ÓBUDAI EGYETEM
ÓBUDA UNIVERSITY

HUN REN | Centre for Energy Research

DEVELOPMENT OF HIGH-SENSITIVITY OPTICAL METHODS FOR THE MONITORING OF INTERFACES

DESHABRATO MUKHERJEE (TK8VY2)

mukherjee.deshabrato@ek-cer.hu

Supervisor:

DR. PÉTER PETRIK

petrik.peter@ek-cer.hu

ÓBUDAI EGYETEM
ÓBUDA UNIVERSITY

HUN REN

Centre for Energy Research

TABLE OF CONTENTS

01 AIM

02 INTRODUCTION

03 FLOW CELL ELLIPSOMETRY

04 JCMWAVE

05 RESULTS

06 FINDINGS

07 CURRICULUM ACTIVITIES

08 FUTURE WORK

AIM

Analyze the Influence of Grating Parameters

Optimize Optical Sensitivity

Investigate Light-Matter Interactions

Compare Simulation with Experimental Data

Enhance Sensing Efficiency

ÓBUDAI EGYETEM
ÓBUDA UNIVERSITY

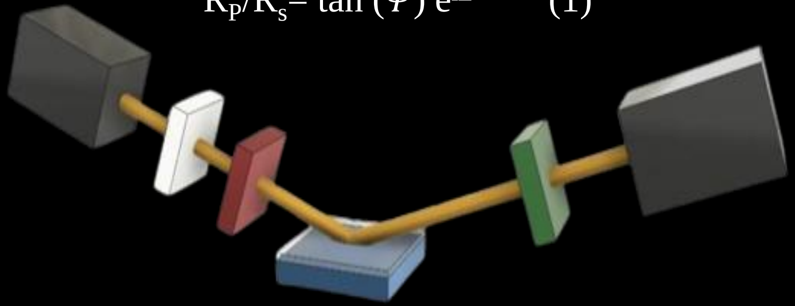
HUN REN

Centre for Energy Research

INTRODUCTION

Ellipsometry measures the change of polarization of an incident beam caused by a sample for determining surface layers.

$$R_P/R_s = \tan(\Psi)\, e^{i\Delta} \qquad (1)$$

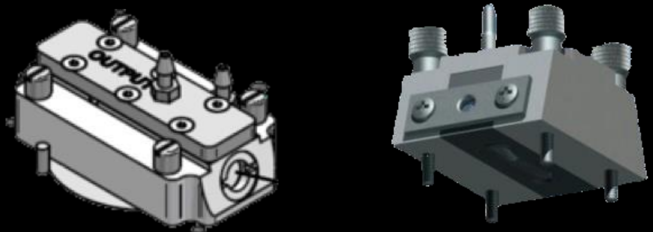


Ellipsometry Phenomenon

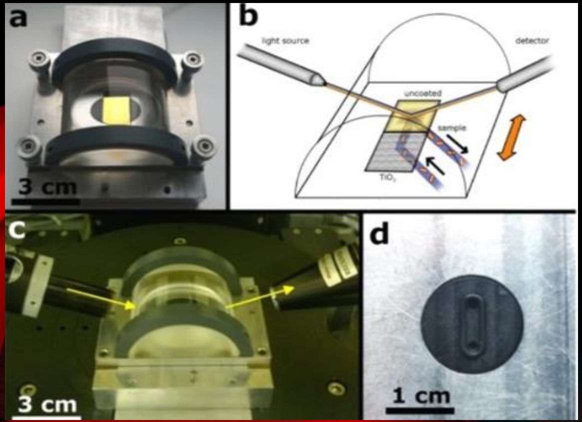
In Situ Spectroscopic Ellipsometry measures a sample "in position" as conditions are varied. The sample can be characterized:

- ❑ Prior to Film Deposition for Accurate Substrate Characterization
- ❑ In Real-time for Thickness and Optical Constants Monitoring
- ❑ Before exposure to Air/Oxidation

