THALES

Gaetano Bellanca, Stefano Trillo
University of Ferrara – Department of Engineering

Luca Stabellini , Wei Lu, Alfredo De Rossi
Thales Research & Technology, Palaiseau, France

Thomas Antoni, Mathieu Carras, Alexandre Nedelcu
Alcatel-Thales III-V Lab, Palaiseau, France

ACCURATE SIMULATION OF QUANTUM WELL INFRARED PHOTODETECTORS BY FDTD

UNIFE

Aim of the Presentation

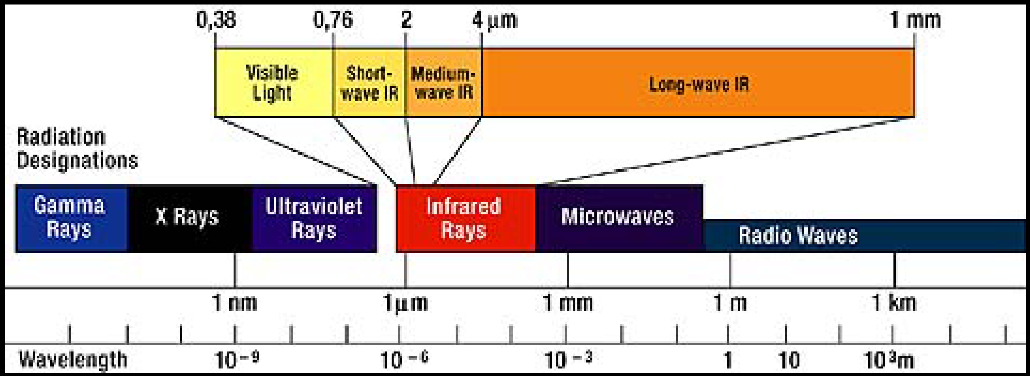
To show our approach based on the Finite Difference Time Domain (FDTD) technique for the design and the optimization of Quantum Well Infrared Photodetector (QWIP) devices

Presentation Outline

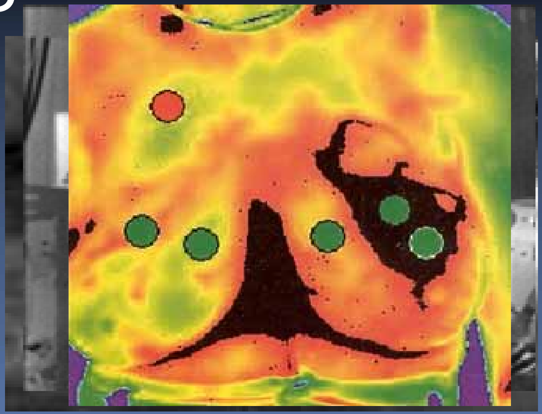
- **Introduction**
- **FDTD technique**
- **QWIP**
- **Results**
- **Conclusions**

Introduction

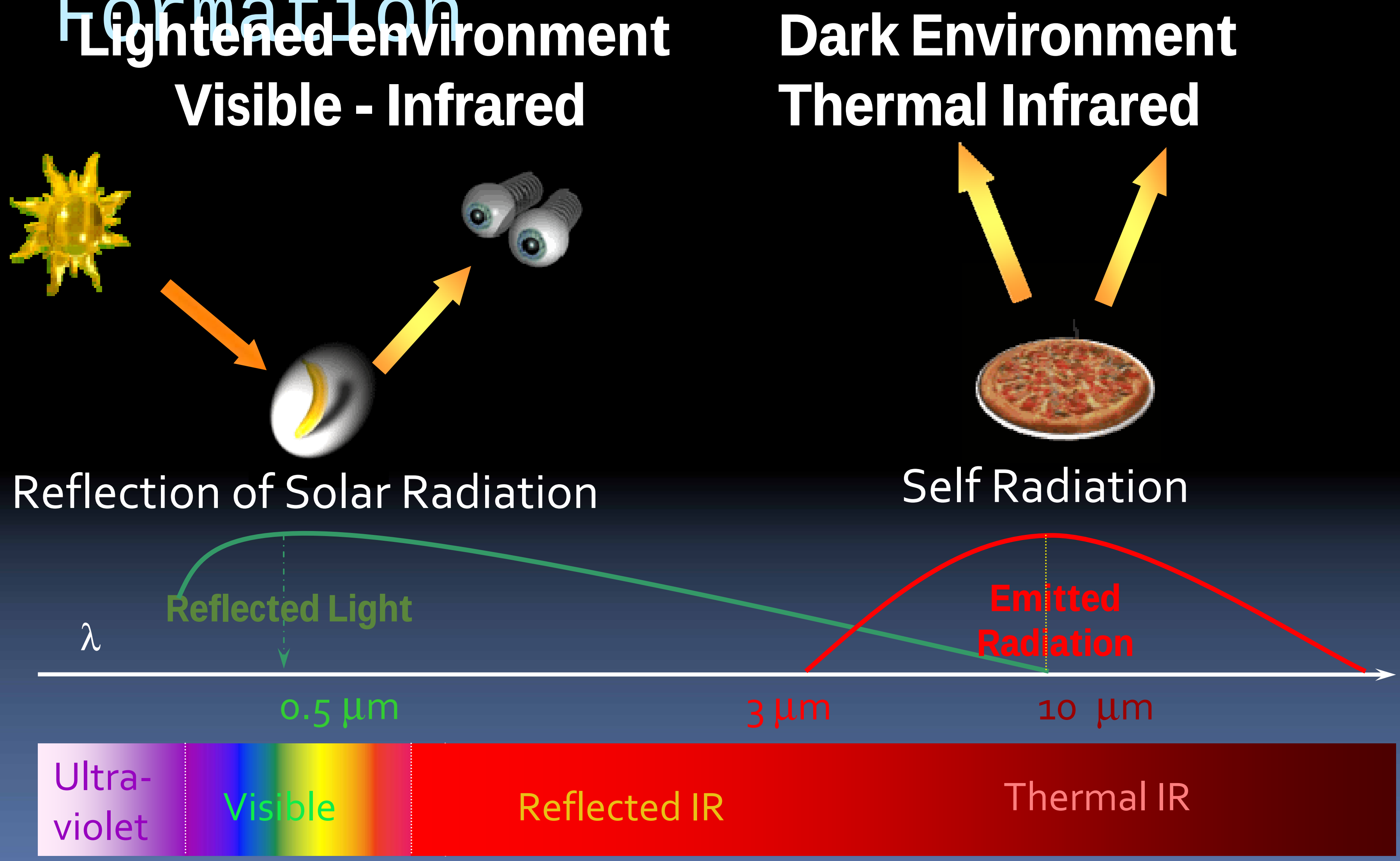
- The Infrared Domain: 0.76 µm ÷ 1000 µm



