Simulation of thin-film quantum dot solar cells with light-trapping in the IR range

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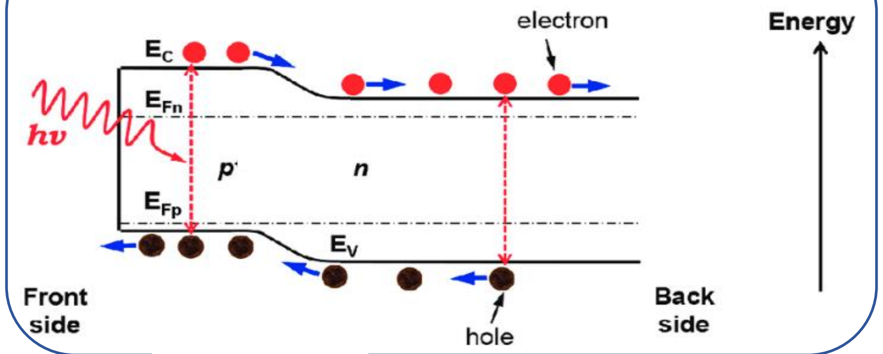
June 12, 2023 - Maïa Pécastaings

1- Topic introduction

QD solar cell with light-trapping

Principle of solar cell in a simple p-n junction:



- Less material
- Less distance for charge carriers to travel

Simulation of thin-film quantum dot solar cells with light-trapping in the IR range

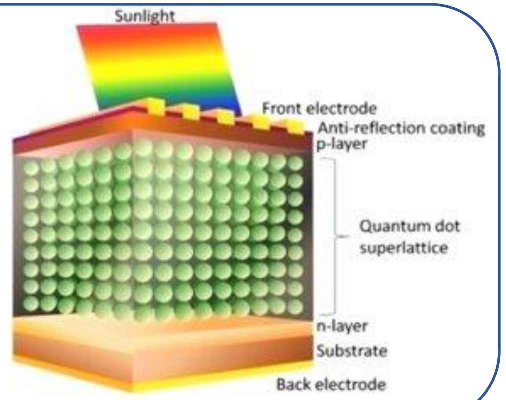
- IR is also interesting: half of the solar spectrum incident on Earth is infrared.
- Requires to be able to absorb photons with lower energy

1- Topic introduction

QD solar cell with light-trapping

quantum dot (QD): tiny nanostructure. When made of semiconductor material, its size determines which wavelengths it absorbs.

p-i-n quantum dot solar cell *: QD layers added in the i-layer to absorb photons.

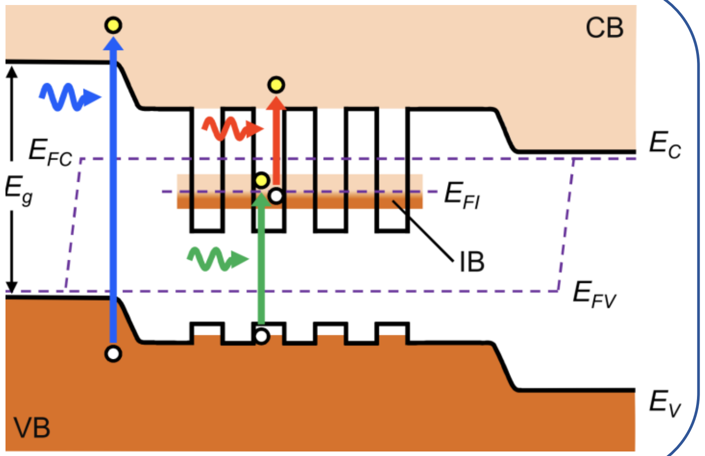


Simulation of thin-film quantum dot solar cells with light-trapping in the IR range

QD solar cells are **intermediate band solar cells.**

With the IB, possibility to **absorb IR photons.**

But in general, too low occupancy of the IB.



*
i (intrinsic): where electron-hole pairs are created
p (positive): where holes are conducted
n (negative): where electrons are conducted

1- Topic introduction

QD solar cell with light-trapping

Simulation of thin-film quantum dot solar cells with light-trapping in the IR range

Goal: increase the absorption in the quantum dots

$$A_{(\lambda)} = \sum^{N_{stacks}} \frac{1}{2} \varepsilon_0 \cdot c \cdot \alpha_{(\lambda)} \cdot d \cdot n_{(\lambda)} \cdot \left| E_{(z,\lambda)} \right|^2$$

Stacking multiple layers
Problem: thicker

Absorption coefficient
- Increase the QD density

Problem: more defects in the material

Field strength
- **Light-trapping strategies**

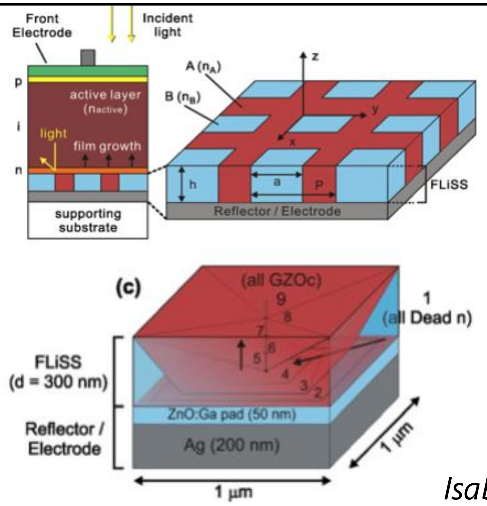
1- Topic introduction

QD solar cell with light-trapping

Goal: increase the absorption in the quantum dots.

Idea: combine two phenomena.

- FLiSS: **light-scattering**



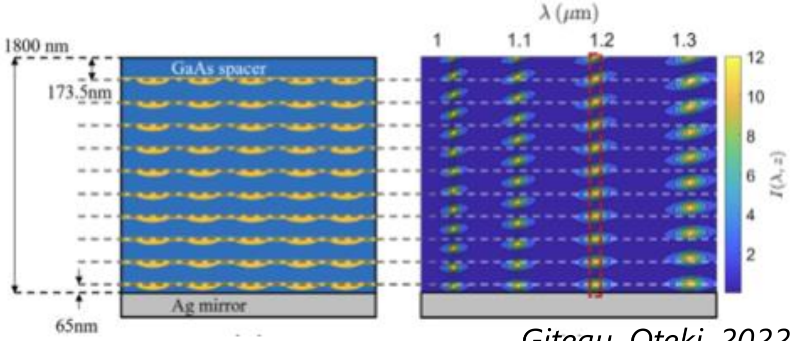
Isabella et al, 2014

A back-grating structure composed of materials with very different refractive indexes can act as **light scatterer.**

= Flattened Light Scattering Substrate (FLiSS)

- Absorption is increased due to higher electric field in the active layer.

- Ag/Au back mirror: **Fabry-Perot resonance**



Giteau, Oteki, 2022

The device, between the air layer and the mirror, forms a cavity with **resonance at specific wavelengths.**

- Absorption is increased when QD layers are positioned on the resonance peaks of a well-chosen wavelength.

Optimize the back-grating to have maximum E-field enhancement.

And then:

Place the QD layers at the peak positions corresponding to this optimized back-grating.