FLOW CELL ELLIPSOMETRY



Flow-cells of 'through-liquid' configuration



Kretschmann–Raether Flow cell

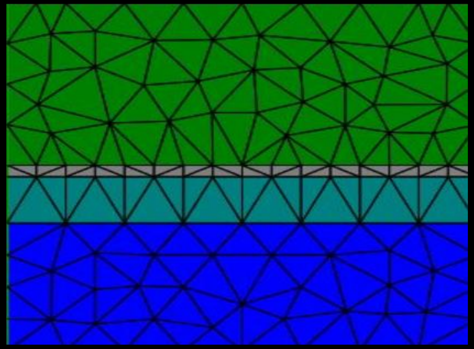
Features of the conventional setup:

- ❑Monitoring of the thickness of adsorbed layers
- ❑Kinetics of adsorption
- ❑Optical Constants (n,k)
- ❑Surface quality before and after processing
- ❑Process conditions that affect optical constants
- ❑Material properties that have an effect on optical constants

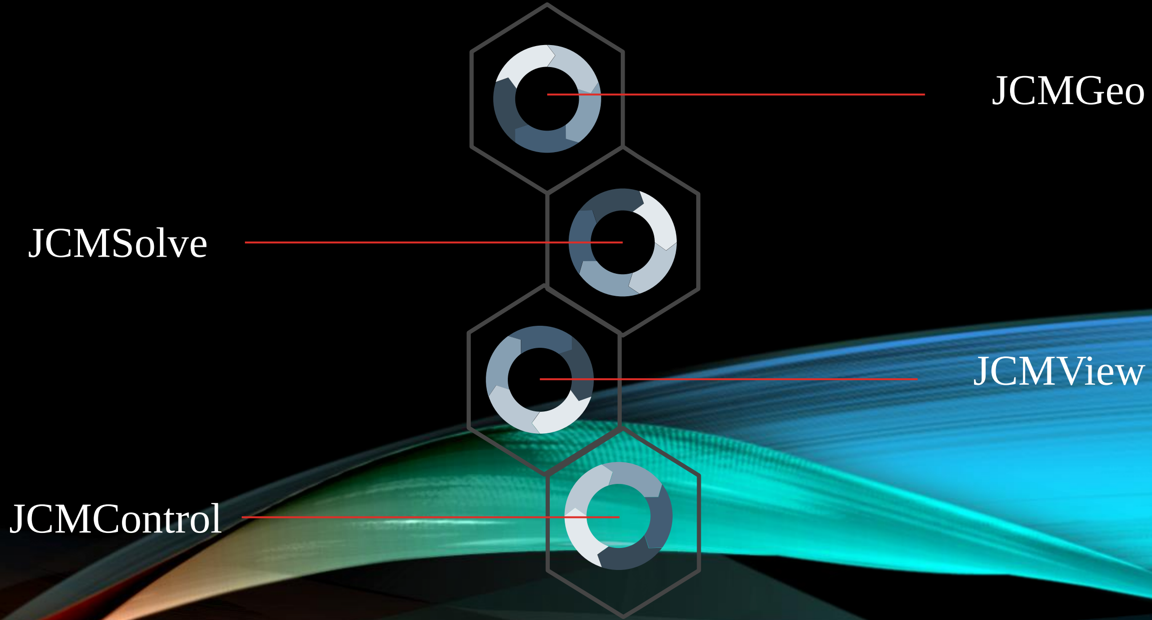
Total Internal Reflection Ellipsometry (TIRE) is a combination of internal reflection and ellipsometry. In the Kretschmann–Raether (K-R) prism geometry, the prism is mounted on a flow cell for measurements in liquids. The surface in contact with the liquid is a thin metal film evaporated on a glass slide, which is in optical contact with the prism by an index matching liquid.

