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

Óbuda University

Doctoral School of Material Science and Technologies

DESHABRATO MUKHERJEE (TK8VY2)

mukherjee.deshabrato@ek-cer.hu

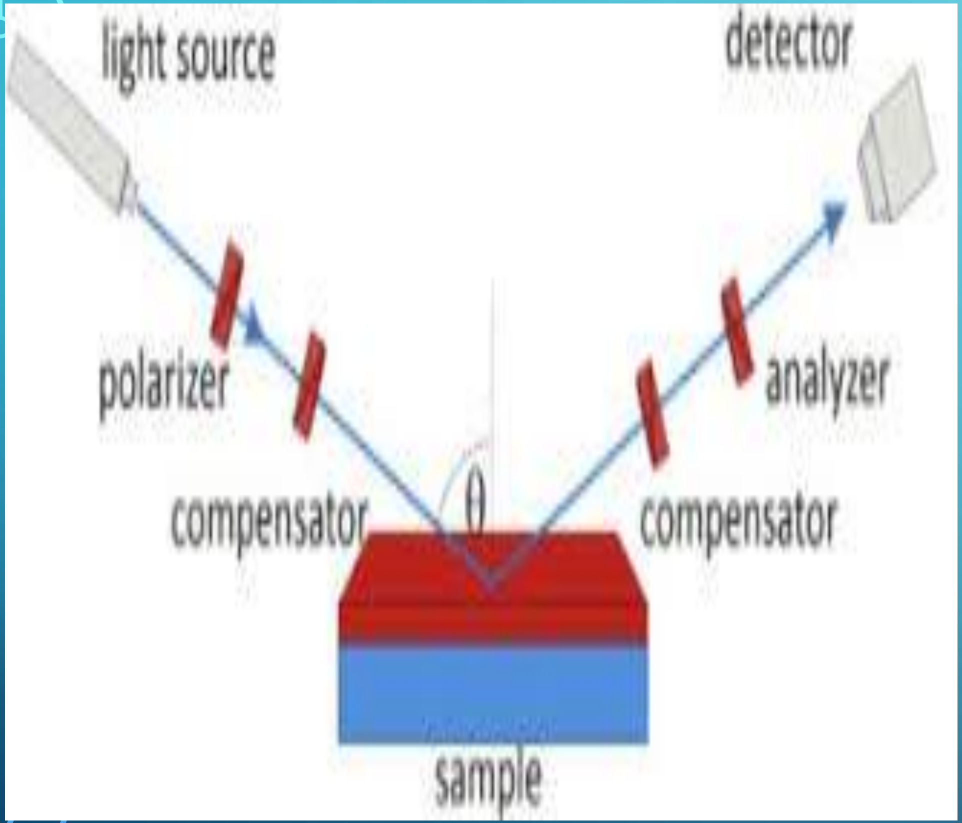
Supervisor:

DR. PÉTER PETRIK

petrik.peter@ek-cer.hu

CONTENTS

INTRODUCTION



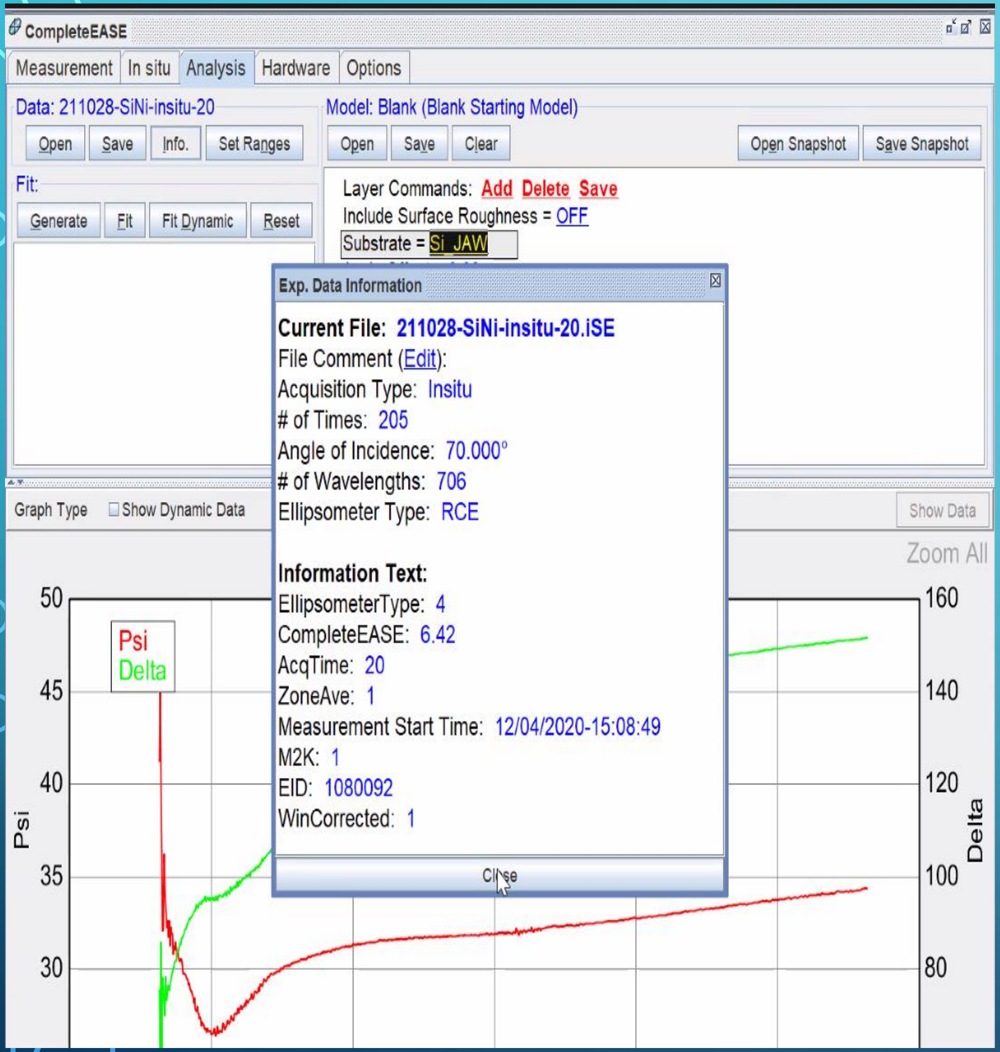
Ellipsometry phenomenon [5]

- **Ellipsometry** measures the change of polarization of an incident beam caused by a sample for determining its geometrical properties.
- Here, a target is illuminated by light with well-defined polarization states to measure a number of field components of the reflected and/or transmitted light. Enabling principle of ellipsometry states that p and s polarized light reflect differently and ellipsometry determines the complex reflectivity ratio of p and s polarized light which is expressed in terms of ellipsometric psi and delta parameters.

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

where, R_p and R_s denote the reflection coefficients of p and s polarized light, $\tan(\Psi)$ is the absolute value of the ratio and Δ is the phase difference between p & s reflected light.

