Babar Ali

Plasmonic ATR–SEIRA Substrates for Oncological Applications

Tutor: Prof. Cutolo Antonello
Co-Tutor: Prof. Marco Pisco

Cycle: XXXVI

Year:21-2022

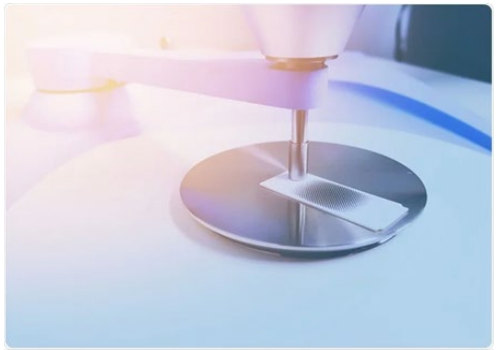
My background

- MSc. degree:Electronics and Communication Engineering
- Research group/laboratory: Information Photonics and Optical Communication
- PhD start date: November,2020
- Scholarship type: UNINA

Summary of study activities

	Courses	Seminars	Research	Tutorship	Total
Bimonth 1	**3**	**1.6**	**10**	**0**	**14.6**
Bimonth 2	**3**	**0**	**8**	**0**	**11**
Bimonth 3	**5**	**0.7**	**6**	**0**	**11.7**
Bimonth 4	**4**	**1**	**5**	**0**	**10**
Bimonth 5	**0**	**0**	**5**	**0**	**5**
Bimonth 6	**0**	**0.8**	**10**	**0**	**10.8**
Total	15	4.1	44	0	63.1
Expected	**10 - 20**	**05-10**	**30- 45**	**0 – 4.8**	

- ***Briefly summarize the study activities of the academic year***
  - *Attended (Courses, Seminars, PhD Schools)*
  - *My research activities for the second year focuses on numerical simulations of suitable SEIRA substrates and the experimental (morphological characterization by AFM and spectral characterization by ATR-FTIR) SEIRA substrates .*
  - ***Ad hoc PhD courses / schools***
  - *Software Defined Radio Applications for Radar and Localization*
  - *Ultra High Field Magnetic Resonance Imaging*
  - *Virtualization technologies and their applications*
  - *Machine Learning for Science and Engineering Research*
- ***Conferences / events attended***
  - *Bio Photonics Conference*
    - *Microscopy and Optical Coherence Tomography ,Biomedical Imaging, Spectroscopy*



FTIR

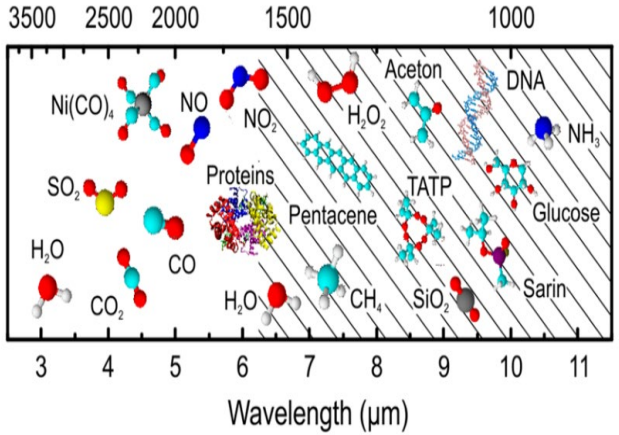
Research activity: Overview

Problem

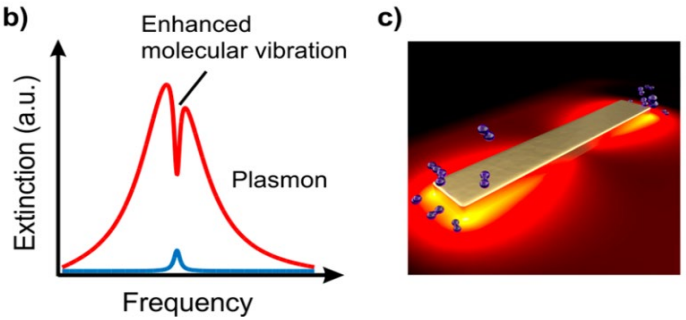
- To access the rich vibrational information of biomolecules and enables the investigation of uniqe structural chracteristic of biosamples
- Identify and develop novel and cost effective and highly efficient plasmonic nanostructures exhibiting good SEIRA properties (namely, the gain factor) in order to improve the detection characteristic of an ATR-FTIR instrument for cell analysis.