- Efficient Technology useful to detect the e.m. radiation in the IR Spectrum Range
- Possible applications:
  - Civil (Security, Surveillance)
  - Medical (Brest Cancer Detection)
  - Military



Introduction: Image Formation



UNIFE

Introduction

- The Image Formation
  - Lightened environment:
    - Detection of the photons emitted by a light source and reflected by the objects
  - Dark environment:
    - Objects at non-zero temperature emit photons

Planck's law

$$E(\lambda,T)=\frac{2hc^2}{\lambda^5}\frac{1}{e^{\frac{hc}{\lambda Tk}}-1}\quad\left[\frac{W}{m^2\mu m}\right]$$

$$c = 310^{-8}\ m/s$$

$$h = 6.62510^{-27}\ erg/s$$

$$k = 1.3810^{-27}\ erg/^{\circ}K$$

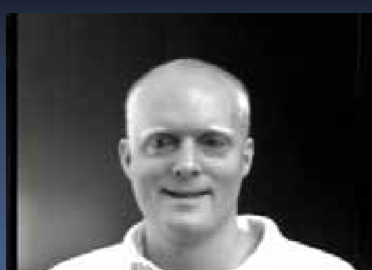
- Using different detectors it is possible to build up different images of the same scenario

Introduction

- Images of the same human head obtained by different detection techniques

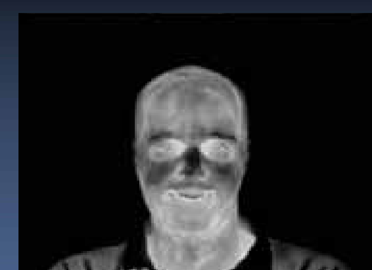
Color Image
Visible Band 0.38 µm ÷ 0.76 µm

B&W Image
Visible Band 0.38 µm ÷ 0.76 µm



Solar Reflection
IR Band 1.0 µm ÷ 1.7 µm

Solar Reflection + Thermal Emission
IR Band 3.4 µm ÷ 5.0 µm



Thermal Emission
IR Band 8.5 µm ÷ 9.5 µm

Infrared Detectors

- **Thermal Detectors**
  - **Absorption of IR radiation** ⇨ Increase of T in the Detector ⇨ External Signal

- **Photonic Detectors**
  - **Absorption of IR radiation** ($f \propto E_g$) ⇒ Electron Current
  - Absorbed λ depend on the semiconductor band-gap

⇨ Only λ: $E_g > E_{go}$ can be absorbed

☹ Problems in obtaining detectors for long wave (λ ≈ 10 μm) IR (small E_g materials: $E_g \approx 0.1$ eV)

👎 'Conventional Detection' (with weak band-gap materials as Hg_x-$Cd_{1-x}Te$) is not efficient (exotic materials, not developed!)

⇨ 'Effective' band-gap materials (GaAs/AlGaAs heterostructures) which use InterSubBand transitions created by **Quantum Wells** in large-band-gap semiconductors