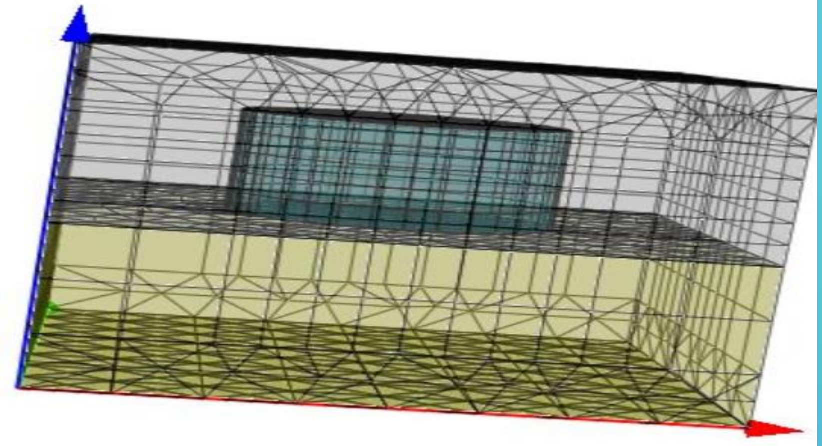
INTRODUCTION



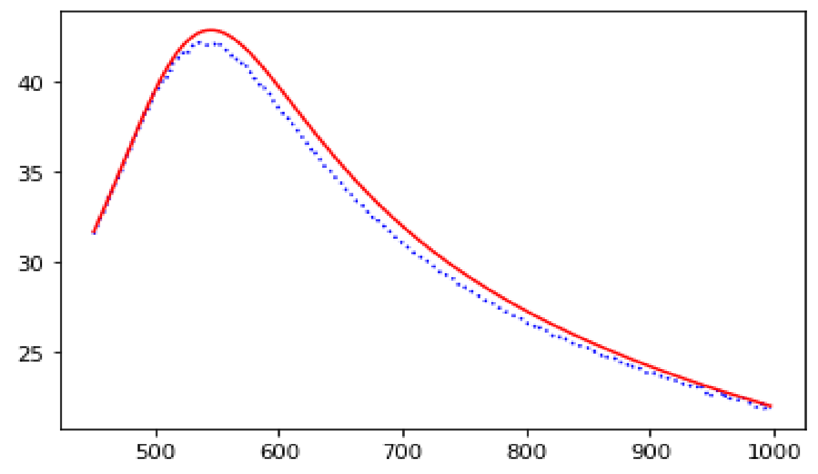
CompleteEASE User Interface

- **CompleteEASE** measures the uniformity of the samples with automated sample mapping and collects in-situ data with spectroscopic ellipsometry on the process chamber or with add-on temperature control stage or liquid cell.
- It includes built-in models covering a wide range of typical samples that conveniently describe how to process the data to determine thin film properties.
- CompleteEASE is the perfect interface for real-time data acquisition, monitoring and control and it has enhanced graphing and model manipulation to handle Mueller-matrix data

INTRODUCTION



Sample JCM model created



Fitting Curve of Psi parameter via Python

JCMsuite is a software package with a focus on fast and highly accurate electromagnetic simulations for finite element analysis. [4] It is based on the Finite Element Method (FEM) and contains following modules:

- JCMgeo
- JCMsolve
- JCMview
- JCMcontrol

Python is an object-oriented high-level programming language first launched in 1992 generally known for its ease of use for writing and understanding coding and programming, Python is an excellent first step with its scope of application is various fields and domains due to:

- Its simple syntax
- Its thriving community
- Its versatility

LITERATURE REVIEW

Modelling effects of non-ideality such as surface roughness

- Here, the ellipsometric response of a large number of random Si surfaces with well-defined root mean square heights and correlation lengths are calculated using finite-element methods (FEM).
- In Effective medium approximation (EMA), the surface roughness is considered a homogeneous layer with an effective dielectric function mixed from the dielectric functions of the two media separating the rough interface.
- The 2D model is simulated using JCM Suite in a wavelength range from 200 to 1000 nm, in steps of 10 nm, for the angles of incidence of 65° and 75°. The simulated topographical parameters for correlation length (ξ) were 2.5, 5, 10 and 20 nm, while for the root mean square height (R_{RMS}) were 0.5, 1, 1.5, 2.5, 3.5, 5, 7.5, 10, 15 and 20 nm with combinations of all these parameter values totaling in 40 points.
- The surface length to be simulated (L) was chosen such that L/ ξ = 500 for achieving adequate Gaussian statistics and diminish deviations
- From the simulation results, for plane wave illumination at an AOI of 75°, and a wavelength of 600 nm small surface features cause high intensity spots that are visible in the near field around the sharp features of surface protrusions of the P polarization that are absent for the S polarization.
- For an identical ξ = 10 nm, the EMA-fitted spectra on simulations with an increasing R_{RMS} value shows an almost perfect fitting for R_{RMS} = 1 nm (d_{EMA} = 0.3 nm), for R_{RMS} = 5 nm case (d_{EMA} = 6.7 nm), small deviations at the UV part of the spectra appears for increasing MSE value. For R_{RMS} = 10 nm case (d_{EMA} = 24 nm), fitting on the whole spectra would be inappropriate, biasing the evaluated roughness.