Research Objective

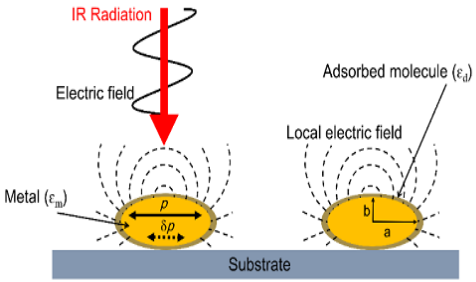
- To reach vibrational signal enhancement, I will exploit the optical properties of specially designed metallic nano particles, which should act as nanoantenna (NA) and the associated field enhancement to obtain a direct detection of bio molecules(**Oncological Applications**).



Different biomolecule in the midinfrared



Characteristic infrared vibrations of selected molecular species. The fingerprint region containing skeletal vibrations is hatched. **(b,c)** Principle (SEIRA)



Schematic representation of the electromagnetic mechanism of SEIRA on metal island film

Chem. Sci., 2020,**11**, 4563-4577

Neubrech et al, Chem. Rev. 2017, 117, 7, 5110–5145

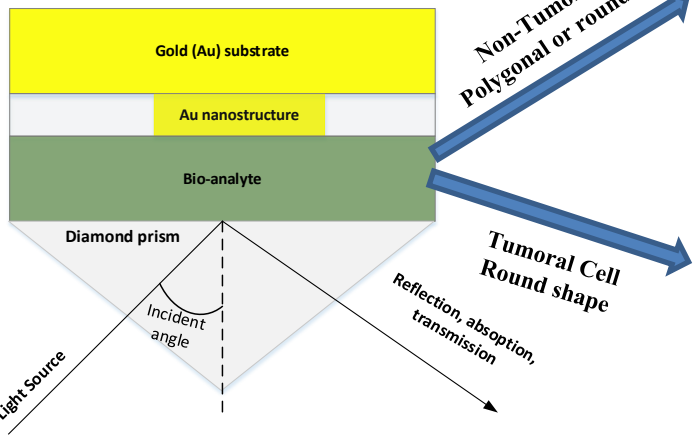
Methodology

- My research activities for the second year focuses on numerical simulations of suitable SEIRA substrates and the experimental characterization SEIRA substrates received from our collaborator from CNR-Milan.
- The two research activities are ongoing concurrently.

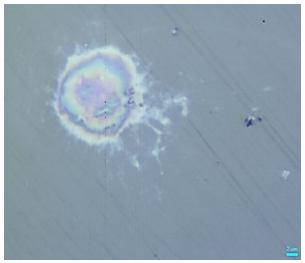
Research activity: ATR-SEIRA Platform

- Identify suitable SEIRA substrate based
  - Nanostructures shape and sizes
  - Spectral Tuning
  - FWHM
  - SEIRA Gain Factor