Quantum Well Infrared Detectors

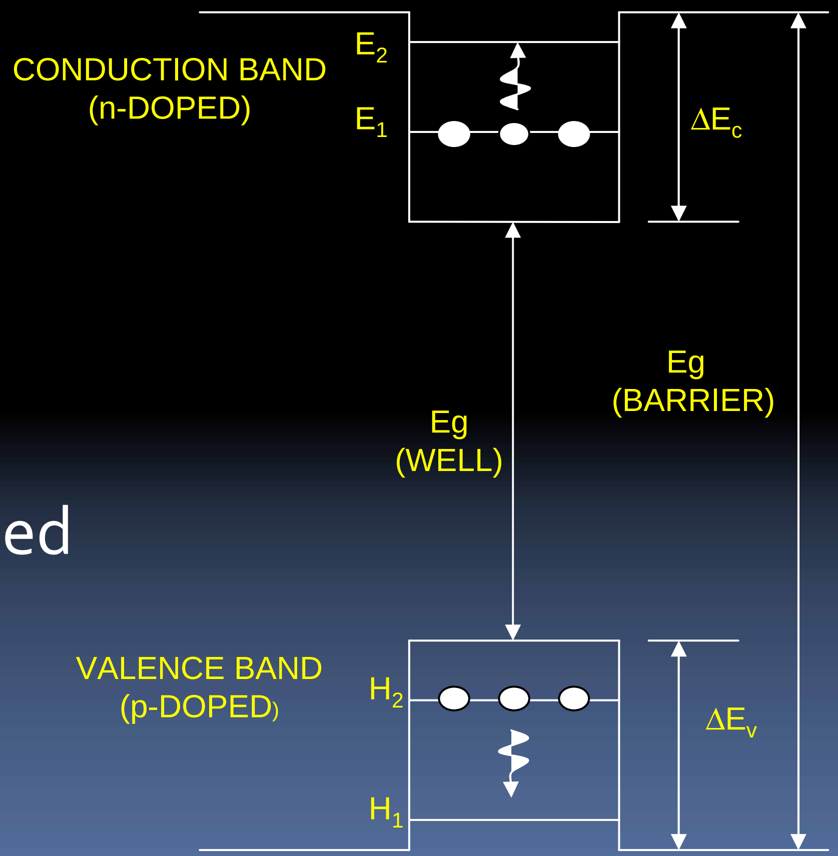
- **Photonic detectors with weak band-gap** (Hg_x-$Cd_{1-x}Te$) (to have detection @ long wave IR)
  - *x* concentration adjusted for λ tuning
  - Electrons excited from VB to CB with inter-sub-band transitions
  - Not very well developed (exotic materials!)
- **Quantum Well detectors** based on GaAs/AlGaAs heterostructures
  - Developed since 1990
  - Multi Quantum Well Photonic detectors (QWIP)

Multi Quantum Well IR Detectors

- The Detection Process: Inter-Sub-Band transitions
  - Involves transitions within the same band

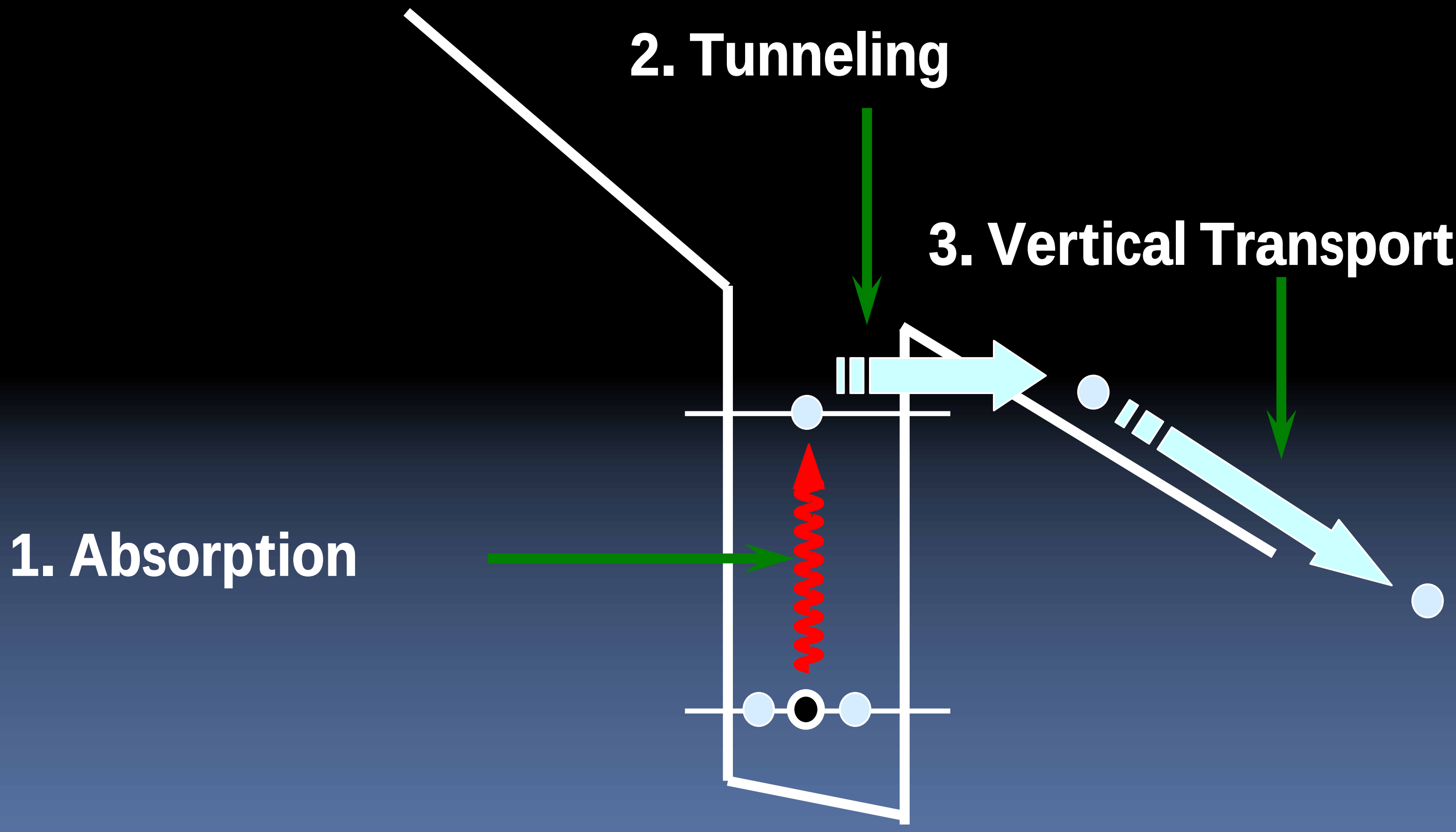
Quantum Well needed

  - Electron (Hole) from the doped QW ground state in CB (VB) to un unoccupied state in the same band