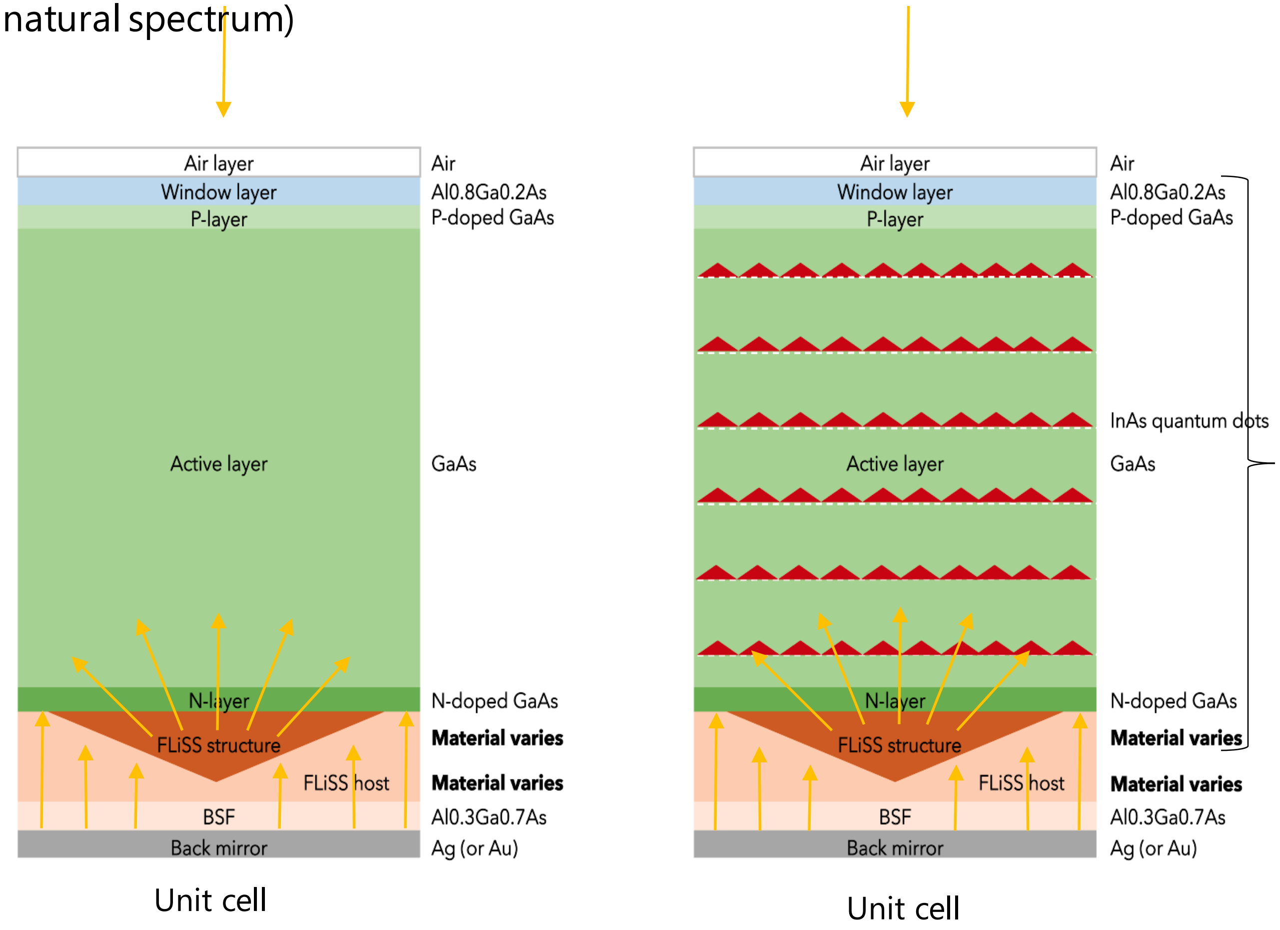
1- Topic introduction

QD solar cell with light-trapping

Goal: increase the absorption in the quantum dots.
In InAs/GaAs QD solar cells with Ag mirror.

For now:

- Incident power 1W (not natural spectrum)
- No quantum dots yet



Optimize the back-grating to have maximum E-field enhancement.

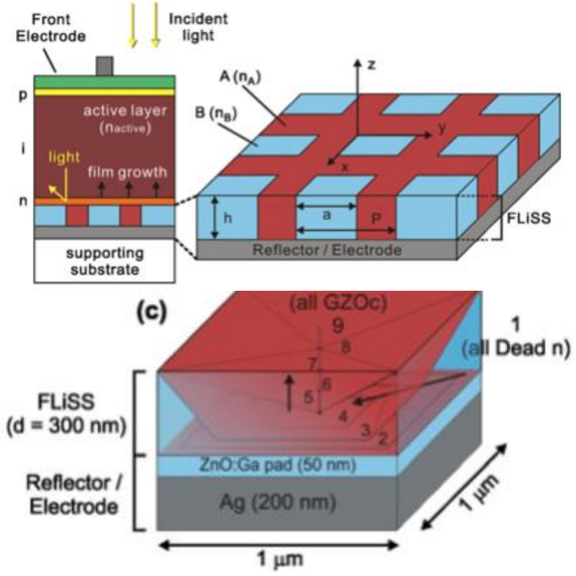
And then:

Place the QD layers at the peak positions corresponding to this optimized back-grating.