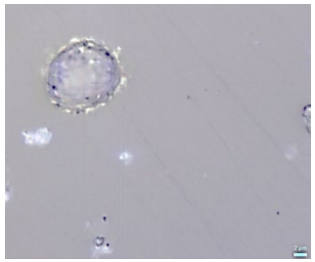
Design based on Otto configuration



Non-Tumoral Cell
Polygonal or round shape



Tumoral Cell
Round shape

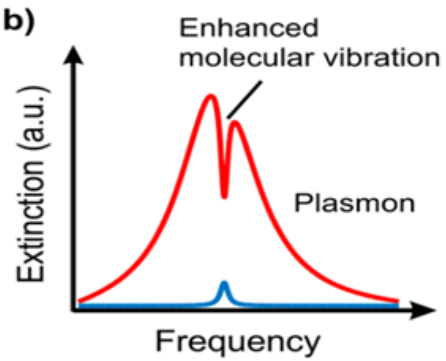


Instrumentation

FTIR instrument

ATR Module

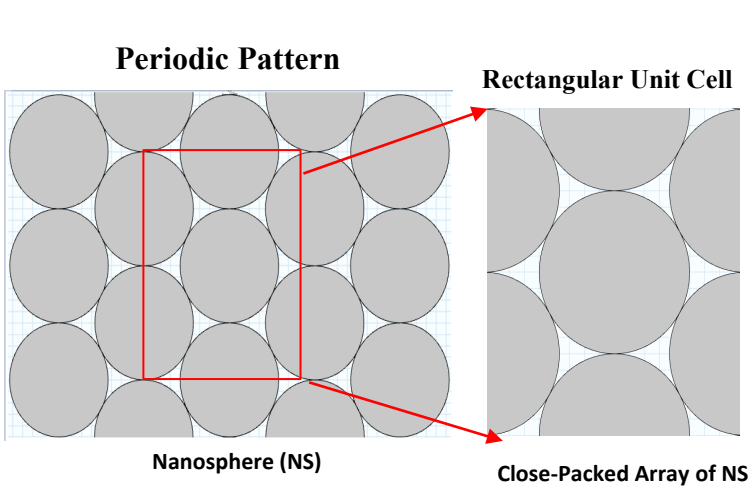
ART-SEIRA vibrational signal of cell are enhanced due to the surface plasmon

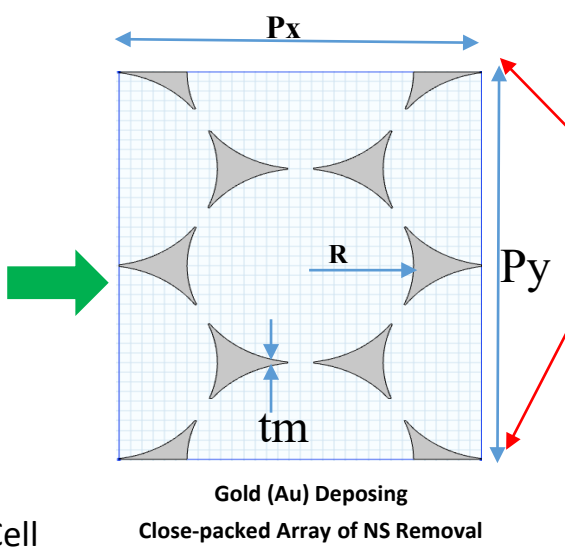


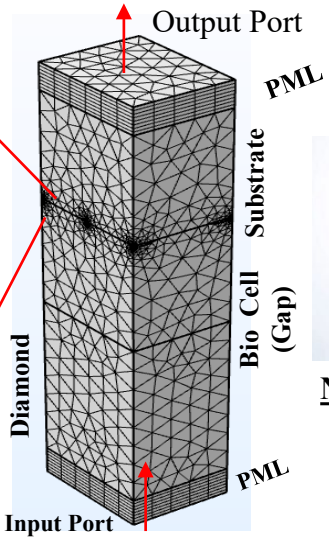
Neubrech et al, Chem. Rev. 2017, 117, 7, 5110–5145

itee PhD information technology electrical engineering

Research activity: Design and Simulation of the SEIRA substrates







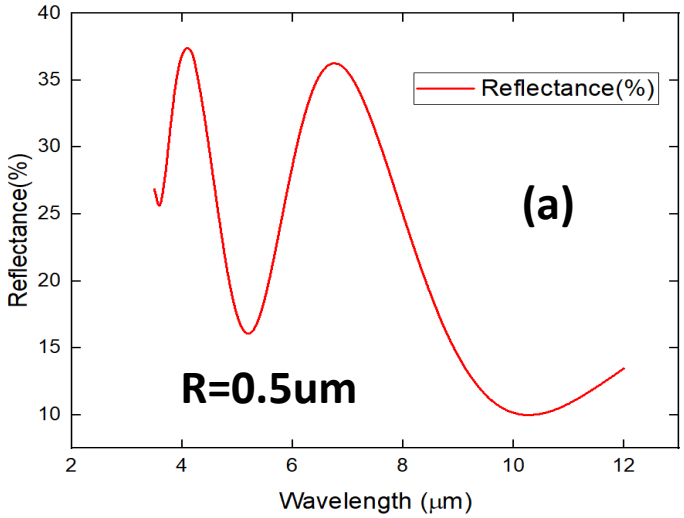
Numerical Tool

Fig. Numerical Procedure of Rectangular Unit Cell

Fig. Design of ATR-SEIRA substrate in COMSOL Multiphysics)

