10. Electron in strong magnetic field (Landau levels, de Haas-van Alphen effect, quantum Hall effect)
11. Electron-phonon interaction, (limits of adiabatic decoupling, obtaining the electron-phonon interaction, polaron, Kohn anomaly).
12. Theory of conduction (Boltzmann equation, relaxation time approximation and its limitations, transport coefficients in metals and semiconductor, scattering of impurities, phonons and electrons, scattering of electron on magnetic impurities, Kondo effect).
13. Interaction of solid materials with photons and neutrons (optical properties, Brillouin and Raman scattering, neutron scattering). Experimental methods for studying the properties of solid materials (Mössbauer effect, NMR, ESR, positron annihilation).
14. The phenomenological theory of superconductivity (thermodynamics of superconductors, I. II. type superconductors, Ginzburg-Landau theory, superconducting vortex)
15. BCS theory of superconductivity, tunnel effect, Josephson effect
16. Many electron systems, electron-electron interaction (Hartree-Fock approximation, correlations, dielectric constant, screening, plasmons, density function theory).

17. Basic properties of magnetism (Hund's rules, splitting of atomic levels in magnetic field, diamagnetism and paramagnetism, paramagnetic resonance, Pauli paramagnetism, exchange interaction, direct exchange, super exchange, RKKY exchange)

18. Ordered magnetic materials (ferro and antiferromagnets, mean field theory, spin waves, magnetic anisotropy, magnetic domains) disordered magnets (spin glasses)

19. Low-dimensional systems (magnetic models in 1 and 2D, super-lattice, magnetic coupling through and non-magnetic layer, 1D electron system, Luttinger liquid)