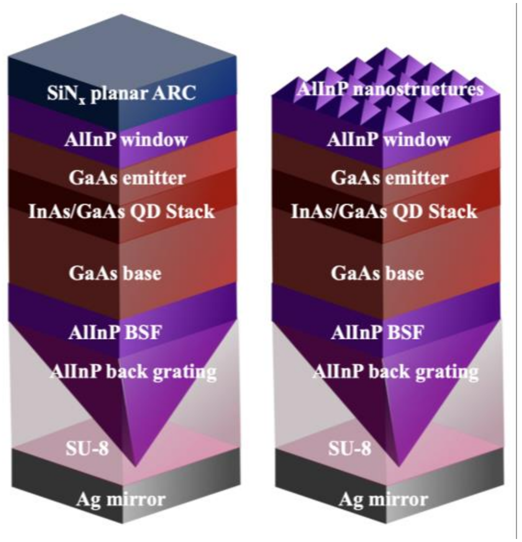
1- Topic introduction

Back-grating pattern

Isabella et al, 2014
In Si solar cell

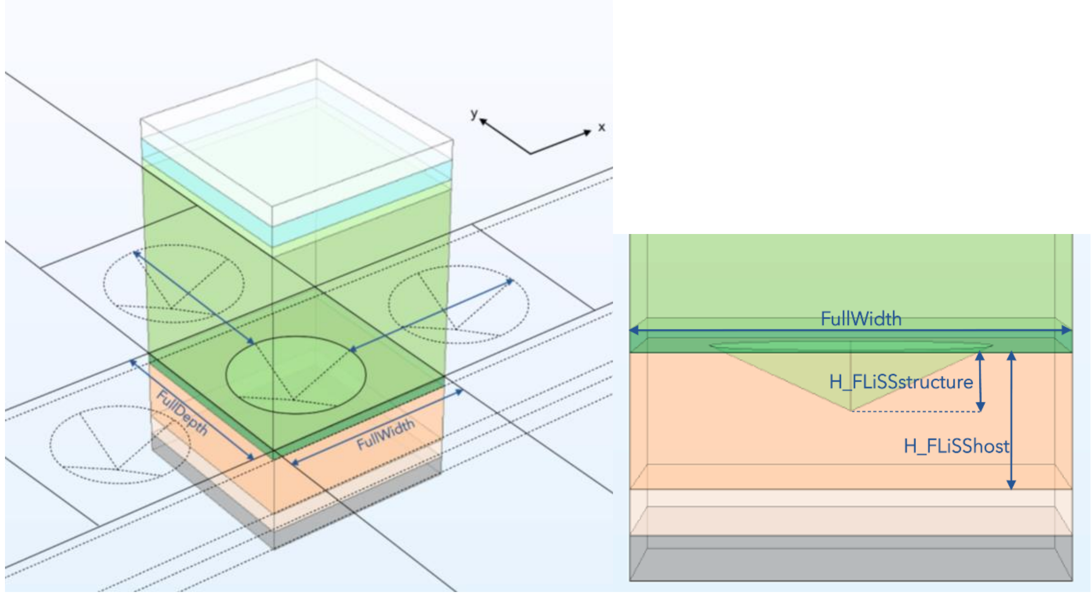


Elsehrawy et al, 2018
In InAs/GaAs QD solar cell



- Structure material: AlInP
- Host material: SU-8

In this study
In InAs/GaAs QD solar cell

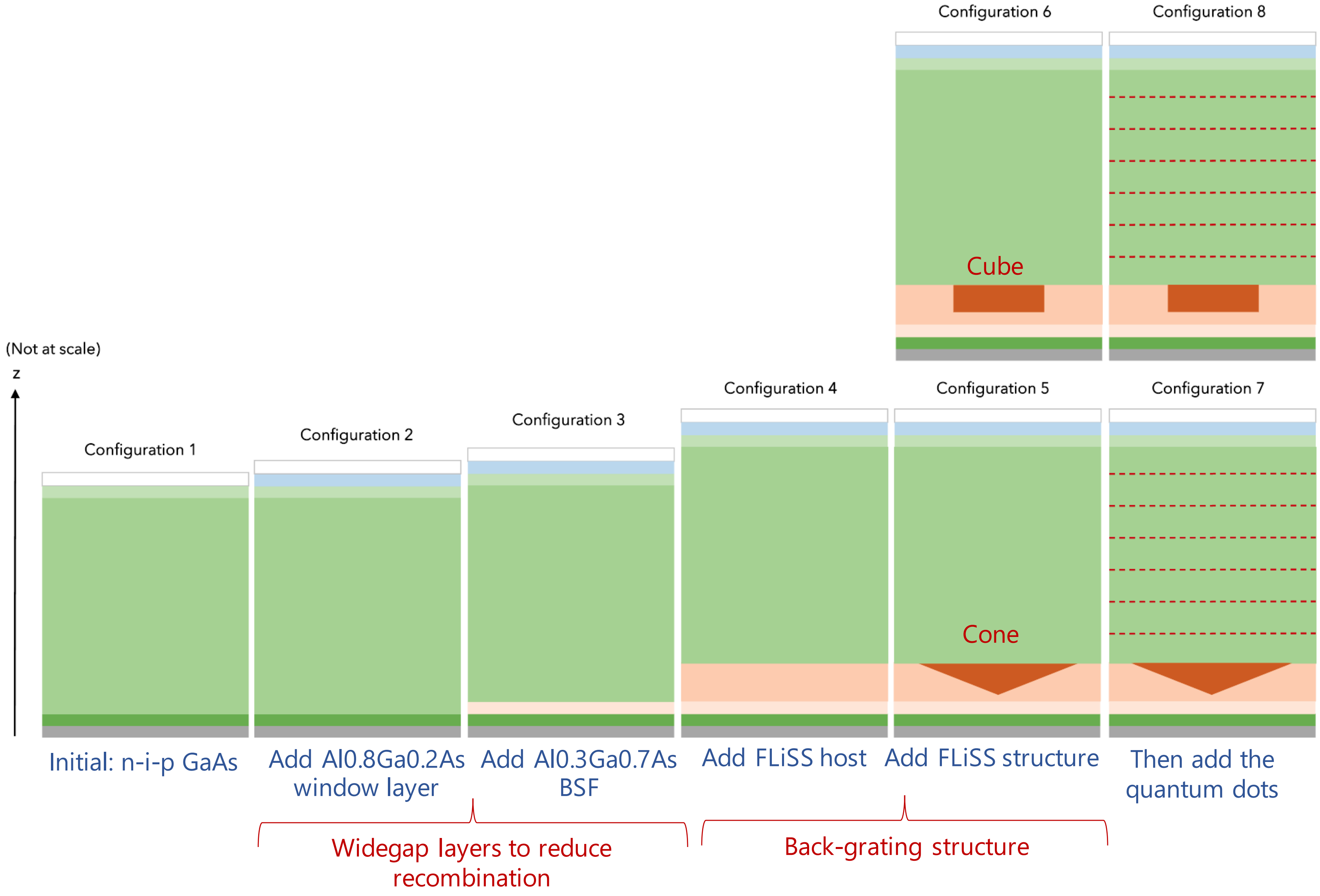


Explore **two shapes**:
- Inverted cone (truncated or not)
- Cube (parallelepiped with square base)