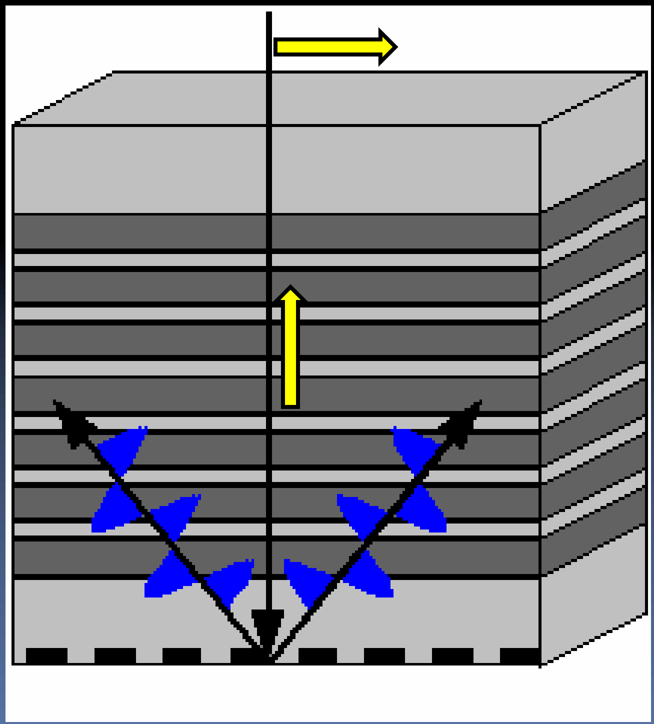
Multi Quantum Well IR Detectors

- QW structure designed to have carrier escaping from the well and collected as a (photo) current



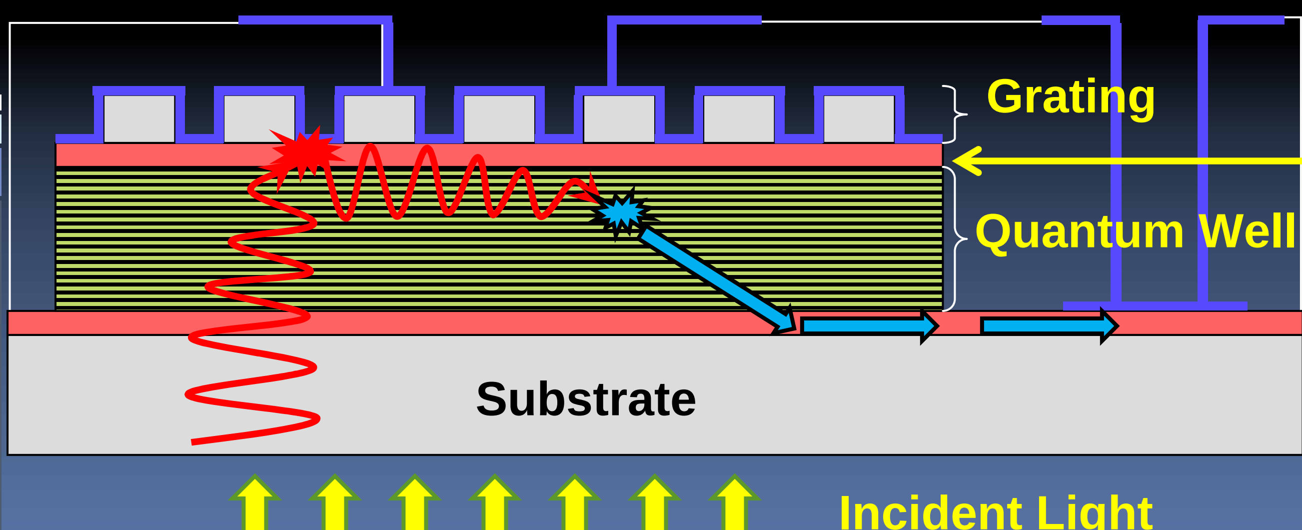
Multi Quantum Well IR Detectors

- InterSubBand Transitions
  - Energy levels inside CB or VB arise from the spatial localization introduced in the QW of a low-band-gap material (GaAs) surrounded by a higher-band-gap semiconductor ($Al_xGa_{1-x}As$)
- Optical Absorption:
  - only the optical field along the superlattice direction (made by the well-barrier structure) is absorbed
  - Light (TEM polarized) orthogonally polarized respect to the direction of interest
  - ⇨ Polarization rotation (TEM ⇨TM) is needed!
  - ⇨ Diffraction gratings are used



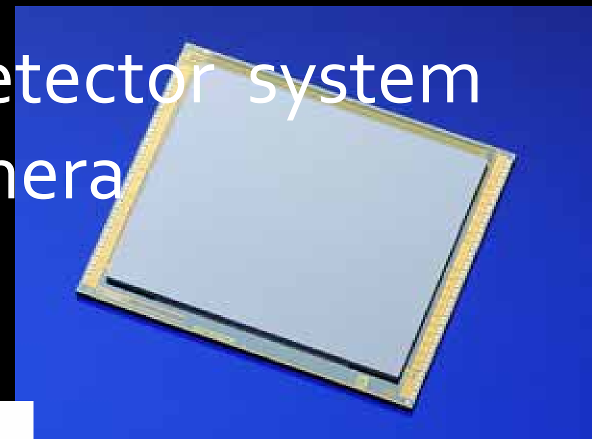
Quantum Well IR Photodetector

- The Structure of a QW IR Photodetector
  - Substrate: GaAs
  - Collector and Emitter: doped GaAs:Si
  - Active zone: 40 QWs (doped GaAs, barrier: AlGaAs)
  - Grating: GaAs + metallic coat (Au, Ni)

