# DS 9: Optical Analysis of Thin Films II

Time: Thursday 9:30–12:45 Location: H3

**Invited Talk** DS 9.1 Thu 9:30 H3

**Inverse Problems and Uncertainty Quantification for the analysis of thin films and nanostructured surfaces** — •Sebastian Heidenreich[1], Nando Hegemann[1], Victor Soltwisch[2], and Markus Bär[1] — [1]Mathematical Modelling and Data Analysis, PTB, Abbestr. 2-12, 10587 Berlin — [2]Radiometry with Synchrotron Radiation, PTB, Abbestr. 2-12, 10587 Berlin

For the analysis of thin films and nanostructured surfaces, indirect optical measurement techniques are often used to determine the optical and geometrical properties by solving an inverse problem. Due to measurement errors and model errors, the results are subjected to uncertainties. In the talk we give an overview about statistical inverse problems with applications in the metrology of thin films and nanostructured surfaces. We start with a discussion of the advantages and disadvantages of frequently used Least-Squares, then consider the Maximum-Likelihood method and introduce the Bayesian approach as a statistical method [1]. We apply the Bayesian approach to thin film examples as well as to line grating structures and show how to deal with measurement uncertainties and model errors. Furthermore, we discuss some drawbacks of the Bayesian method and present recent developments like polynomial chaos, transport maps or neural networks to tackle these drawbacks [2]. –[1] Soltwisch, Fernandez Herrero, Pflüger, Haase, Probst, Laubis, Krumrey, Scholze, J. Appl. Cryst. 50, 2017; Heidenreich, Gross, Bär, Metrologia 55(6), 2018. [2] Hegemann, Heidenreich, J. Open Software 8 (89), 2023; Hagemann, Hertrich, Casfor, Heidenreich, Steidl, Mach. Learn:Sci. Technol. 5, 2024.

**Invited Talk** DS 9.2 Thu 10:00 H3

**Metrological spectroscopic and imaging Mueller matrix ellipsometry for the analysis of thin films and nanostructured surfaces** — •Bernd Bodermann[1], Matthias Wurm[1], Manuela Schiek[2], Jana Grundmann[1], and Tim Käseberg[1] — [1]Optical Nanometrology, PTB, Bundesallee 100, 38116 Braunschweig — [2]Center for Surface and Nano-Analytics (ZONA) Johannes Kepler University Linz, Austria

Spectroscopic Mueller ellipsometry is a widely used method for analysing thin films and nanostructured surfaces. The extension to imaging ellipsometry enables measurements on small measurement objects << 1 mm2 and investigations of local parameter variations. However, as an integral and indirect measurement method, the determination of the corresponding measurement uncertainties is challenging and requires complex analysis methods. Imaging ellipsometry, involves an even higher level of complexity both in terms of data analysis and the necessary metrological system characterisation. We give an overview of various experimental sources of uncertainty including structure-induced contributions and how these can be characterised. Both deterministic and stochastic contributions of the measurement system as well as the samples under test will be discussed. Additionally, we present investigations of sensitivity-enhanced ellipsometry, by e.g. exploiting local plasmonic or dielectric resonances in the sample structure, and advanced methods that use additional structures to amplify and/or guide resonances for the detection and characterisation of periodic and non-periodic structures.

**session break**

DS 9.3 Thu 10:45 H3

**Structured Light Microscopy for Optical and Topological Characterization** — •Denis Ukolov, Polina Gromova, and Peter Lemmens — IPKM, TU-BS, Braunschweig, Germany

Structured light beams with orbital angular momentum (OAM) are applied to study topological properties of thin films and metasurfaces. Using a laser confocal microscope with integrated interferometry, we investigate phase distributions and topological features of chiral structures.

Experimental data are compared with simulations to understand the interaction of OAM with surface geometry and its topological effects. This method offers a novel approach to characterizing surface properties in complex systems.

Work supported by DFG EXC-2123 QuantumFrontiers - Light and Matter 390837967.