JCMWAVE

JCMsuite is a software package with a focus on fast and highly accurate electromagnetic simulations for finite element analysis. It is based on the following modules:



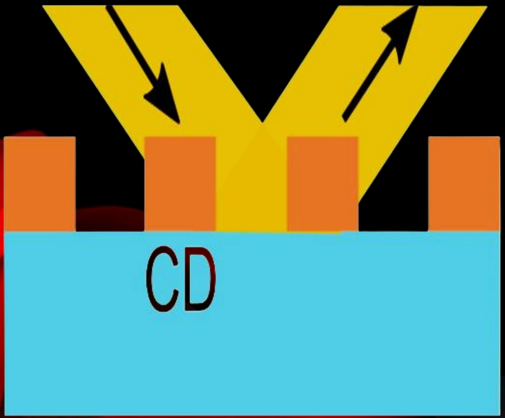
JCM Modelled Kretschmann-Raether Configuration



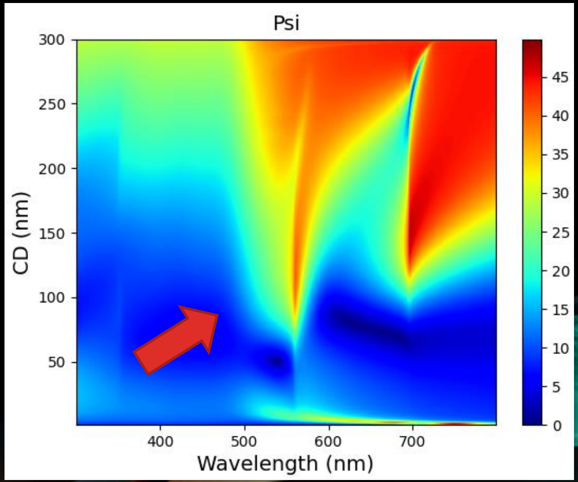
CONVENTIONAL CONFIGURATION

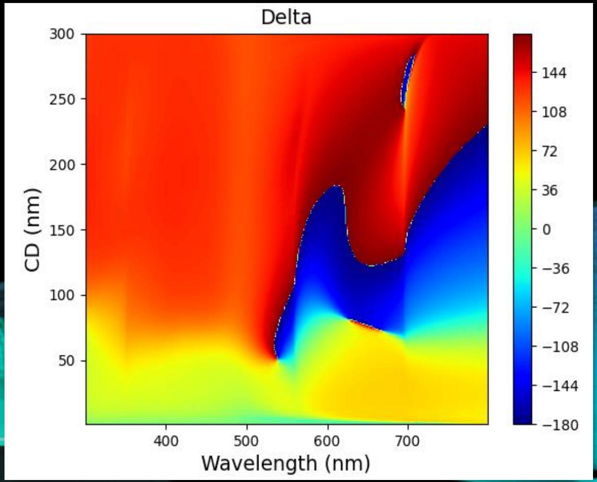
For our experiment, Thickness (d_Au) = 40 nm Au on glass in reflection setup, i.e. air/Au-grating/glass, is modelled using JCMsuite. The parameters used are as follows:

Angle of Incidence (AOI) = 60°, Period = 300 nm, Unit cell = 300 nm x 300 nm, Critical Dimension (CD): Au line width.