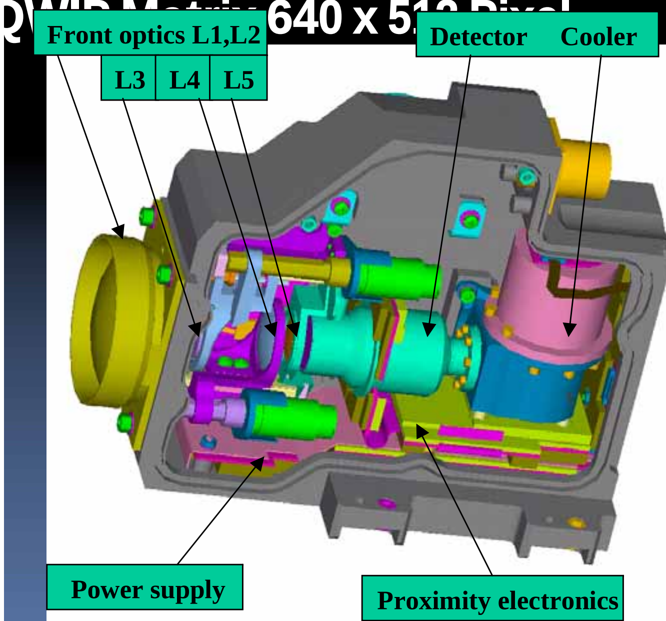


Thermal Imager (IR Camera)

- Matrices are then put in the detector system and installed inside the IR Camera
  - Photodetectors are assembled in Matrices
  - Each Pixel is a QWIP



QWIP Matrix 640 x 512 Pixel

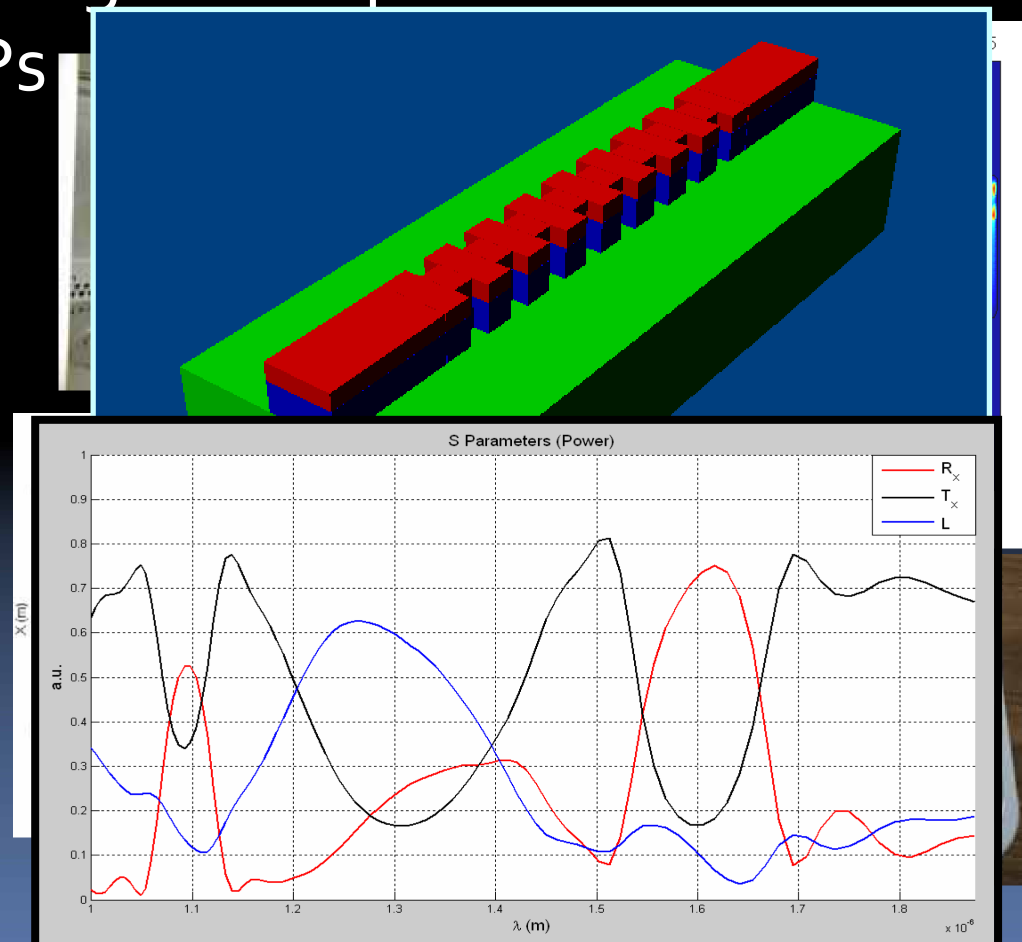


The FDTD Approach

- The Finite Difference in the Time Domain (FDTD) approach is used to design and optimize the performance of QWIPs
- Why FDTD?
  - Available in our group
  - FDTD Properties

Microwave Heating Applications

Optics



The FDTD Approach

- **The FDTD Properties**

☺ Generality and Versatility

☺ Dissipative, Dispersive and Non Linear materials can be 'easily' included

- Temporal evolution of the e.m. fields
- Frequency Domain results available by Fourier Transform