DS 9.4 Thu 11:00 H3

**Synchrotron-based VUV ellipsometry on passivated Si samples for optical thin film metrology** — •Julian Plaickner[1], Alexander Gottwald[2], Mattia Mulazzi[2], Jörg Rappich[3], Karsten Hinrichs[3], Christoph Cobet[4], Johanna Reck[5], and Norbert Esser[1] — [1]Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin — [2]Physikalisch-Technische Bundesanstalt, Abbestr. 2-12, 10587 Berlin — [3]Nanoscale Solid-Liquid Interfaces, Helmholtz Zentrum Berlin für Materialien und Energie GmbH, Albert Einstein Str. 15, 12489 Berlin — [4]Center for Surface and Nanoanalytics, Johannes Kepler Universität, Altenbergerstr. 69, 4040 Linz — [5]SENTECH Instruments GmbH, Schwarzschildstr. 2, 12489 Berlin

The vacuum ultraviolet (VUV) spectral range spectral range is characterized by a lack of reliable data on optical properties due to the extreme surface sensitivity and the requirements of a high brightness light source. A method for determining traceble optical data with well-defined uncertainty budget is tested on novel reference materials. For this purpose, chemically passivated vicinal silicon surfaces were measured between 2 and 30 eV with the synchrotron-based VUV ellipsometer[1] at the Metrology Light Source (MLS) of the PTB. X-ray photoelectron spectroscopy (XPS) and IR ellipsometry measurements serve as quality cross checks for the prepared surfaces. In the spectral range between 2 and 6 eV, results are compared to reference measurements made with commercial SENTECH ellipsometers.

DS 9.5 Thu 11:15 H3

**Tailoring Properties of Epitaxially Grown Bismuth Telluride Thin Films through Stoichiometric Control** — •Felix Hoff, Christoph Ringkamp, Alexander Kiehn, Thomas Schmidt, Dasol Kim, Jonathan Frank, Timo Veslin, and Matthias Wuttig — I. Institute of Physics (IA), RWTH Aachen University, Germany

The Earth's crust contains a significant number of minerals formed by elements such as Bi and Te, which is surprising given their scarcity. This rich mineral diversity can be attributed to strong interlayer interactions within layered chalcogenides, leading to complex phase diagrams. Bismuth tellurides, in particular, exhibit various stacking sequences that influence their properties as thermoelectrics and topological insulators. While their structural and thermoelectric properties are well-studied in bulk forms, high-quality thin films and their optical and vibrational properties remain underexplored. We address this gap by examining the vibrational and dielectric properties of epitaxially grown thin films of nine distinct BiTe compositions grown on Si (111). Using Raman and fs pump-probe spectroscopy, we characterized the lattice dynamics while optical spectroscopy was employed to determine the dielectric properties. The variation in phonon frequencies with respect to the Bi share can be attributed to the differing strengths of the interlayer bonds. The height of the dielectric absorption peak increases with increasing Bi share, accompanied by a shift in the absorption maximum to lower photon energies. Our results demonstrate the potential of the BiTe system as a versatile and tunable platform for thin film applications.

DS 9.6 Thu 11:30 H3

**VUV ellipsometry for the determination of thin film optical constants** — •Mattia Mulazzi[1], Julian Plaickner[2], Jörg Rappich[3], Alexander Gottwald[1], and Norbert Esser[2] — [1]Physikalisch-Technische Bundesanstalt, Abbestr. 2-12, 10587, Berlin, Germany — [2]Technische Universität Berlin, Hardenbergstr. 36, 10623, Berlin, Germany — [3]Helmholtz-Zentrum-Berlin für Materialien und Energie, Hahn-Meitner Platz 1, 14109 Berlin, Germany

Motivated by the purpose of determining the optical constants of thin films materials, we present our investigation method based on spectroscopic ellipsometry in the vacuum-ultraviolet spectral range using monochromatised synchrotron radiation. The measurements are characterised by low noise and high accuracy, both quantified according to state-of-the-art metrological procedures, and are well-suited to be fit by numerical methods to obtain the refractive index and the absorption coefficient in a non-parametric way, i.e., independent of the underlying physics of the material under investigation. We show exemplary measurements on surfaces of hydrogen-passivated Si, native SiO2 on Si, graphene on Si and the evaluation steps necessary to determine the optical constants from the measured data.