Vary:
- The structure size ad height
- The period of the pattern

2- First simulation results

Simulation steps



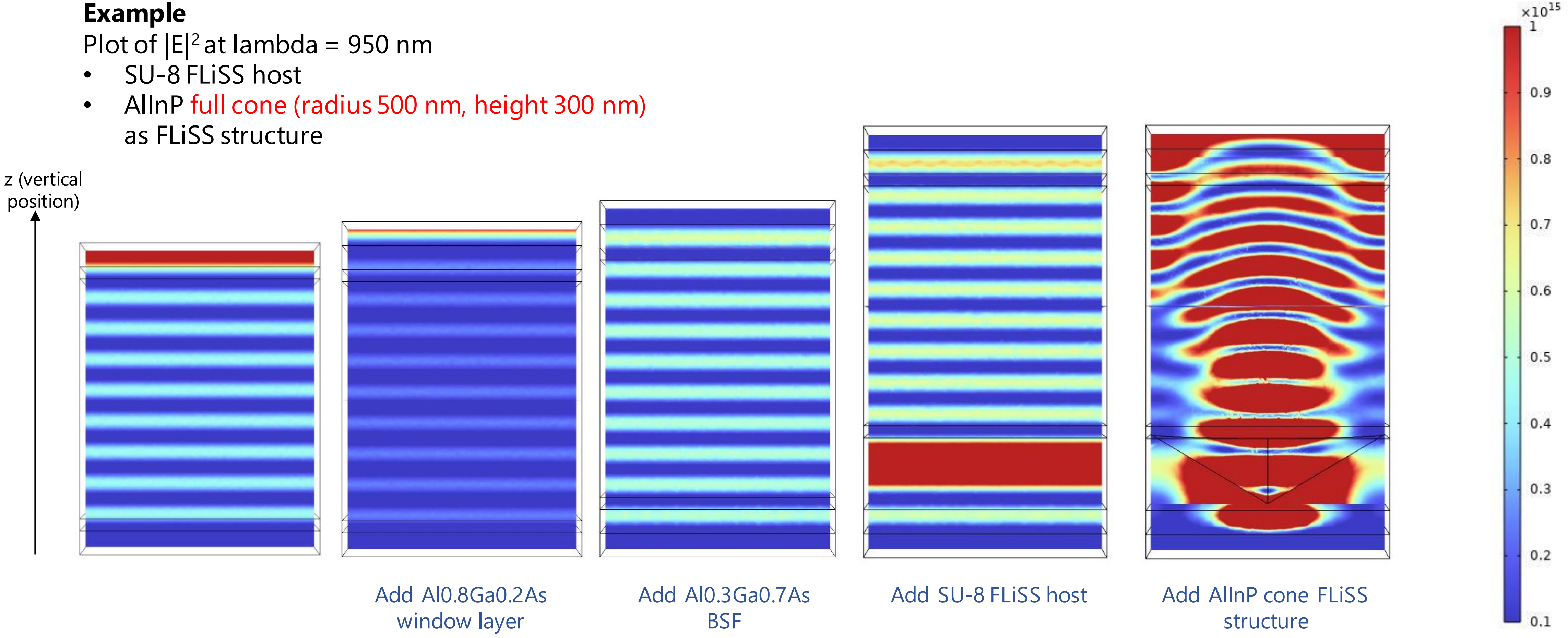
2- First simulation results

E-field distribution in the successive configurations (cone)

Example

Plot of $|E|^2$ at lambda = 950 nm

- SU-8 FLiSS host
- AlInP full cone (radius 500 nm, height 300 nm) as FLiSS structure



One choice of lambda is not representative but:

- In general for almost all wavelengths, the FLiSS structure **enhances** and **distorts** the distribution of **the E-field.**
- However, there is a small displacement of the resonance wavelengths.

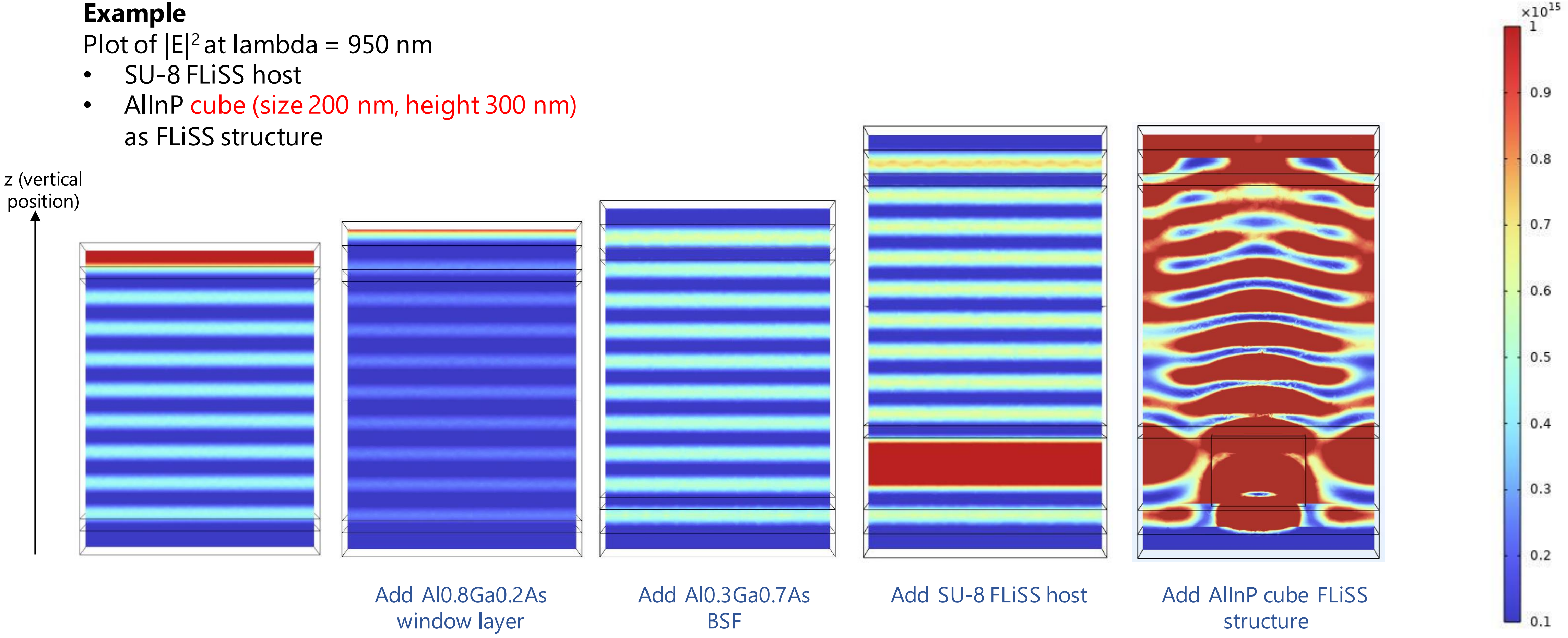
2- First simulation results

E-field distribution in the successive configurations (cube)

Example

Plot of $|E|^2$ at lambda = 950 nm

- SU-8 FLiSS host
- AlInP cube (size 200 nm, height 300 nm) as FLiSS structure



One choice of lambda is not representative but:

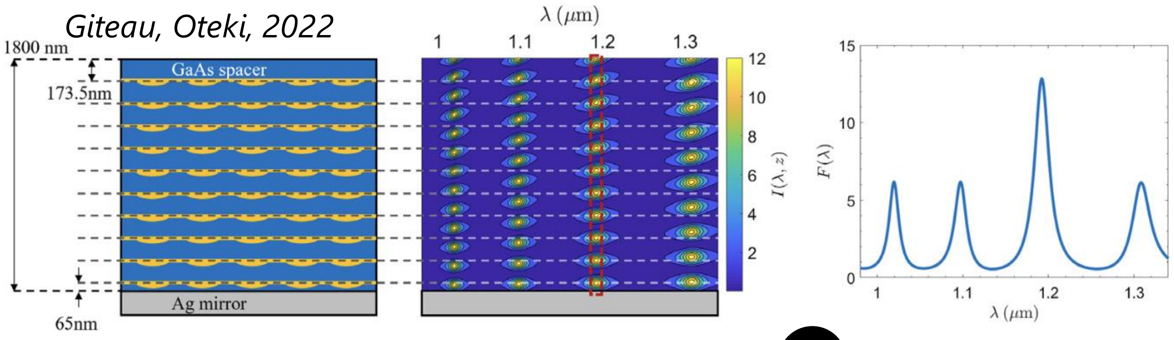
- In general for almost all wavelengths, the FLiSS structure **enhances** and **distorts** the distribution of **the E-field.**
- However, there is a small displacement of the resonance wavelengths.