Design Parameters

tm =Thickness of Nanoantenna, **R**= Centre Radius , **Px** =Width of Unit Structure, **Py** = Width of Unit Structure



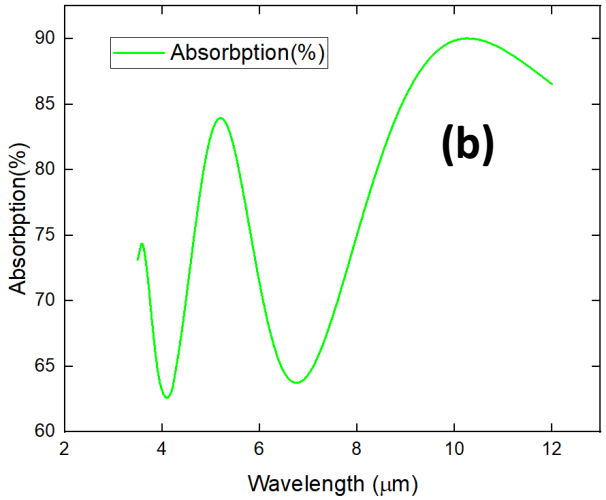


Fig. Reflectance**(a)** and Absorptance**(b)**

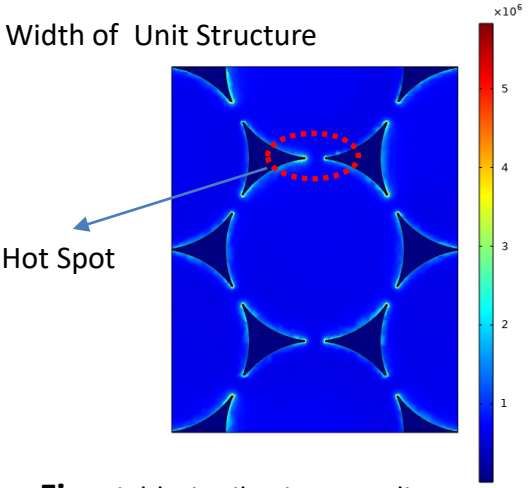
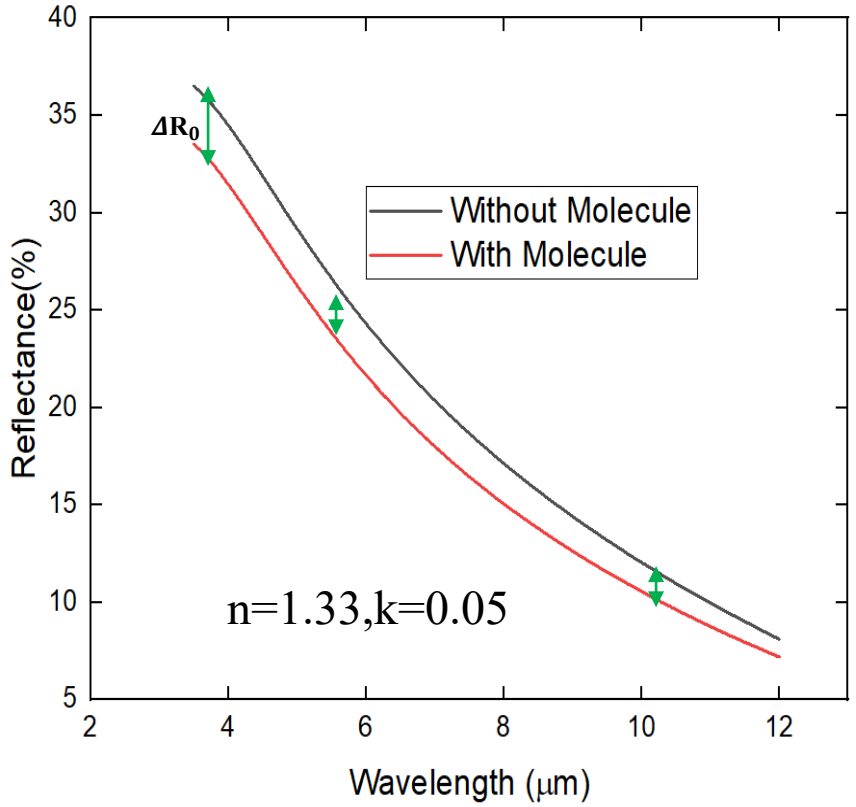


