# DS 21: Optical Analysis of Thin Films

Time: Friday 9:30–12:30 Location: REC/C213

DS 21.1 Fri 9:30 REC/C213

**From Semiconductors to Quantum Materials: Ultrafast Optical Signatures Across Chalcogenide Classes** — •Timo Veslin[1], Felix Hoff[1], Jonathan Frank[1], and Matthias Wuttig[1,2] — [1]I. Institute of Physics (IA), RWTH Aachen University, Germany — [2]Peter Grünberg Institute - JARA-Institute Energy Efficient Information Technology (PGI-10), Jülich, Germany

Optical pump probe spectroscopy provides a powerful means to investigate and compare ultrafast dynamics in diverse material classes, ranging from covalently bonded semiconductors to quantum materials. In this study, we contrast the optical and structural responses of sesquichalcogenides like In2Te3 films with those of quantum materials such as Bi2Te3 or Sb2Te3. Femtosecond pump probe and complementary spectroscopic analyses reveal that In2Te3 exhibits remarkably stable optical and vibrational properties across a wide thickness range, attributed to its predominantly covalent bonding network. In contrast, quantum materials based on Bi or Sb display pronounced thickness-dependent responses and strong coupling between coherent phonons and electronic states. These materials demonstrate tunable coherent lattice motions through variations in pump fluence, polarization, and pulse sequencing, offering routes for ultrafast manipulation of quantum states. The comparison highlights a clear distinction between structurally robust semiconducting chalcogenides and highly responsive quantum materials. Together, these findings delineate how bonding character and electronic topology govern ultrafast optical behavior.

DS 21.2 Fri 9:45 REC/C213

**Orientation-Dependent Near-Field Infrared Properties of a Chiral SURMOF** — •Nadine von Coelln[1], Ana C. Fingolo[2], Benedikt Zerulla[3], Marjan Krstić[4], Christian Huck[1], Carsten Rockstuhl[3,4], Christof Wöll[2], and Petra Tegeder[1] — [1]Institute for Physical Chemistry, Heidelberg University, Germany — [2]Institute of Functional Interfaces — [3]Institute of Nanotechnology — [4]Institute of Theoretical Solid State Physics, Karlsruhe Institute of Technology, Germany

Chiral surface-anchored metal organic frameworks (SURMOFs) are promising candidates for enantioselective separation, molecular sensing and optoelectronic applications with circularly polarized light. Given the large possible design space, it is highly important to understand their spectral response and to be able to predictively model SURMOF structures to determine interesting candidates for experimental screening. In this work, we employ infrared scanning near-field optical microscopy (IR-SNOM) to probe anisotropic infrared properties. Crystallites with two distinct molecular orientations exhibited pronounced differences in their near-field infrared spectra. A controlled manipulation of crystal orientation confirmed that molecular orientation is the origin of these spectral differences. A multi-scale modeling approach, spanning single MOF unit cell simulations to thin-film Maxwell scattering calculations, was validated as it reproduced the spectral signatures and strong orientation sensitivity of the material [1].

[1] A. Fingolo, N. von Coelln et al., *Adv. Funct. Mater.* e24088 (2025).

DS 21.3 Fri 10:00 REC/C213

**Pressure-dependent photoluminescence and Raman spectra of GeSn alloys** — •Stefan Zollner[1], Sonam Yadav[1], Meghan A. Worrell[1], Preston T. Webster[2], Rigo A. Carrasco[2], and Perry C. Grant[3] — [1]New Mexico State University, Las Cruces, NM, USA — [2]AFRL Space Vehicles Directorate, Albuquerque, NM, USA — [3]Arktonics LLC, Fayetteville, AR, USA

Optical spectra of $\mathrm{Ge}_{1-x}\mathrm{Sn}_x$ alloys ($x$<10%) grown on Si by chemical vapor deposition were acquired in a gas-membrane diamond anvil cell at pressures up to 10 GPa. The Si substrate contracts hydrostatically under pressure and imposes a biaxial stress on the thin epitaxial layer. The tetragonal distortion of the layer can be calculated from the bulk modulus of the substrate and the elastic constants of the layer. Room temperature Raman spectra of bulk Ge with 532 nm excitation show a parabolic blueshift from 300 $\mathrm{cm}^{-1}$ at atmospheric pressure to 335 $\mathrm{cm}^{-1}$ at 10 GPa. The blueshift due to pressure is linear and slightly larger for Ge on Si. We also acquired photoluminescence spectra of $\mathrm{Ge}_{1-x}\mathrm{Sn}_x$ alloys as a function of temperature and pressure. We observe a blueshift of the infrared $\mathrm{Ge}_{1-x}\mathrm{Sn}_x$ emission at 10 K of 46 meV/GPa which quenches at 0.6 GPa. For MWIR III/V multiple quantum wells, the blueshift is larger at 77 meV/GPa and the emission quenches at 1.3 GPa.