2- First simulation results

Position of the resonance wavelengths

Expectations: (FP resonance)

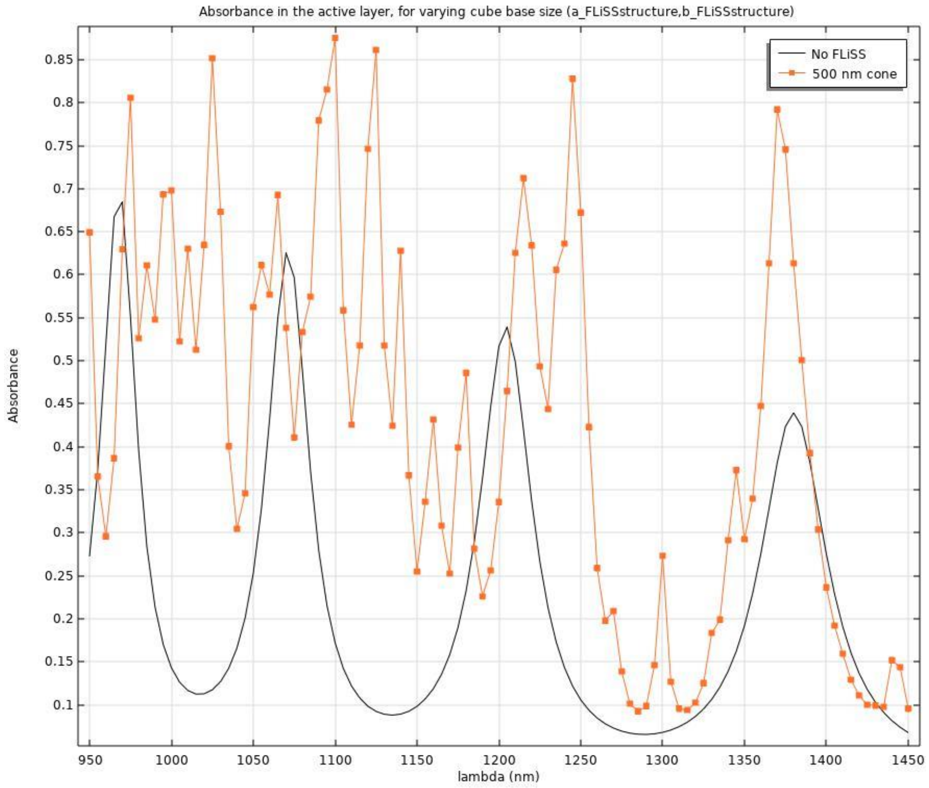
Giteau, Oteki, 2022



1 Resonance wavelengths

2 At these wavelengths, peaks and nodes depending on vertical position z

1 **Absorption in active layer -** Comparison with or without the FLiSS



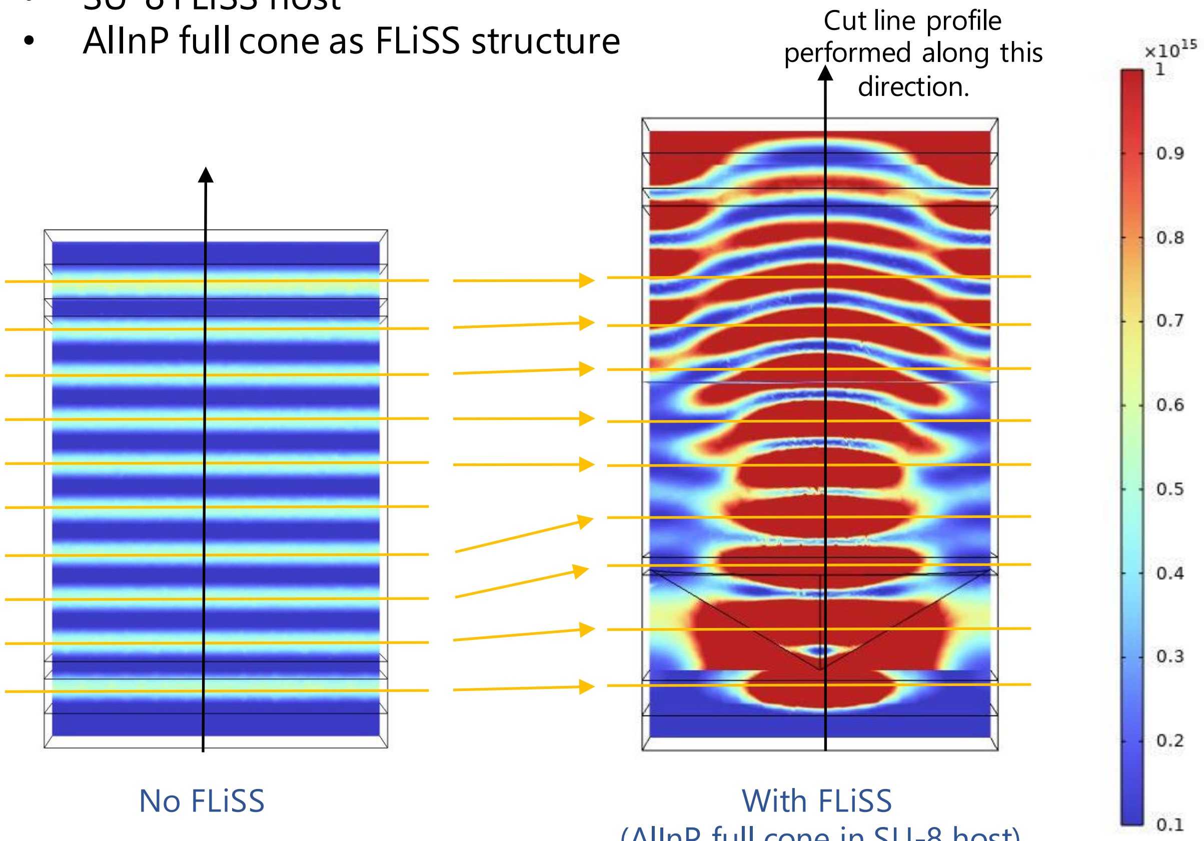
Resonance wavelengths are still observed but their position is modified due to the FLiSS.