Optical configuration





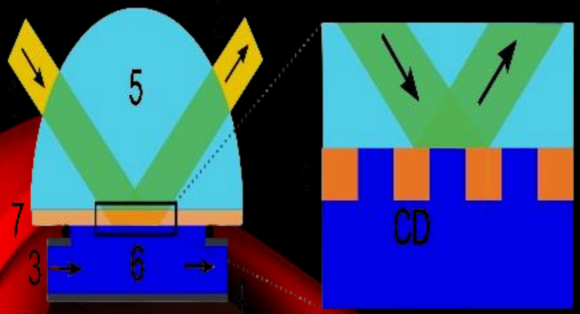
ÓBUDAI EGYETEM
ÓBUDA UNIVERSITY

HUN REN

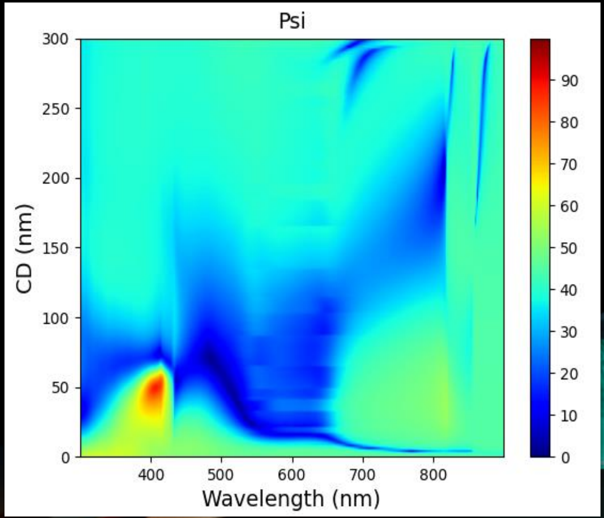
Centre for Energy Research

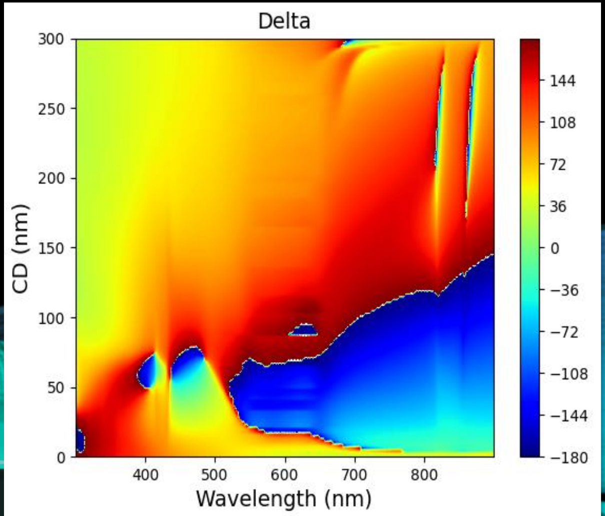
K-R CONFIGURATION

For our experiment, Thickness (d_Au) = 40 nm Au on glass in Kretschmann-Raether setup, i.e. glass/Au-grating/water, is modelled using JCMsuite. The parameters used are as follows:
Angle of Incidence (AOI) = 75°, Period = 300 nm, Unit cell = 300 nm x 300 nm, Critical Dimension (CD): Au line width.