**15 min. break**

DS 21.4 Fri 10:30 REC/C213

**VIPR: A Modular Machine Learning Framework for Inverse Problems with Application to Reflectometry** — •Sascha Creutzburg[1,6], Jeyhun Rustamov[2], Alexandros Koutsioumpas[4], Jens Bornschein[1,6], Marina Ganeva[4], Stefan Häusler[4], Bernd Helm[1,6], Alexander Hinderhofer[5], Mykhailo Levytskyi[4], Valentin Munteanu[5], Robert Juzak[1,6], Vedhas Pandit[2], Frank Schreiber[5], Jeffrey Kelling[2,3], and Nico Mothes[1,6] — [1]Helm & Walter IT-Solutions GmbH, Dresden — [2]Helmholtz-Zentrum Dresden-Rossendorf — [3]Chemnitz University of Technology — [4]Jülich Centre for Neutron Science, Heinz Maier-Leibnitz Zentrum — [5]University of Tübingen — [6]Saxony.AI

Ambiguous inverse problems are ubiquitous in experimental physics, where multiple parameter configurations can reproduce the same measurement and classical iterative approaches are often too slow for online analysis. We present the VIPR framework, a modular machine-learning approach for such problems in thin-film reflectometry. Its reflectometry plugin for X-ray and neutron reflectometry combines three approaches: (i) Reflectorch for fast parameter estimation, (ii) prior-amortized neural posterior estimation, and (iii) neural spline flows to capture multimodal posteriors and reveal alternative plausible structures. VIPR features streaming mode for near-real-time beamline feedback and is deployed at Heinz Maier-Leibnitz Zentrum for routine analysis. The framework integrates seamlessly into existing workflows and can be extended to other inverse problems via its plugin architecture. Code: https://codebase.helmholtz.cloud/vipr/vipr-framework

DS 21.5 Fri 10:45 REC/C213

**Spectroscopic Imaging Ellipsometry at Cryogenic Temperatures: Uncovering a Structural Phase Change in 2D Polar Ga** — •Jakob Henz[1], Arpit Jain[2], Joshua A. Robinson[2], Su Y. Quek[3], and Ursula Wurstbauer[3] — [1]University of Münster — [2]Center for 2DLM, PennState University — [3]Centre for Advanced 2D Materials, National University of Singapore

2D polar metals are a class of atomically thin 2D materials, realized by confinement heteroepitaxial growth (CHet). Hereby, metal atoms are intercalated between a graphene and 6H-SiC interface[1]. This results in a large area, stable 2D metal film with a bonding gradient ranging from covalent over metallic to a vdW-interaction within only two to three atomic layers[2].

Here, we use cryogenic spectroscopic imaging ellipsometry to investigate the temperature dependent light-matter interaction in bilayer 2D polar gallium down to 1 K.

Contrary to theoretical expectations[1], we find a change in the local dielectric response of the material from a homogenous behavior at room temperature to a heterogenous regime at low temperatures, characterized by two absorption peaks localized to distinct surface areas on the sample[3]. This change is interpreted to indicate a structural phase transition in the material.

1 N. Briggs et al., Nat. Mater. **19**.6, 637-643 (2020).
2 M. A. Steves et al., Nano Letters **20**.11, 8312-8318 (2020).
3 J. Henz et al., in preparation (2025).

DS 21.6 Fri 11:00 REC/C213

**Adsorption-Driven Vibrational and Electronic Changes on Cu(110)** — •Sarang Bhasme, Mariella Denk, and Peter Zeppenfeld — Johannes Kepler University, Linz, Austria

Surface resonant Raman spectroscopy (SRRS) provides a sensitive approach for probing phonons and electron-phonon interactions on metal surfaces through resonant coupling to the surface electronic states.[1] In this work, SRRS combined with reflectance difference spectroscopy is employed to investigate adsorption induced modifications of the vibrational response of Cu(110) under ultra-high-vacuum conditions. Time-resolved SRRS measurements during controlled CO and Oxygen exposure reveal systematic evolution in phonon-related features, indicating changes in surface electronic structures and scattering pathways as adsorption progresses. These data enable comparative assessment of molecule-specific interactions and adsorption dynamics on the same surface.

[1] M. Denk et al., Phys. Rev. Lett. 128, 216101 (2022).

**15 min. break**

DS 21.7 Fri 11:30 REC/C213

**Refining the Tanguy dispersion model for strong direct interband interactions** — •Beáta Hroncová and Stefan Zollner — New Mexico State University, Las Cruces, NM, USA

In semiconductors, absorption near the band gap energy is dominated by electron valence-to-conduction band transitions. Exciton formation effectively reduces the band gap and enhances the absorption coefficient. A sharp excitonic peak corresponding to this bound state is observed in the spectral function, especially at low temperatures and low carrier concentrations [1]. At higher temperatures, the bound state is broadened and the peak disappears, but the Sommerfeld enhancement of the absorption persists.

A dispersion model of Wannier–Mott excitons with a screened Coulomb potential was derived by Tanguy [2]. However, if the band gap is small, the interactions between the conduction and valence bands are more prominent. This leads to deviations from the parabolic band curvature, and the effective mass approximation used for the calculation of the excitonic spectra is no longer accurate.