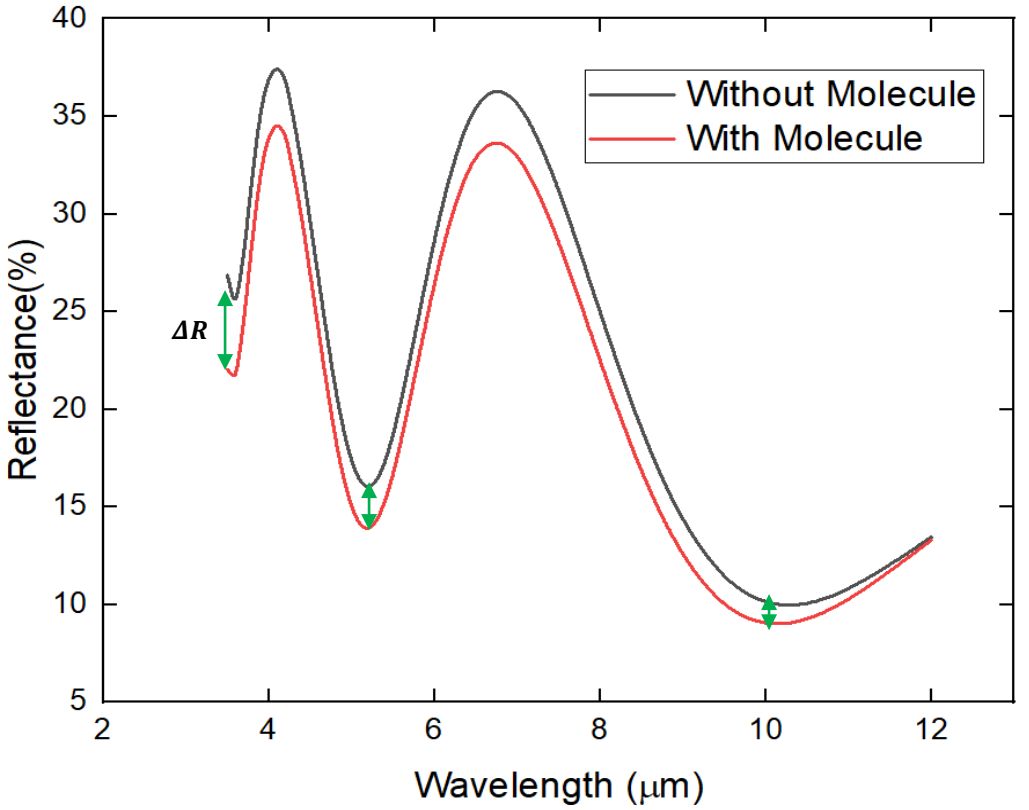
Fig. Field Distribution at z-distance

Noble-metal nanostructures allows a significant enhancement of the local scattered electromagnetic field at nanoscale "hot-spots".