☹ Time and Memory consuming

Problems with devices of several λ on each side are impractical on a simple PC

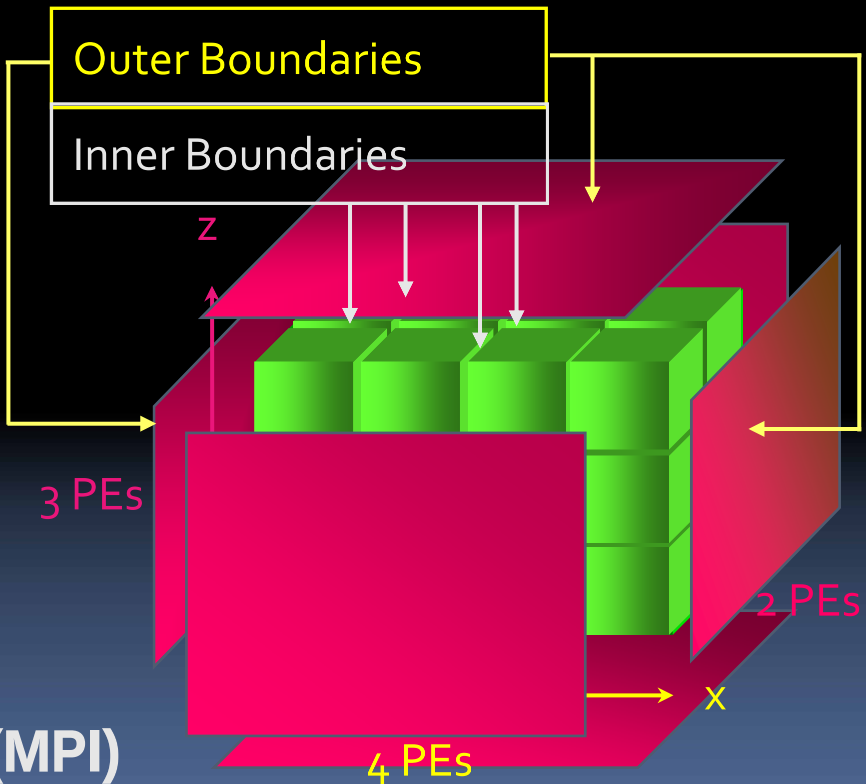
- Lack of Computer Memory (RAM)
- Long CPU time

⇨ Use of Parallel Computing

Parallel FDTD Technique

- FDTD is well suited for Parallel Computation as the solving algorithm mainly involves 'local data'

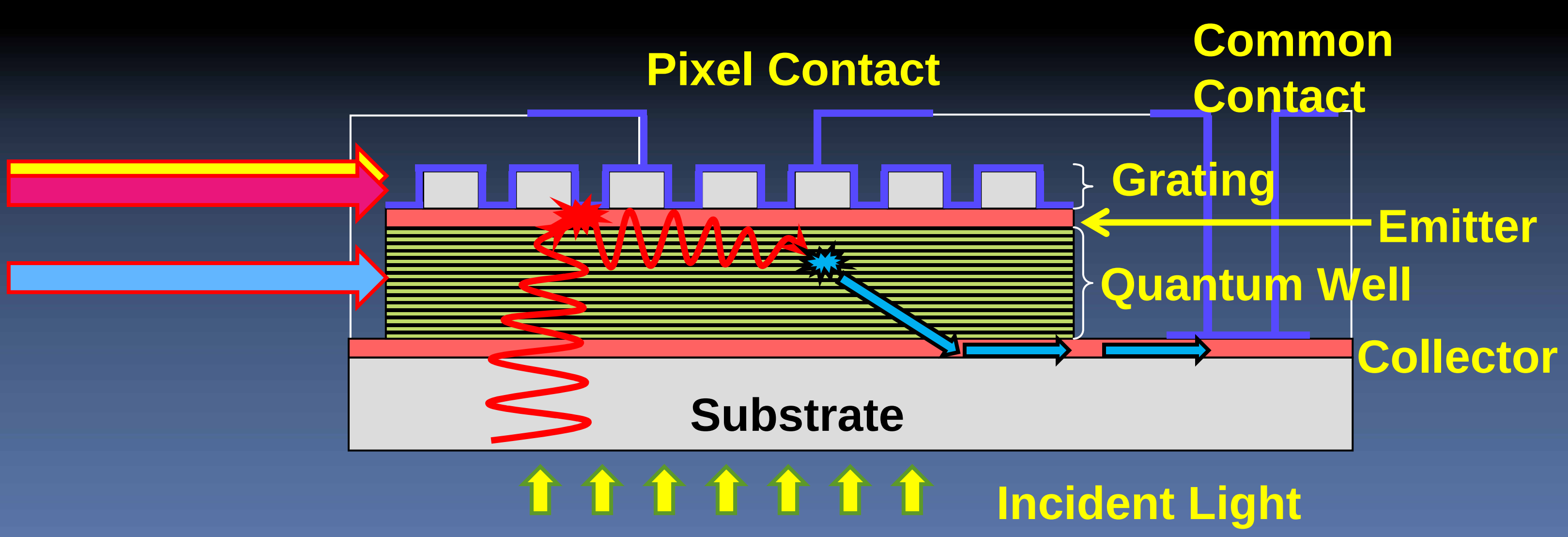
- Domain Decomposition
  - **Each Block belongs to a single PE**
- **Boundary Conditions**
  - **Outer Boundaries**
    - ⇨ **ABC - PML**
  - **Inner Boundaries**
    - ⇨ **Data Communication**
  - **Message Passing Interface (MPI)**