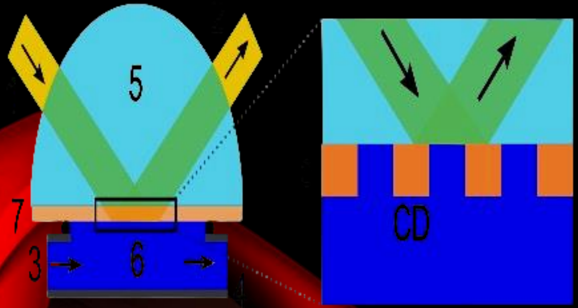
Optical configuration



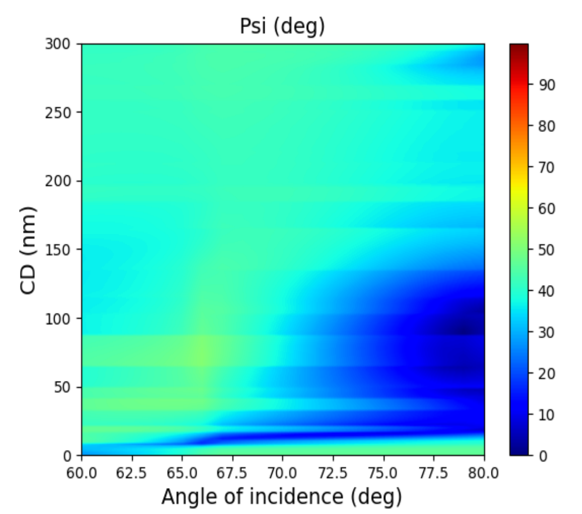


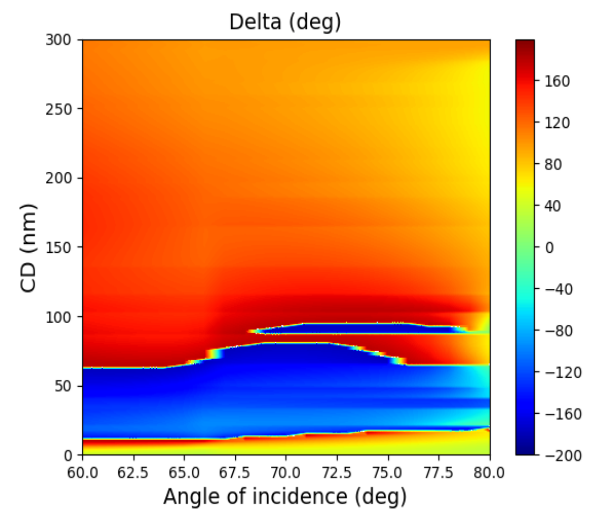
K-R CONFIGURATION

For our experiment, Thickness (d_Au) = 40 nm Au on glass in Kretschmann-Raether setup, i.e. glass/Au-grating/water, is modelled using JCMsuite. The parameters used are as follows:
Angle of Incidence (AOI) = 75°, Period = 300 nm, Unit cell = 300 nm x 300 nm, Critical Dimension (CD): Au line width.



Optical configuration





FINDINGS

ENHANCED RESONANCE SHARPNESS: As the Critical Dimension (CD) increases from 0 to 200 nm, the resonance peaks in the 300-800 nm range become sharper, indicating improved optical performance.

RESONANCE WAVELENGTH SHIFT: A noticeable shift in resonance wavelength is observed from ~500 nm to ~650 nm with increasing CD, highlighting a tunable optical response.

IMPROVED HOMOGENEITY AND FWHM REDUCTION: The homogeneity of the optical response improves with a corresponding reduction in the FWHM of resonance peaks by ~ 50 nm as CD increases.

PHASE CONTROL AND TUNABLE RESONANCE REGIONS: The ability to control phase difference and shift resonance regions by varying the grating parameters provides pathways for optimizing them for specific sensing applications such as biosensing in the K-R configuration, heavy metal sensing applications, etc.