- PBC (Periodic boundary conditions) PML (Perfectly matched layer)

Research activity: SEIRA Gain Factor Calculation





$$SEIRA\ EGF = \frac{\Delta R}{\Delta R_0}$$

ΔR: *Difference of Resonance peak with and without Molecule presence on NA*

ΔR_0: *Difference of Resonance peak with and without Molecule on presence Flat Gold*

Name	Resonance Peak (um)	SEIRA Gain Factor
Peak0	3.6	1449
Peak1	5.2	748
Peak2	10.2	566

Fabrication Process and Experimental characterization

Fabrication Procedure

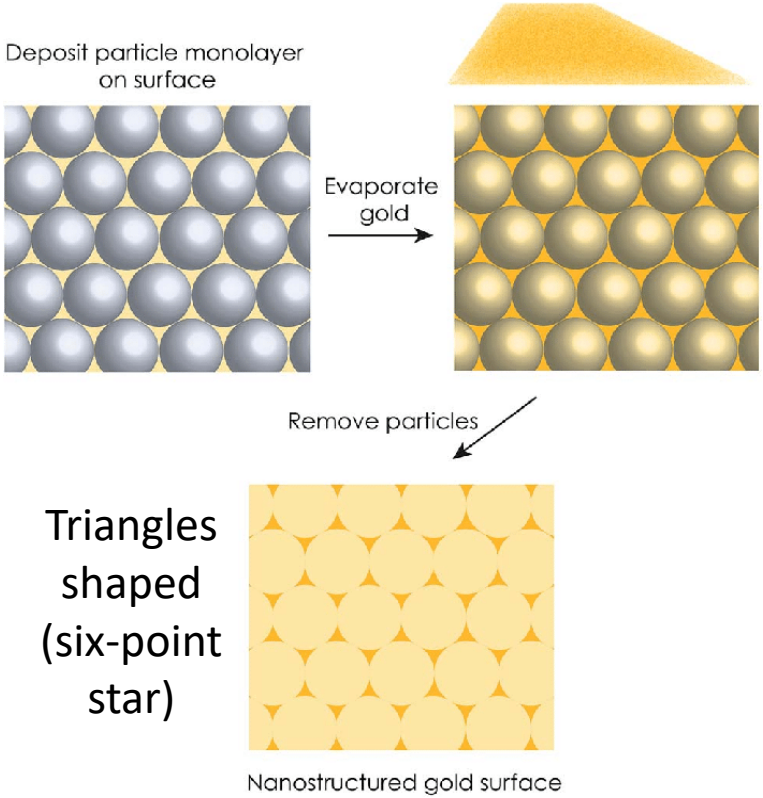


Fig. Schematic Representing the Fabrication Procedure (**Nanosphere lithography**)

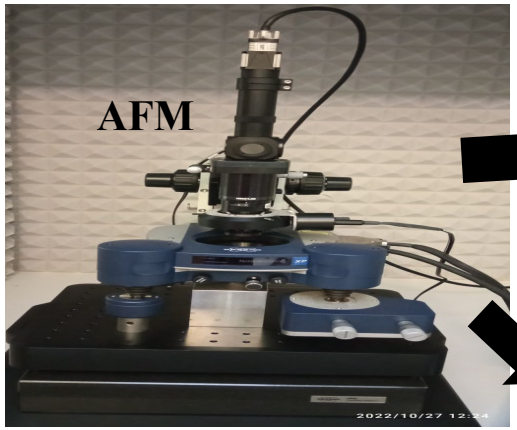
Fabricated Sample from SCITEC-CNR in Milan

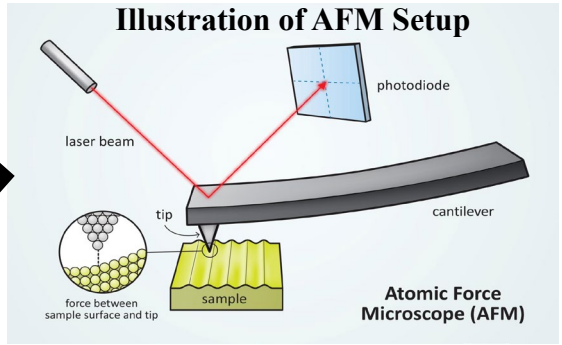
Morphological characterization by AFM

Bruker The Nano Wizard® 4 XP Nanoscience atomic force microscope

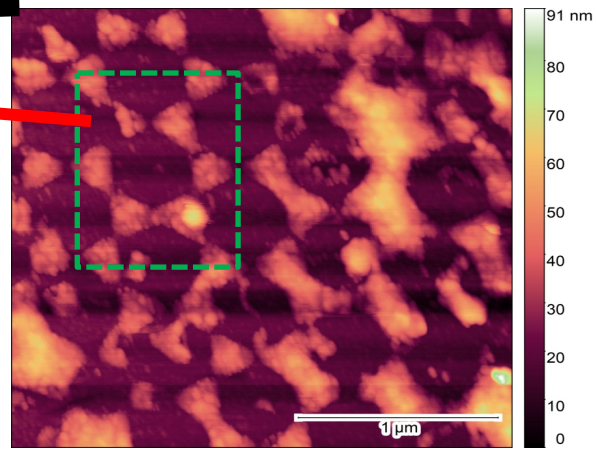
Performance:

- Fast scanning with rates of up to 150 lines/sec, 100µm scan range
- Nested Scanner Technology for high-speed imaging of surface structures up to 16.5µm
- V7 Software with revolutionary new workflow-based user interface
- Vortis™ 2 controller for high-speed signal processing and lowest noise levels





Tapping Mode Scan Measurement



Single rectangular cell

Instrument settings:

- Tapping Mode™ with Phase Imaging™
- Laser align
- Detector align
- 510x510 pixels
- Scan size 2um
- Data processing in Gwyddion

Nanostructure thickness=30nm

Research activity: Experimental characterization

Spectral characterization by ATR-FTIR

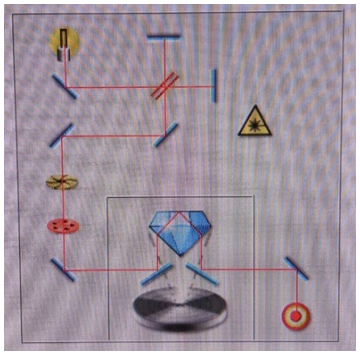
The PerkinElmer Spectrum™ 3 FT-IR spectrometer

- Model: L1280127
- Wavelength range:8500 - 30 cm-1
- Exceptional signal-to-noise ratio and photometric performance
- High reproducibility of spectral data without spectral interferences
- Best-in-class sensitivity, even when using room temperature detectors
- Characterize fast reactions with scan speed up to 100 scans/sec
- Optimize sensitivity and spectral resolution performance

FTIR instrument

ATR Module

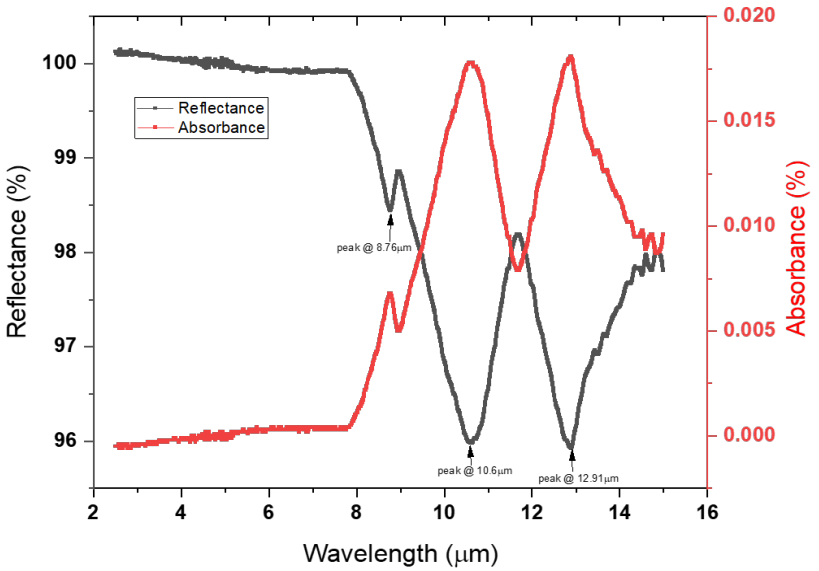
Scheme IR beam path



ATR-FTIR (at CeRICT SCRL-Benevento)

Instrument settings:

- Resolution=4cm^{-1}
- Measurement range = 2.5-16.67 micrometers
- Measured=Reflectance
- Accumulation: 16
- CO_2/H_2O settings
- Scan speed (cm/s)=0.2
- Phase correction=magnitude
- Apodization=strong



Reflectance and Absorbance Spectra