Tot = 24 PEs

FDTD Simulation of QWIPs

- Simulation Strategy:
  - Optimization of the Metallic Grating
    - PEC metallic surface
    - Real metal (Drude Model)
  - Lorentz Model for the InterSubBand Absorption
  - TFSF Approach for Field Excitation



Grating Optimization

- Coupling grating fundamental component of a QWIP (only TM waves are absorbed, but the incident light is mainly TEM Polarized)
  - TEM to TM Polarization Rotation
  - Increasing of the e.m. field in the active region (Surface Plasmons + Surface Cavity Effect)

⇨ Grating optimization is essential for good QWIP performance

L. Stabellini, M. Carras, A. De Rossi and G. Bellanca, "Design and Optimization of High-Q Surface ModeCavities on Patterned Metallic Surfaces", IEEE JQE, 2008, in press

Real Conductor

- Drude model used to describe the interaction between the light and the 'real' conductor

$$\varepsilon_0 \frac{\partial \vec{E}}{\partial t} = \nabla \times \vec{H} - \vec{J}_p$$

$$\frac{\partial \vec{J}_p}{\partial t} = -\upsilon \vec{J}_p + \varepsilon_0 \omega_p{}^2 \vec{E}$$

$$\hat{\varepsilon} = \varepsilon_0 \left[1 + \frac{\omega_p{}^2}{\omega(j\upsilon - \omega)} \right] = \varepsilon_0 \left[1 + \hat{\chi}(\omega) \right]$$

ω_p: Plasma frequency

υ: Collision frequency

Parameters for Gold

ω_p: $2\,\pi\,2.175\;10^{15}$ rad/s

υ: $2\,\pi\,6.5\;10^{12}$ rad/s

- Implemented in FDTD using the Auxiliary Differential Equation (ADE) technique

Lorentz Model for InterSubBand Absorption

- A Lorentz model can be used to describe InterSubBand absorption of a Quantum Well IR Photodetectors (A. Nedelcu, 'Detection Infrarouge, Imaginerie Infrarouge' , Thales Internal Report)

$$\varepsilon_0 \frac{\partial \vec{E}}{\partial t} = \nabla \times \vec{H} - \vec{J}_p$$

$$\frac{\partial \vec{J}_p}{\partial t} = -\upsilon_1 \vec{J}_p + (\varepsilon_s - \varepsilon_\infty)\varepsilon_0 \omega_1^2 \vec{P} \qquad \frac{\partial \vec{P}}{\partial t} = \vec{J}_p$$

$$\hat{\varepsilon} = \varepsilon_0 \varepsilon_\infty + \frac{(\varepsilon_s - \varepsilon_\infty)\varepsilon_0 \omega_1^2}{\omega_1^2 + j\omega\upsilon_1 - \omega^2} = \varepsilon_0 [1 + \hat{\chi}(\omega)]$$

ω_1: Resonant frequency

υ_1: Damping frequency

ε_s: Static relative permittivity

ε_∞: Infinite relative permittivity

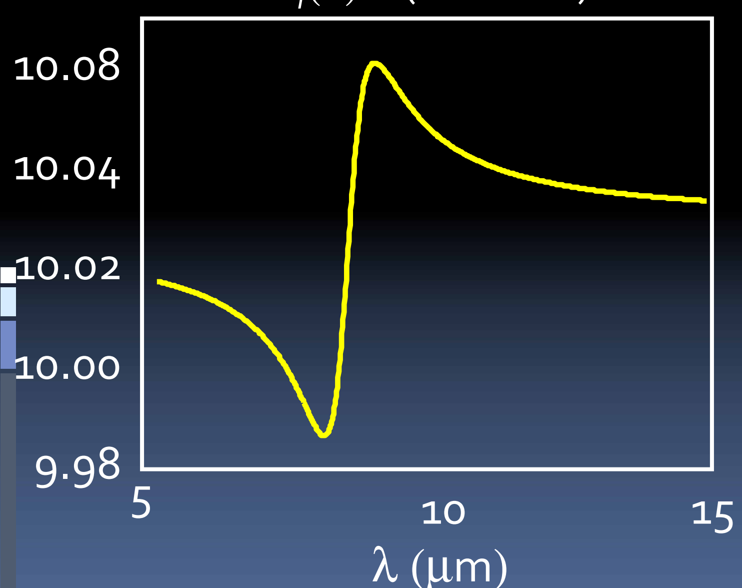
- Implemented in FDTD using the ADE Technique
- Same model for both Drude and Lorentz media
- ⇨ Multi-Pole Lorentz model integrates the two different material representations in a single procedure (Drude material = zero order pole)

Parameters for the Lorentz Model

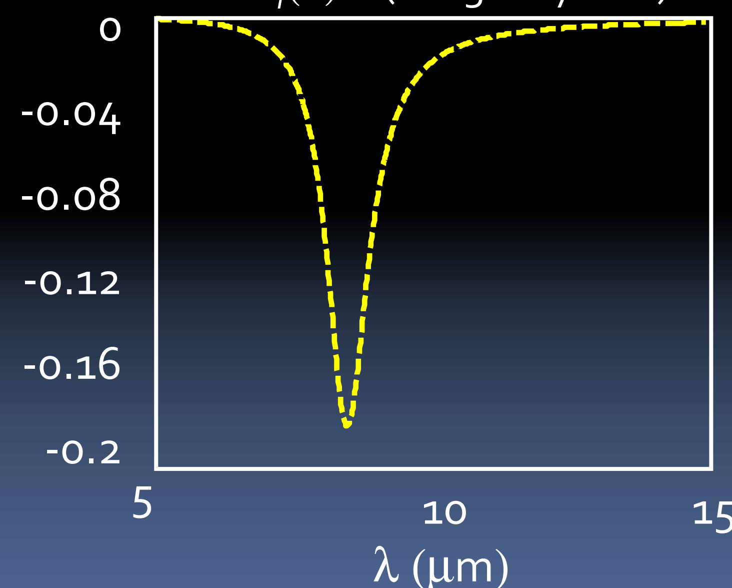
- The parameters ω_1, υ_1, ε_∞ and $\Delta\varepsilon = \varepsilon_s - \varepsilon_\infty$ can be obtained starting from the Density Matrix formalism and considering the doping parameters and the refractive index of the semiconductors used in the active region