2- First simulation results

At fixed wavelength, position of the E-field peaks

2 **Example**

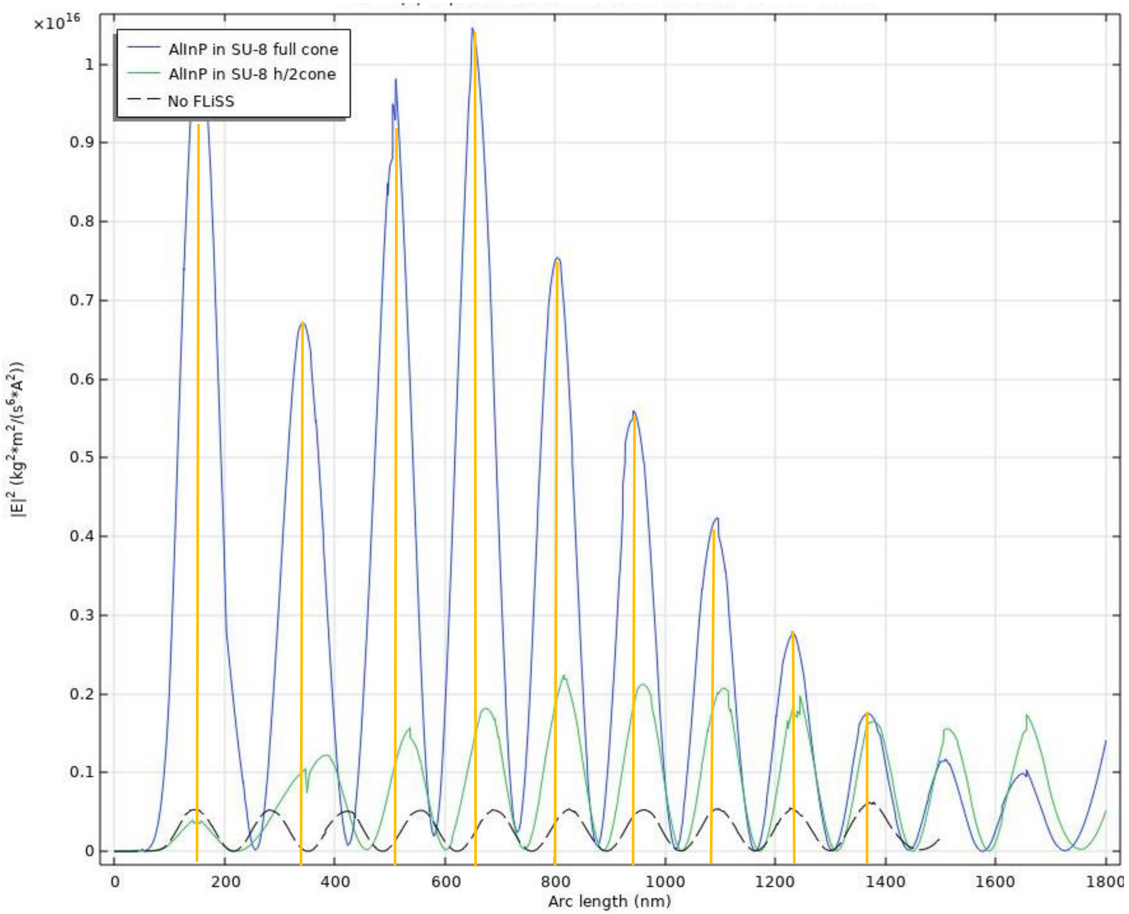
Plot of $|E|^2$ at lambda = 950 nm
- SU-8 FLiSS host
- AlInP full cone as FLiSS structure



No FLiSS

With FLiSS (AlInP full cone in SU-8 host)

Cut line profile $|E|^2$ at lambda = 950 nm



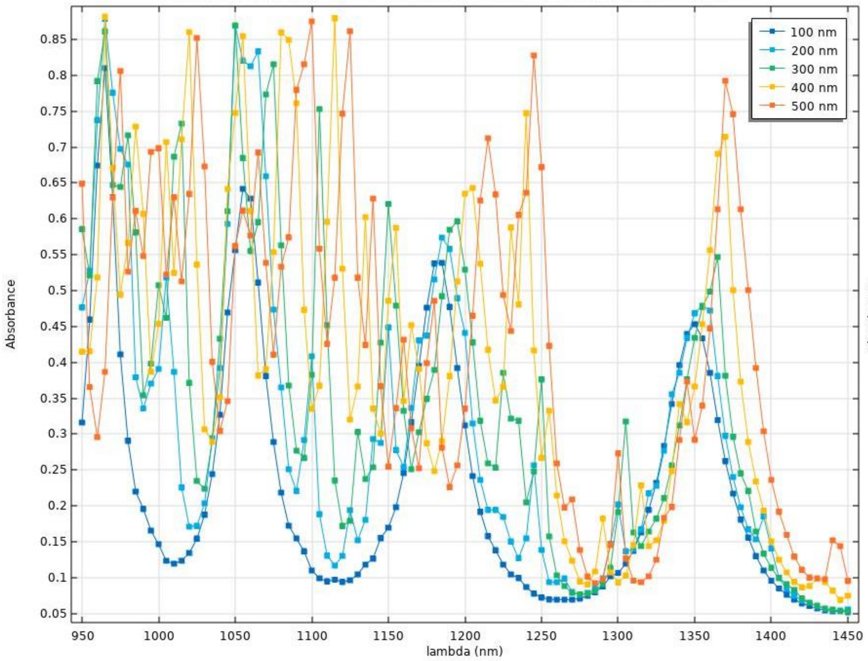
For each wavelength, **position and number of the resonance peaks is changed** when adding the light-scattering structure.

- ➢ For a chosen FLiSS (shape, size), the position of the QD layers can be optimized accordingly after choosing one wavelength of interest.

3- Parametric studies

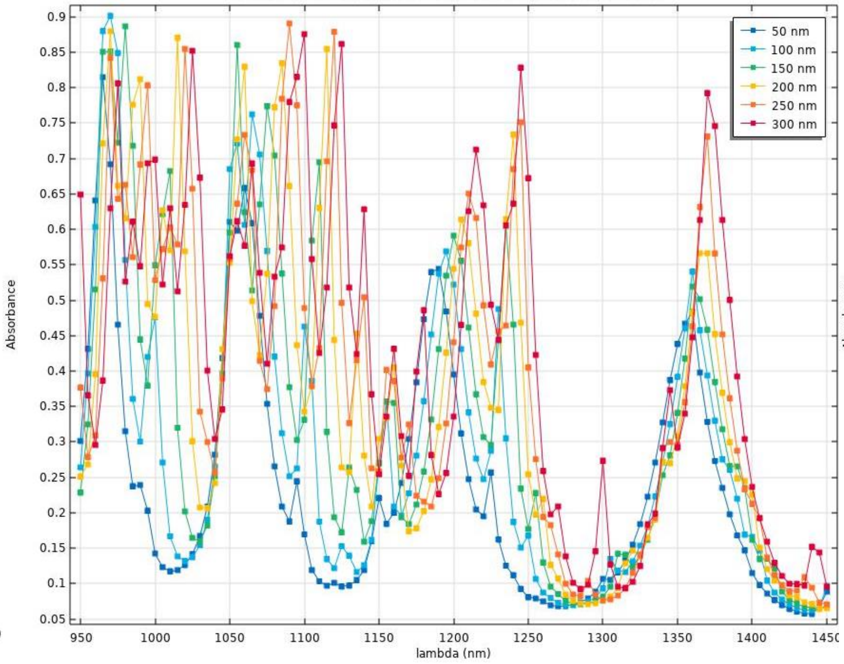
Absorption in the active layer – Cone pattern