LITERATURE REVIEW

Finite element modeling approach for computational nano-optics

- The finite-element method (FEM) is a numerical method mostly used to solve partial differential equations (PDEs) and used for simulations of optical effects and optical device properties.
- The examined micro cavities consist of a square shape silicon waveguide perforated with a finite number of periodically arranged cylindrical air pores that forms a finite 1D PhC with a band gap in the relevant wavelength range and supported by a silica substrate.
- Numerical results indicate bandgap between 1,200 and 1,600 nm is formed in the transmission spectrum due to the 1D PhC arrangement and a distinct transmission peak in the bandgap is evident at resonance wavelength of about 1,489.2 nm.
- On closer examination of the wavelength range of 1489.0–1489.5 nm, depicts a 50 picometer FWHM of the resonance in correspondence to a resonance Q-factor of about 30,000.
- It can be thus concurred with various convergence checks that a satisfactory resonance wavelength of 1,479 nm is obtained although the experimental Q-factor value of about 147,000 is significantly higher than the simulation result which can be attributed to the experimental error budgets and the difference between the model geometry and the experimentally realized device
- The reviewed example establishes the fact that higher-order finite elements have very good convergence properties that yields results of very high accuracy while unstructured meshes allow for spatial adaptivity.

RESEARCH PLAN

Sensitivity, miniaturization, and costs are some of the key components that drive the optical biosensor market. In spite of a number of innovative biosensors developed so far, the biosensors market is still far from meeting some of the key requirements such as:

- Biosensors capable of detection and monitoring of multiple analytes, simultaneously.
- Development of integrated lab-on-chip bio-sensing platforms.
- Standardization and multiproduct interoperability among biosensors.
- Availability of wireless options.
- Availability of tracking and communicating bio-sensing data at real time.
- Sensor driven automatic decision analytics through analysis and control.

WORK DONE

In my first semester of doctoral studies for the 2021-2022 session, I have been able to accomplish the following work and objectives:

- Reviewing the related literature of ellipsometry and finite element modelling.
- Operating an ellipsometer and learning the applications of its software known as CompleteEASE
- Learning and running Python to create datasets of obtained ellipsometric data and evaluate simulated data.
- Learning to use the JCMSuite modelling software and creating sample 2D and 3D structures with meshes for finite element modelling.

FUTURE WORK

I am looking forward to build upon my preliminary work and studies conducted in this semester and I propose to accomplish the following work for the next semester:

- Preparing a review article: in-situ ellipsometry on solid-liquid interfaces
- Designing a python program for optical models in ellipsometry
- Finite element simulation of the ellipsometry response of 2D structures
- Experiments with in-situ ellipsometry

REFERENCES

- Sven Burger, Jan Pomplun, Frank Schmidt, "Finite Element Methods for Computational Nano-optics"; (2012).
- B. Fodor, P. Kozma, S. Burger, M. Fried, P. Petrik, "Effective medium approximation of ellipsometric response from random surface roughness simulated by finite-element method"; Thin Solid Films 617, 20–24, (2016).
- B. Kalas, J. Nador, E. Agocs, A. Saftics, S. Kurunczi, M. Fried, P. Petrik, "Protein adsorption monitored by plasmon-enhanced semi-cylindrical Kretschmann ellipsometry"; Applied Surface Science 421 (2017) 585–592.
- www.jcmwave.com/docs/
- Matthias Wurm, Tobias Grunewald, Sven Teichert, Bernd Bodermann, Johanna Reck, and Uwe Richter, "Some aspects on the uncertainty calculation in Mueller ellipsometry"; **Optics Express** Vol. 28, Issue 6 pp. 8108-8131, (2020)
- Hiroyuki Fujiwara**,** **"**Spectroscopic Ellipsometry Principles and Application" Japanese Edition, Copyright 2003, ISBN 4 621 07253 6, Published by Maruzen Co. Ltd, Tokyo, Japan
- H. Raether, Surface Plasmons on Smooth and Rough Surfaces and on Gratings, Springer-Verlag Berlin Heidelberg, 1988.