**session break**

DS 9.7 Thu 12:00 H3

**Optical absorption by two-dimensional excitons (with and without screening)** — •Stefan Zollner and Carlos Armenta — New Mexico State University, Las Cruces, NM

Two-dimensional excitons form not only in 2D layered materials (such as transition metal dichalcogenides) or in quantum wells. They also dominate the visible absorption by 2D van Hove singularities in 3D semiconductors. As an example, we measured and calculated the optical absorption of germanium near the $E_1$ and $E_1 + \Delta_1$ transitions. The 2D character of these transitions stems from the large optical mass along the (111) direction, where the highest valence bands and the lowest conduction band are nearly parallel. Elliot's formalism for the Sommerfeld enhancement of optical absorption (as modified by Tanguy for 2D excitons) provides an excellent description of these absorption peaks, if the momentum matrix element from $\vec{k} \cdot \vec{p}$-theory is used as the optical dipole matrix element. We also discuss how band filling with Fermi-Dirac statistics after intense laser excitation reduces the absorption. We are not aware of a (Banyai-Koch) theory that can be applied to the screening of 2D excitons. This work was supported by the US Air Force (FA-9550-24-1-0061).

DS 9.8 Thu 12:15 H3

**All-optical quality-control of indenene intercalation into graphene/SiC** — •Cedric Schmitt[1,2], Simone Sotgiu[3], Stefan Enzner[2,4], Jonas Erhardt[1,2], Elena Stellino[3], Domenico Di Sante[5], Giorgio Sangiovanni[2,3], Ralph Claessen[1,2], Simon Moser[1,2], and Leonetta Baldassarre[3] — [1]Physikalisches Institut, Universität Würzburg — [2]Würzburg-Dresden Cluster of Excellence ct.qmat — [3]Department of Physics, Sapienza University of Rome — [4]Institut für Theoretische Physik und Astrophysik, Universität Würzburg — [5]Department of Physics and Astronomy, University of Bologna

Intercalating two-dimensional quantum materials beneath a sheet of graphene provides effective environmental protection and facilitates ex situ device fabrication. However, developing a functional device requires rapid, large-scale screening methods to evaluate the quality of the intercalant, which to date can be monitored only by slow, UHV-based surface science techniques. In this study, we utilize ex situ Raman micro-spectroscopy to optically and non-destructively identify the quantum spin Hall insulator indenene, a monolayer of indium sandwiched between a SiC(0001) substrate and a single sheet of graphene. Color modulation combined with indenene's distinctive low-frequency Raman fingerprint enables rapid assessment of its homogeneity and crystalline quality. Density functional perturbation theory indicates that this Raman signature originates mainly from indenene's shear and breathing modes, while additional higher-order modes are tentatively attributed to defect-assisted and two-phonon Raman processes.

DS 9.9 Thu 12:30 H3

**Moiré lattice of twisted bilayer graphene as template for non-covalent functionalization** — •Tobias Dierke[1], Stefan Wolff[1], Roland Gillen[1], Tamara Nagel[2], Jasmin Eisenkolb[2], Sabine Maier[1], Milan Kivala[3], Frank Hauke[2], Andreas Hirsch[2], and Janina Maultzsch[1] — [1]Chair of Experimental Physics, FAU Erlangen-Nürnberg, Erlangen — [2]Department of Chemistry and Pharmacy, FAU Erlangen-Nürnberg — [3]Organisch-Chemisches Institut, Centre for Advanced Materials, Universität Heidelberg

We present an innovative approach to achieve spatial variations in the degree of non-covalent functionalization of twisted bilayer graphene (tBLG). The tBLG with local twist angle variations between * 5° and 7° was non-covalently functionalized with 1,4,5,8,9,11- hexaazatriphenylenehexacarbonitrile (HATCN) molecules. We observe a correlation between the twist angle of tBLG and the degree of functionalization, determined through Raman spectroscopy. We propose that the adsorption of HATCN molecules follows the moiré pattern of twisted bilayer graphene, preferentially avoiding AA-stacked regions and primarily attaching to regions with local AB-stacking order, resulting in an overall ABA-stacking arrangement. This hypothesis, is further supported by density functional theory (DFT) calculations [1]. [1] Dierke et al., Angew. Chemie Int. Ed., accepted (2024), DOI: 10.1002/anie.202414593