ÓBUDAI EGYETEM
ÓBUDA UNIVERSITY

HUN REN Centre for Energy Research

PUBLICATIONS

No	Publication	IF	Total credit	MTMT ID	Personal credit
1	Mukherjee, Deshabrato, and Peter Petrik. "Real-Time Ellipsometry at High and Low Temperatures" ACS Omega 8, no. 4 (January 31, 2023): 3684–97. https://doi.org/10.1021/acsomega.2c07438.	4.223	36	33570770	36
2	Mukherjee, Deshabrato, Benjamin Kalas, Sven Burger, G. Safran, M. Serenyi, Miklos Fried, and Peter Petrik. "Nanostructures for In-Situ Surface-Enhanced Kretschmann-Raether Ellipsometry" In Photonic Instrumentation Engineering X, edited by Yakov Soskind and Lynda E. Busse, 37. San Francisco, United States: SPIE, 2023. https://doi.org/10.1117/12.2649080.	0.367	24	33699389	24
3	Labadi, Zoltan, Csaba Bakos, Mate Szucs, Attila Bonyar, Deshabrato Mukherjee, Hajnalka Jankovics, Ferenc Vonderviszt, and Peter Petrik. "Ellipsometry Monitoring of Sensor Processes Based on Gold Nanoparticle Bonded Proteins" In Colloidal Nanoparticles for Biomedical Applications XVIII, edited by Marek Osiński and Antonios G. Kanaras, 24. San Francisco, United States: SPIE, 2023. https://doi.org/10.1117/12.2649990.	0.367	24	33724105	24
4	Merkel D.G., Sájerman K., Váczi T., Lenk S., Hegedűs G., Sajti S., Németh A., Gracheva M.A., Petrik P., Mukherjee D., Horváth Z.E., Nagy D.L., Lengyel A. "Laser irradiation effects in FeRh thin film" (2023) Materials Research Express, 10 (7), Art. no. 076101. https://doi.org/10.1088/2053-1591/ace4a3	1.991	36	34536298	18
5	Chou Ta-Shun, Bin Anooz Saud, Grüneberg Raimund, Rehm Jana, Ahktar Arub, Mukherjee Deshabrato, Petrik Peter , Popp Andreas. "In - situ spectral reflectance investigation of heteroepitaxial grown β-Ga_2O_3thin films on c-plane Al_2O_3 via MOVPE process" (2024) Applied Surface Science. https://doi.org/10.1016/j.apsusc.2024.159370	6.779	36	34503364	18
6	Bin Anooz Saud, Petrik Peter, Wang Yankun, Mukherjee Deshabrato, Schmidbauer Martin, and Schwarzkopf Jutta "Dielectric function and interband critical points of compressively strained ferroelectric $K_{0.85}Na_{0.15}NbO_3$ thin film with monoclinic and orthorhombic symmetry". Optics Express, Vol. 32, Issue 9, pp. 15597-15609, (2024), https://doi.org/10.1364/OE.520426	3.420	36	34791151	18
7	Mukherjee Deshabrato, Kertész Krisztián, Zolnai, Kovács Zoltán, Deák András, Pálinkás András, Osváth, Olasz Dániel, Romanenko Alekszej, Fried Miklós, Sven Burger, Sáfrán György, Petrik Peter " Optimized Sensing on Gold Nanoparticles Created by Graded-Layer Magnetron Sputtering and Annealing" Sensors and Actuators B-Chemical, Vol. 425, 136875, (2025),https://doi.org/10.1016/j.snb.2024.136875	8.464	36	35459601	36

ÓBUDAI EGYETEM
ÓBUDA UNIVERSITY

HUN REN Centre for Energy Research

CURRICULUM ACTIVITIES

No	Neptun Code	Subject	Professor	Semester
1	OATBESZ7ND	Research Report VII.	Dr. Recskiné Dr. Borsa Judit Ilona	7
2	OATKUTP7ND	Research Project VII.	Dr. Recskiné Dr. Borsa Judit Ilona	7

CONFERENCES ATTENDED

- Presented my work titled **“Finite element simulations for the optical sensing performance of gold gratings”** at the **23rd ISCMP-2024, August 26-30, 2024, Varna, Bulgaria.**
- Presented my work titled **“The power of using combinatorial materials science and finite element methods in the optimization of sensing by gold nanostructures”** at the **EUROSENSORS XXXVI, September 01-04, 2024, Debrecen, Hungary.**
- Presented my work titled **“Modeling of dimensions and sensing properties of gold gratings by spectroscopic ellipsometry and finite element method”** at the EOSAM-2024, **September 09-13, 2024, Naples, Italy.**