We study the dielectric response of InAs and InSb near the band edge measured by spectroscopic ellipsometry in a wide range of temperatures 50-800 K. With the use of $k \cdot p$ theory, we find the non-parabolicity of the electronic band structure, and describe how to include it in the Tanguy model. Herewith we achieve a better agreement between the theory and the experimental data.

[1] Schweizer et. al., Phys. Rev. Lett. **51**, (1983)
[2] Tanguy, Phys. Rev. B **60**, (1999)

DS 21.8 Fri 11:45 REC/C213

**A Novel Characterization Tool for Optical Coatings and Thin Films** — •Fabian Felixberger[1,2], Ayesha Khan[1,3], Jonathan Noé[1], Michael Förg[1], Manuel Nutz[1], Simone Strohmair[1], Ines Amersdorffer[1,3], David Hunger[3], Theodor Hänsch[2], and Thomas Hümmer[1] — [1]Qlibri GmbH, Munich — [2]Ludwig Maximilian University of Munich — [3]Karlsruhe Institute of Technology

Thin films and nanostructured surfaces play a crucial role in modern science and technology, with their applications ranging from optical components to biosensors. Their precise characterization is therefore essential for understanding and optimizing their function.

We show that inserting such materials in an optical resonator [1] offers a platform which allows the investigation of minimal amounts of scattering and absorption. In addition, it can be utilised for the detection of defects, deviations from surface flatness and local changes of the refractive index.

By raster-scanning the sample, we obtain spatially resolved maps that allow us to distinguish between point-like defects and extended surface features.

Our results prove that we have developed a versatile and open-access tool for non-destructive and quantitative analysis of optical coatings and thin films, suitable for a wide range of materials.

[1] T. Hümmer et al., Nat Commun. 7, 12155 (2016)

DS 21.9 Fri 12:00 REC/C213

**Measuring sub-nanometer oscillations of a thin gold film by a combination of ultrafast imaging ellipsometry and interferometry** — •Markus Olbrich[1,2], Theo Pflug[1,3], Andy Engel[1], Andrés Lasagni[2,4], and Alexander Horn[1] — [1]Laserinstitut Hochschule Mittweida, Hochschule Mittweida, Technikumplatz 17, 09648 Mittweida, Germany — [2]Institut für Fertigungstechnik, Technische Universität Dresden, George-Bähr-Str. 3c, 01069 Dresden, Germany — [3]Carl Zeiss SMT GmbH, Carl-Zeiss-Promenade 10, 07745 Jena, Germany — [4]Fraunhofer-Institut für Werkstoff- und Strahltechnik IWS, Winterbergstr. 28, 01277 Dresden, Germany

Measuring the transient dielectric function of laser-excited surfaces by ultrafast optical metrology is crucial for understanding fundamental processes such as the absorption of laser radiation, the dynamics of the electron-phonon non-equilibrium, or material ablation. Thereby, the measured transient dielectric function always represents the sum of changes in the optical properties and topography. To distinguish between these two contributions, a combination of ultrafast ellipsometry and ultrafast interferometry enables solving this problem. To demonstrate the advantage of the combination of both methods, the transient changes in the dielectric function and the surface topography in terms of periodic oscillations due to the induced shock and rarefaction waves are exemplarily demonstrated for an excited thin gold film upon single-pulsed irradiation with ultrafast laser radiation ($\lambda = 800\,\mathrm{nm}$, $\tau_H = 40\,\mathrm{fs}$) at a fluence of 50 % of the ablation threshold.

DS 21.10 Fri 12:15 REC/C213

**Long-term studies of the defect types in tritiated graphene using Raman microscopy** — •Genrich Zeller[1], Magnus Schlösser[1], and Helmut H. Telle[2] — [1]KIT-IAP, Karlsruhe, Germany — [2]UAM, Madrid, Spain

Tritium loading of graphene and graphene-like materials is of interest, e.g., in astroparticle physics, where such materials are proposed as sources and targets for neutrino experiments like KATRIN or PTOLEMY, or in hydrogen-isotope separation membranes for nuclear fusion. Although hydrogenation of graphene is well established, the radioactive nature of tritium introduces additional experimental challenges and open questions.

Only in recent years has tritiation of graphene been demonstrated using self-radiolysis of tritium. In that initial proof-of-principle study, we found that tritium exposure not only led to the adsorption of atomic tritium but also to the creation of vacancy defects. A key component of the analysis of tritiated graphene is high-resolution Raman spectroscopy, which allows us to measure defect densities and to determine the nature of the defects. In this work, we follow up on our initial studies, and we observe the evolution of defect types during three years of storage under ambient conditions. We find that graphene adsorption sites become strongly depleted, evidenced by the recovery of the characteristic 2D band and an overall decrease in defect density as tracked by the D/G band ratio. The magnitude of this depletion substantially exceeds the annual reduction expected from tritium $\beta$-decay alone, indicating additional removal pathways besides radioactive decay.