Changing the radius of the cone



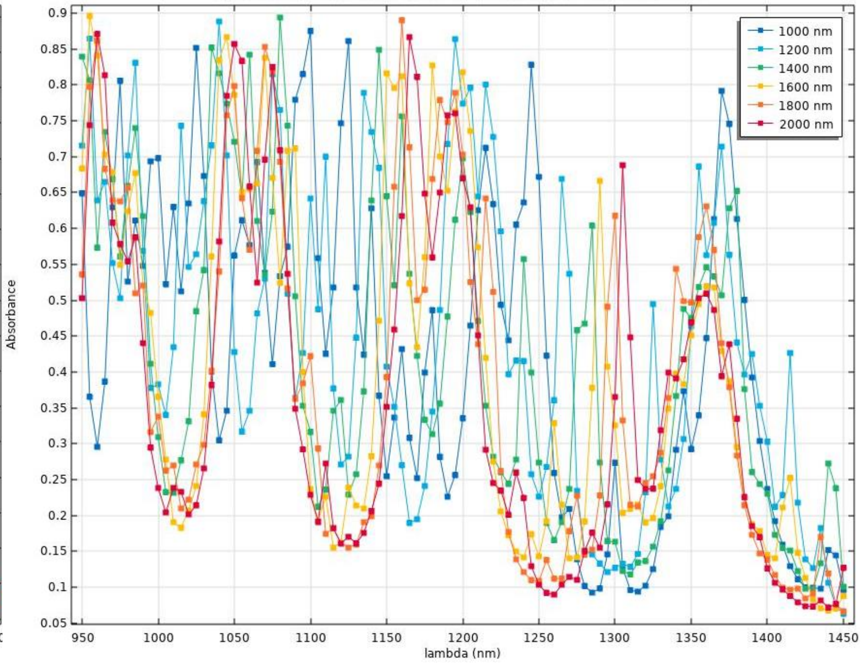
Absorption is higher when the **radius** of the FLiSS cone is **larger**.

Changing the height of the cone



Absorption is higher when the **height** of the FLiSS cone is **larger**.

Changing the pattern periodicity



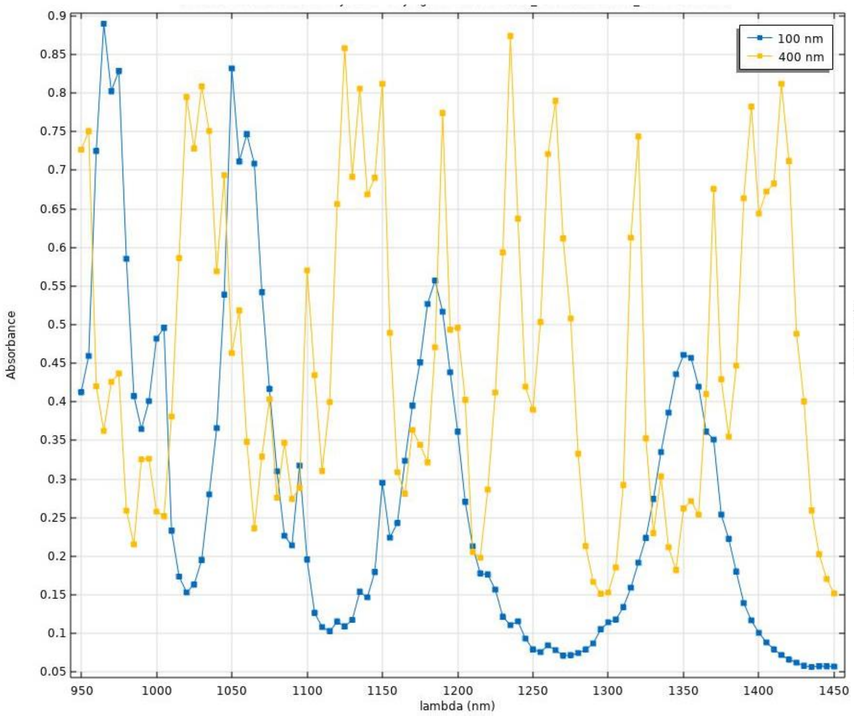
Absorption is higher when the **periodicity** of the pattern is **lower**.

- The data seems **noisy** but this reflects the complexity of the light-scattering.
- The denser the pattern, the more complex and the higher this scattering.

3- Parametric studies

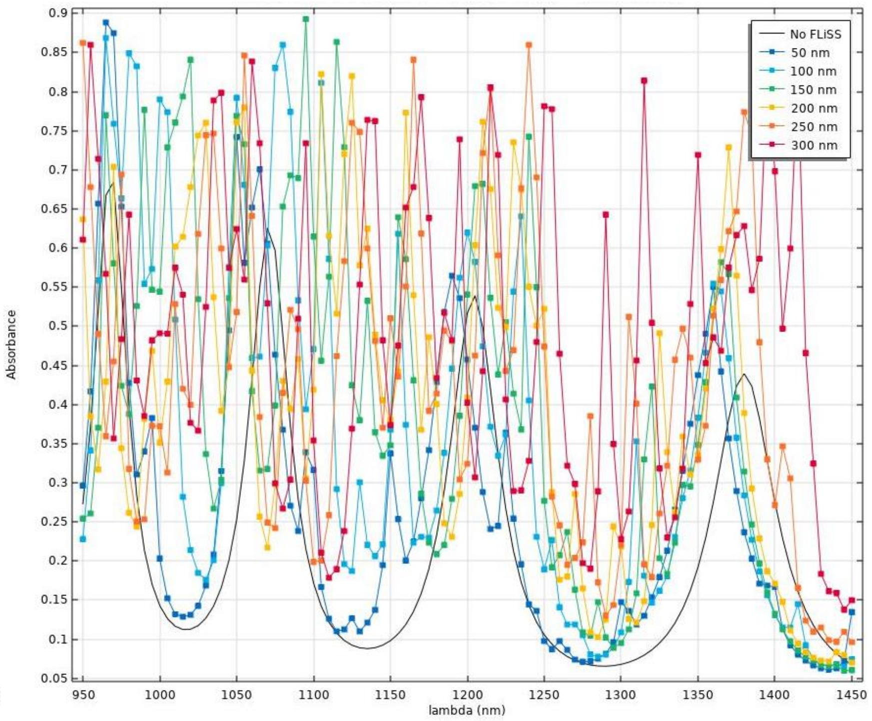
Absorption in the active layer – Cube pattern

Changing the square base size of the cone



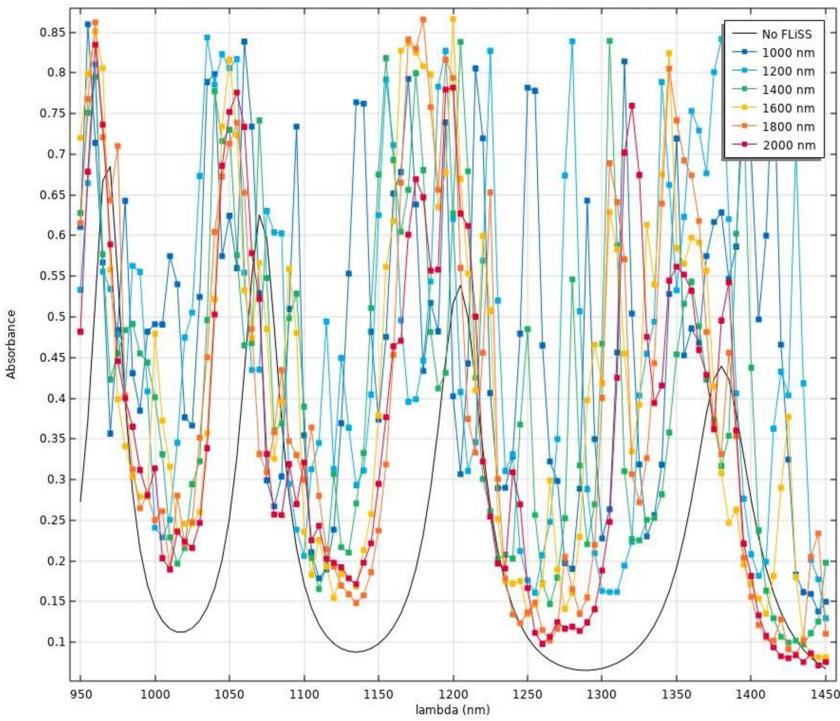
Absorption is higher when the **square size** of the FLiSS cube is **between 200 and 400 nm**.