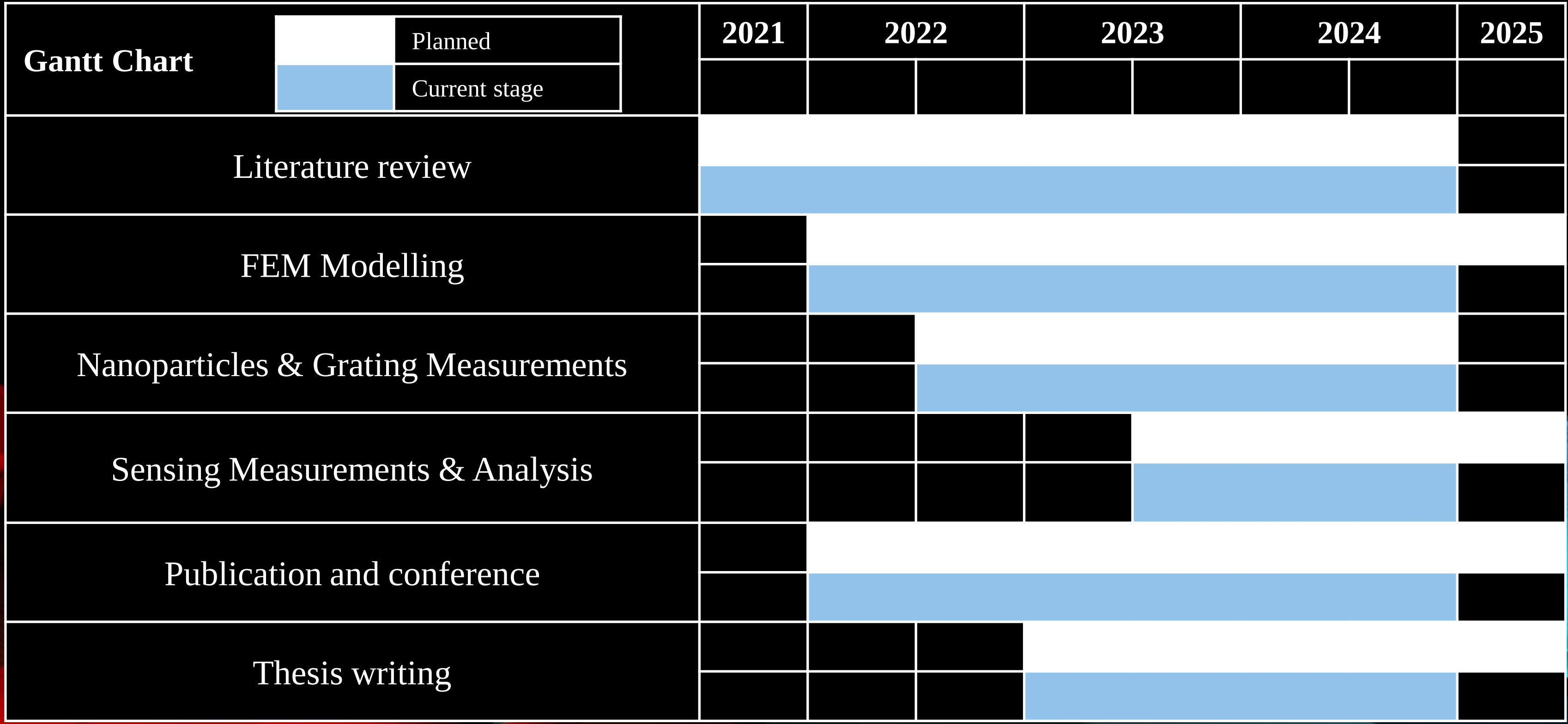
CURRICULUM ACTIVITIES

- Reviewing the related literature of ellipsometry and finite modelling for my future publications and progress.
- Involved in investigations combining spectroscopic ellipsometry with cyclic voltammetry.
- Conducting various measurements on new samples from Leibniz-Institut für Kristalzüchtung (IKZ), Berlin using the J.A. Woollam M-2000 DI ellipsometer in combination of TSEL-1000 heat cell stage ranging up to temperatures of 1000 ^{o}C. The samples were also measured with the J.A. Woollam Mark II IRS ellipsometer.
- Self-development of a novel non-depolarizing Kretschmann-Raether (KR) flow cell for ellipsometry and the preliminary set of sensing measurements of heavy metals were done which will be followed up with further studies and results for a publication. Certain experiments have already been completed for heavy metal sensing in an optical flow cell using monomers of genetically engineered flagellar filaments.
- The first grating structures that arrived from POLight project last semester were measured using M-2000DI SE and these set of experiments were mirrored to study the modeling capabilities for periodic plasmonic nanostructures on JCMSuite. Currently for the modelled grating structure, simulations are being carried out with modification of all the grating parameters such as Critical Dimension (CD), thickness of Au, Wavelength, Angle of Incidence (AOI) and Pitch.

