

PhD STUDIES COURSE UNIT DESCRIPTION

Name of subject	Field of science, code	Faculty / Center	Department
Thin film XRD	Chemistry N 003	FTMC	Characterization of Materials Structure
Student's workload	Credits	Student's workload	Credits
Lectures		Consultations	3
Independent study	7	Seminars	

Course annotation
Methods of examination of thin layers based on X-ray diffraction are presented. The grazing (glancing) incidence method is used for X-ray diffraction measurements of thin layers (30 to 1500 nm) of polycrystalline materials. A parallel X-ray beam falling to the surface of a flat sample at a small angle ($0,3$ to $0,9^\circ$) slips over the surface of the sample over a large area, causing the x-rays diffraction in a much larger volume of material than θ/θ or $\theta/2\theta$ methods and yields sufficiently intense X-ray diffraction peaks even in the case of thin layers. By changing the incidence angle of the X-rays, it is possible to get diffraction from different depths. Layers of only 1 to 10 nm thick can be analysed by the In-plane diffraction method, since special optics produce X-ray diffraction from the crystallographic planes of the layer perpendicular to the surface of the sample i.e. in contrast to the parallel planes in case of the θ/θ or $\theta/2\theta$ methods. These methods of studying thin layers provide information on the phase composition of thin layers, the size of crystallites, the prevailing orientation of crystallites. The X-ray reflectivity method examines the thickness, density and surface(s) roughness of thin layers (3-300 nm) or thin layer packets. This method may also cover non-crystal thin layers.
Reading list
- Thin Film Analysis by X-Ray Scattering. Mario Birkholz. WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim, 2006. - Fundamentals of powder diffraction and structural characterization of materials. Vitalij K. Pecharsky, Peter Y. Zavalij. Springer Science+Business Media, Inc. 2003.

The names of consulting teachers	Science degree	Main scientific works published in a scientific field in last 5 year period
Martynas Skapas	Doctor	M. Skapas, E. Luna, S. Stanionyte, K. Graser, R. Butkute. In Situ TEM Study of Size-Controlled Bi Quantum Dots in an Annealed GaAsBi/AlAs Multiple Quantum Well Structure. <i>ACS Omega</i> 2025, 10, 10, 10432–10437. DOI:10.1021/acsomega.4c10631 S. Stanionytė, T. Malinauskas, G. Niaura, M. Skapas, J. Devenson, A. Krotkus. The Crystalline Structure of Thin Bismuth Layers Grown on Silicon (111) Substrates. <i>Materials</i> 15 (2022) 4847. DOI: 10.3390/ma15144847. I. Uogintė, S. Pleskytė, M. Skapas, S. Stanionytė, G. Lujanienė. Degradation and optimization of microplastic in aqueous solutions with graphene oxide-based nanomaterials. <i>Int. J. Environ. Sci. Technol.</i> (2022). DOI: 10.1007/s13762-022-04657-z V. Karpus, B. Čechavičius, S. Tumėnas, S. Stanionytė, R. Butkutė, M. Skapas and T. Paulauskas. Optical anisotropy of CuPt-ordered GaAsBi alloys. <i>J. Phys. D: Appl. Phys.</i> 54 (2021) 504001. DOI: 10.1088/1361-6463/ac244a. N. Žurauskienė, V. Stankevič, S. Keršulis, V. Vertelis, M. Koliada, V. Rudokas, M. Skapas, M. Vagner, V. Plaušinitienė, A. Guobienė, Š. Meškinis. Hybrid manganite-graphene sensor for magnetic field magnitude and direction measurement. <i>Sci Rep</i> 15, 9100 (2025). DOI:10.1038/s41598-025-94248-y

Vidas Pakštas	Doctor	1. G. Lujanienė, R. Novikau, K. Karalevičiūtė, V. Pakštas, M. Talaikis, L. Levinskaitė, A. Selskienė, A. Selskis, J. Mažeika, K. Jokšas. Chitosan-minerals-based composites for adsorption of caesium, cobalt and europium. <i>Journal of Hazardous Materials</i> 462, 15 (2024), 132747 doi.org/10.1016/j.jhazmat.2023.132747 2. R. Kondrotas, R. Juškėnas, A. Krotkus, V. Pakštas, A. Suchodolskis, A. Mekys, M. Franckevičius, M. Talaikis, K. Muska, Xiaofeng Li, M. Kauk-Kuusik, V. Kravtsov. Synthesis and physical characteristics of narrow bandgap chalcogenide SnZrSe₃. <i>Open Res Eur.</i> (2023) doi: 10.12688/openreseurope.15168.2 3. R. Levinas, V. Pakštas, A. Selskis, T. Murauskas, R. Viter, A. Anspoks, I. Pudza, A. Kuzmin, L. Tamasauskaite-Tamasiunaite, H. Cesiulis. Plasma Electrolytic Oxidation Synthesis of Heterostructured TiO₂/Cu₂O Films for Photoelectrochemical Water Splitting Applications. <i>J. Electrochem. Soc.</i> 171 (2024) 036501 doi. Org/10.1149/1945-7111/ad2ba7 4. V. Pakštas, G. Grincienė, A. Selskis, S. Balakauskas, M. Talaikis, L. Bruc, N. Curmei, G. Niaura, M. Franckevičius. Improvement of CZTSSe film quality and superstrate solar cell performance through optimized post-deposition annealing. <i>Scientific Reports</i> 12, (2022) 16170. doi.org/10.1038/s41598-022-20670-1 5. Ž. Jurgelėnė, D. Montvydienė, S. Šemčuk, M. Stankevičiūtė, J. Pažusienė, G. Sauliutė, A. Morkvėnas, R. Butrimienė, K. Jokšas, V. Pakštas, N. Kazlauskienė, V. Karabanovas. The impact of co-treatment with graphene oxide and metal mixture on <i>Salmo trutta</i> at early development stages: The sorption capacity and potential toxicity. <i>Science of The Total Environment</i> 838, (2022), 156525. doi.org/10.1016/j.scitotenv.2022.156525
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Approved by the Doctoral Committee in Chemistry of Vilnius University and the Center for Physical Sciences and Technology on 30 April 2026, Protocol No. 15600-KT-1611.
Committee Chairman Prof. habil. dr. Audrius Padarauskas.