Changing the height of the cube



Absorption is higher when the **height** of the FLiSS cube is **larger**.

Changing the pattern periodicity

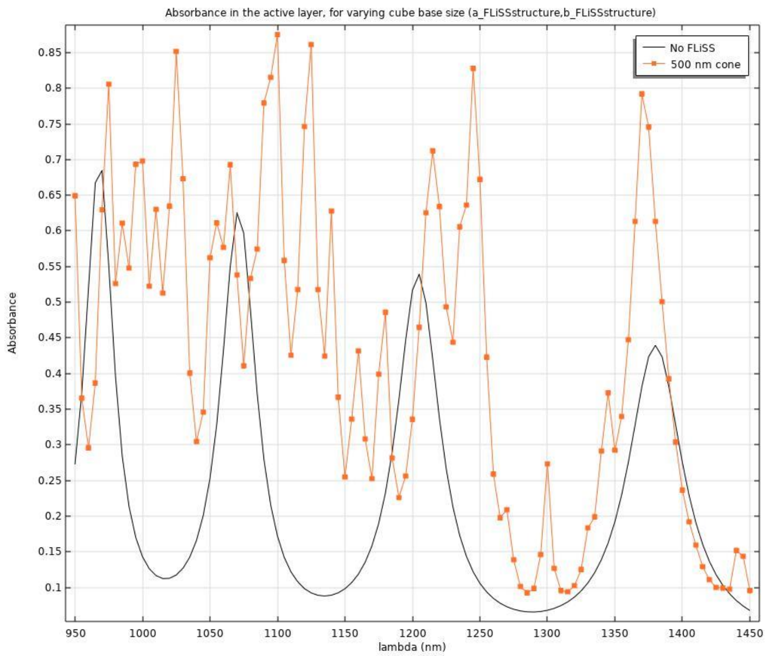


Absorption is higher when the **periodicity** of the pattern is **lower**.

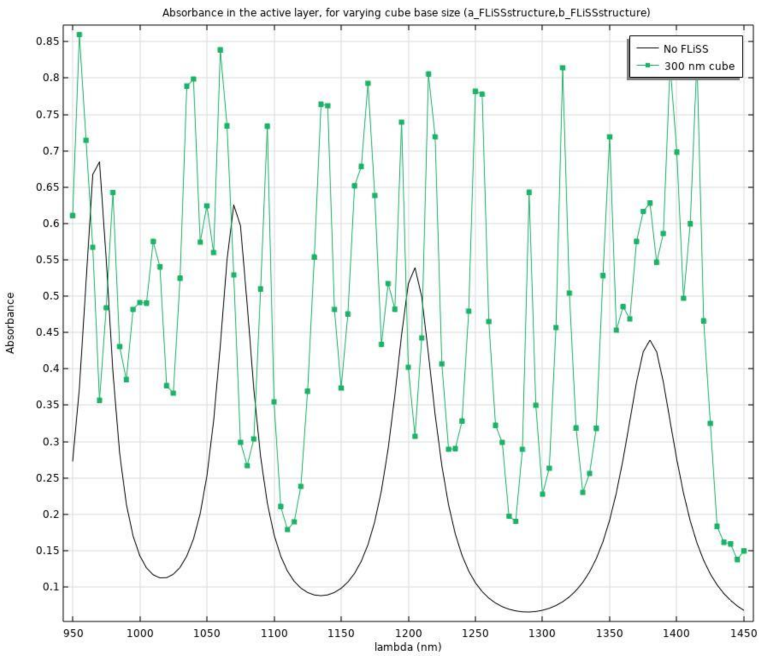
- The data seems **noisy** as well but this is the light-scattering.
- The denser the pattern but with a medium size, the more complex and the higher this scattering.

3- Parametric studies

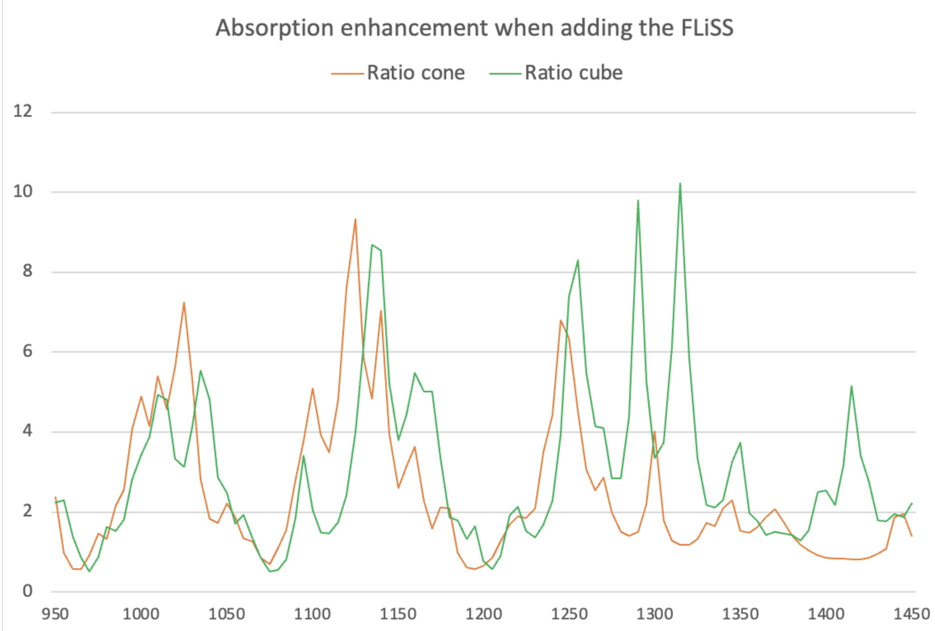
Comparison cone vs cube FLiSS



Absorption
FLiSS cone (radius 500 nm and height 300 nm)
VS no FLiSS



Absorption
FLiSS cube (square 300 nm and height 300 nm)
VS no FLiSS



Absorption enhancement
FLiSS cone (radius 500 nm and height 300 nm)
VS FLiSS cube (square 300 nm and height 300 nm)

- As targeted, **increased absorption with the FLiSS**, for almost all wavelengths.
- For now, difficult to compare between best cube and cone FLiSS.

Summary

Results:

- High, large FLiSS cone results in the highest absorption.
- ➢ Try even higher values?
- High, medium sized cube results in the highest absorption.
- Hard to compare between cone and cube for now.

Problems:

- Find good meshing for calculations in finite elements on Comsol.
- Find more accurate refractive indexes for AlInP and SU-8 with wavelength dependency.

Next:

- Add quantum dots and solar incident spectrum in the model.
- Do finer simulations around the interesting values.