FUTURE WORK

- Submission of review article titled **"In-situ ellipsometry at solid-liquid interfaces"** by the end of this month.
- Final analysis of IKZ samples with SE and IRSE characterization along with heat treatment whose results will lead to an upcoming publication this year.
- Further experiments on the self-developed novel non-depolarizing KR flow cell for sensing measurements of heavy metals and results for another publication.
- Experiments related to heavy metal sensing in an optical flow cell using monomers of genetically engineered flagellar filaments.
- New grating samples from the POLight project has arrived recently which will be measured using M-2000DI SE and these will be again mirrored to study the modeling capabilities on JCMSuite. After the modulation of the grating parameter results obtained in this semester, it will be followed with simulations and experiments for interactions with biomolecules for determining of sensing with and overlayer present. This will be a work which I propose to publish in another D1 journal before the submission of my thesis.
- A culmination of my research work over the last couple of years and the the summarization of my forthcoming research will be presented at the 10th International Conference on Spectroscopic Ellipsometry, ICSE-10 hosted in Denver, USA in June.

GANTT CHART


Gantt Chart
Planned
Current stage
2021
2022
2023
2024
2025
Literature review
FEM Modelling
Nanoparticles & Grating Measurements
Sensing Measurements & Analysis
Publication and conference
Thesis writing

ACKNOWLEDGEMENTS

This research was funded by the National Research, Development and Innovation Office (NKFIH) in Hungary via the Grants Nr. K-146181, K-143216, K-134258 and PD 146479.

The work in the frame of the 20FUN02 "POLight" project has received funding from the EMPIR programme co-financed by the Participating States and from the European Union's Horizon 2020 research and innovation programme.

Project no. TKP2021-EGA04 has been implemented with the support provided by the Ministry of Innovation and Technology of Hungary from the National Research, Development and Innovation Fund, financed under the TKP2021 funding scheme.

- On behalf of the 'MFA-Fotonika-1' project we are grateful for the possibility to use HUN-REN Cloud.
- Project no. C1792954 has been implemented with the support provided by the Ministry of Culture and Innovation of Hungary from the National Research, Development and Innovation Fund, financed under the KDP-2021 funding scheme. A.P. acknowledges the János Bolyai Research Scholarship from the Hungarian Academy of Sciences.

REFERENCES

- www.jcmwave.com/docs/
- qd-uki.co.uk/wp-content/uploads/2019/07/In-Situ-EllipsometryJ-A-Woollam-In-Situ-Brochure-small.pdf
- Matthias Wurm, Tobias Grunewald, Sven Teichert, Bernd Bodermann, Johanna Reck, & Uwe Richter, "Some aspects on the uncertainty calculation in Mueller ellipsometry"; **Optics Express** Vol. 28, Issue 6 pp. 8108-8131, (2020)
- Postava, K., Maziewski, A., Yamaguchi, T., Ossikovski, R., Visnovsky, S., & Pistora, J. "Null ellipsometer with phase modulation"; **Optics Express**, 12(24), 6040, (2004).
- Chen, Y., Meng, Y., & Jin, G. "Optimization of off-null ellipsometry for air/solid interfaces"; **Applied Optics**, 46(35), 8475, (2007).
- Nador, J., Kalas, B., Saftics, A., Agocs, E., Kozma, P., Korosi, L., … Petrik, P. "Plasmon-enhanced two-channel in situ Kretschmann ellipsometry of protein adsorption, cellular adhesion and polyelectrolyte deposition on titania nanostructures"; **Optics Express**, 24(5), 4812, (2016).
- Arwin, H., Poksinski, M., & Johansen, K. "Total internal reflection

THANKS