Current subject area:

Solid State Physics

Status	Course code / number in the book: ELECTRONIC STRUCTURE AND PHYSICAL PROPERTIES OF THE MATERIALS			
	Taught by:			
	Ivan Shcherba			
Acad. cycle	**ECTS** credits	**Duration**	**Semester**	**Contact hours**
Barchelor	**4**	**1 semester**	**Winter, spring**	**64**
Year of study	Weekly lectures/seminars		Prerequisites	
5, 6	32/ 32		**Structure of bulk solids, physical properties of crystalline materials, Material science**	
Languages	**Examination**	**Assessment**		
English	Written exam	100 point scale		

Aims and objectives: **Provide with knowledge concerning electron structure, valence state and physical properties of different types of materials. The objective of the course is also to describe the Kondo effect, which are important for mixed valence.**

Description: Basic physical principles of high-energy spectroscopy are reviewed. The book deals with informational content of X-ray emission and absorption spectra of elements. Physical principles of the X-ray photoelectron spectroscopy are considered. Quantitative X-ray electron diagnostics of the material surfaces is analyzed. Substantial attention has been paid to description of results of theoretical and experimental study of physical properties, valence state and electronic structure of binary and ternary intermetallic compounds.

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Reading list:

1. I. D. Shcherba HIGH – ENERGY SPECROSCOPY OF MATERIALS, Lviv, 2018. 320 p.

ELECTRONIC STRUCTURE AND PHYSICAL PROPERTIES OF THE MATERIALS

Education program

(Prof. Dr Ivan Shcherba)

Lecture 1. X-ray emission spectroscopy

- Informational content of X-ray emission spectra
- Moseley's Law
- Theory of spin doublets
- Form and width of the X-ray spectrum lines
- Basic features of design of high resolution x-ray spectrometers

Lecture 2. Interpretation of X-ray spectra in solids

- Main lines and bands of the X-ray emission spectrum.
- Modern methods of obtaining X-ray emission spectra.
- Tube spectrometer with the RKD-01-1 X-ray coordinate detector.
- The RKD-01-1 complex for X-ray registration.
- Techniques of the M-spectra study.
- X-ray spectroscopy of elements of the second large period.
- X-ray emission spectra in the unified energetic scale

Lecture 3 X-ray absorption spectroscopy

- Informativeness of X-ray absorption spectra
- Long wavelength structure of the absorption edge.
- Long wavelength structure of the absorption edge.
- Technique of the X-ray absorption spectra measurement.
- X-ray absorption spectra of rare-earth elements
- Technique for calculation of the rare-earth elements valence

Lecture 4. X-ray photoelectron spectroscopy of solids

- Physical principles of the x-ray photoelectron spectroscopy
- Design features of electron spectrometers
- X-ray photoelectron spectroscopy of metals and their alloys
- X-ray photoelectron spectra of the first transition period metals.
- X-ray photoelectron spectra of compounds with metallic conductivity.
- X-ray photoelectron spectroscopy of crystals with non-metallic conductivity.
- Qualitative x-ray electron diagnostics of surface of solids.
- X-ray spectral and photoelectron study of copper halides.
- The peculiarities of x-ray emission spectra of gallium garnets
- X-ray spectra and electronic structure of the $Ca_3Ga_2Ge_3O_{12}$ compound

Lecture 5. Auger spectroscopy

- Energy of Auger-electrons of a free atom
- Auger-electron energy in solids
- Auger-spectra with participation of valence electrons
- Chemical shifts in Auger-spectra.
- Broadening of lines in Auger-spectra of solids.
- Line broadening related to a final lifetime.
- Phonon broadening.
- Variations of the polarization energy.
- Heterogeneous charge distribution.

Lecture 6. Messbauer spectroscopy

- Method of gamma-resonant spectroscopy.
- Quadruple interaction.

Lecture 6. Electronic structure, chemical binding and physical properties of intermetallides with tetragonal-antiprismatic coordination

- Study of electronic structure of the $Sc_2Fe_3Si_5$ type compounds
- Moessbauer spectra of ^{57}Fe in compounds of $Sc_2Fe_3Si_5$ and $ScFeSi_2$
- Crystalline and electronic structure, and physical properties of the $R_2M_3Si_5$ (M=Co, Ni) type compounds.

Lecture 7. Band structure and properties of compounds with the $CeGa_2Al_2$ structure

- X-ray spectrometry of electronic structure of the RM_2Si_2 compounds
- Band structure and p-d resonance in the RCu_2Si_2 compounds
- Calculation of band structure and shape of the X-ray emission bands of components of the RM_2Si_2 compounds by the LMTO-method.
- Moessbauer spectroscopy of the $ScFe_2Si_2$ compound
- Effect of the d-and f-levels population on the valence state of Ce and Yb in compounds with the $ThMn_{12}$ structure.
- Determination of the Ce and Yb valence state
- Structure of the copper K-edge of absorption in the RCu_4Al_8 compounds
- Structure of the valence band of the RM_4Al_8 compounds.

Lecture 8. Electronic structure and x-ray spectroscopic properties of $R.E.Ni_2P_2$

- Electronic structure and x-ray spectroscopic properties of $YbNi_2P_2$
- Valence State of Ce and Electron Structure of CeM_2P_2 (Fe, Co, Ni) Compounds
- Peculiarities of electron structure of $R.E.M_2P_2$ (R.E.=Y, Ce; M=Fe, Co, Ni, Pd, Rh) components