Parameters for the Doped Quantum Well (GaAs)

$\varepsilon_r(\lambda)$ – (Real Part)



$\varepsilon_r(\lambda)$ – (Imaginary Part)



V. Berger, 'Proprietes des Doubles Puits Quantiques et Utilisation dans des Dispositif Optoelectroniques', PhD Thesis, Paris VI, 1992)

Spectral Response of a QWIP

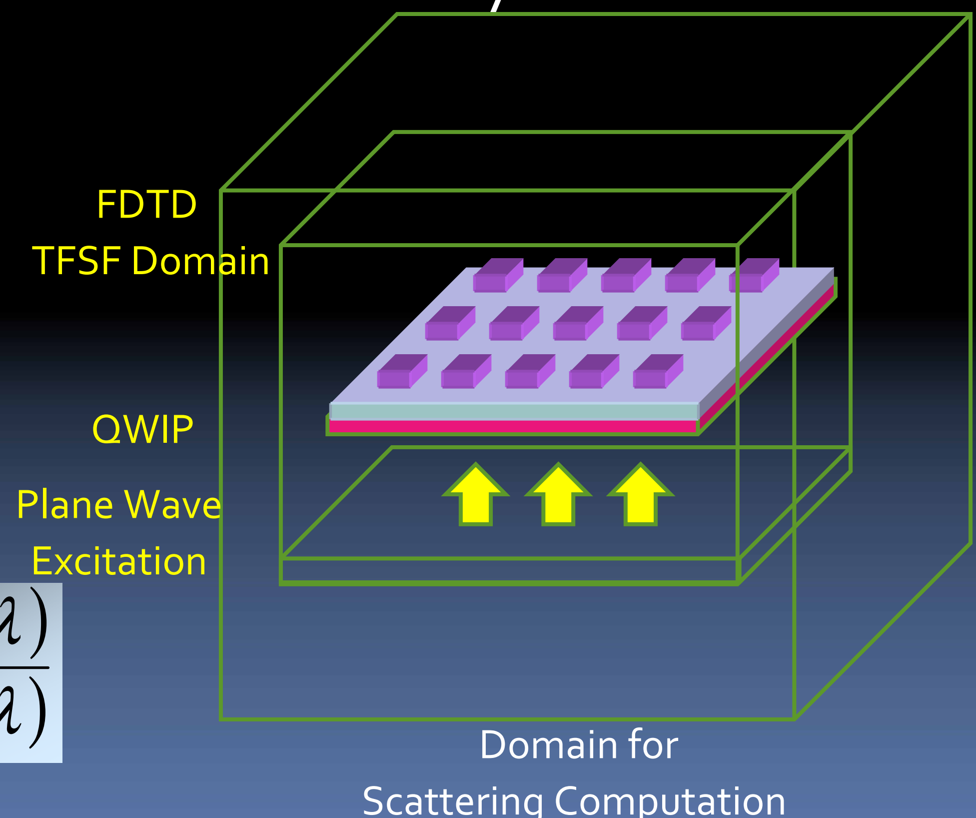
- Excitation of a ‘Plane Wave’ propagating in *y* direction
- Computation of the field ‘Scattered’ by the QWIP
- Computation of the field ‘absorbed’ by the semiconductor

$$P_a(\lambda) = P_0(\lambda) - \sum_{i=1..6} P_i(\lambda)$$

$$P_i(\lambda) = \mathrm{Re}\left\{ \iint_{S_i} \frac{\tilde{\mathbf{E}}_{\parallel} \times \tilde{\mathbf{H}}_{\parallel}^{*}}{2} \, ds \right\}$$

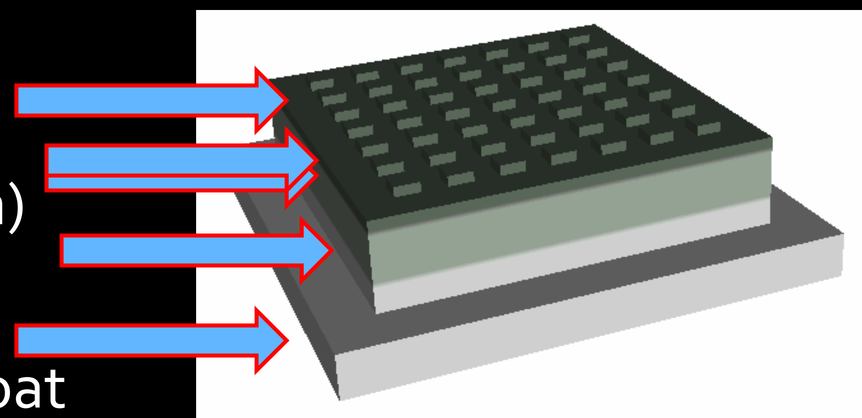
Normalized Absorbed Flux A

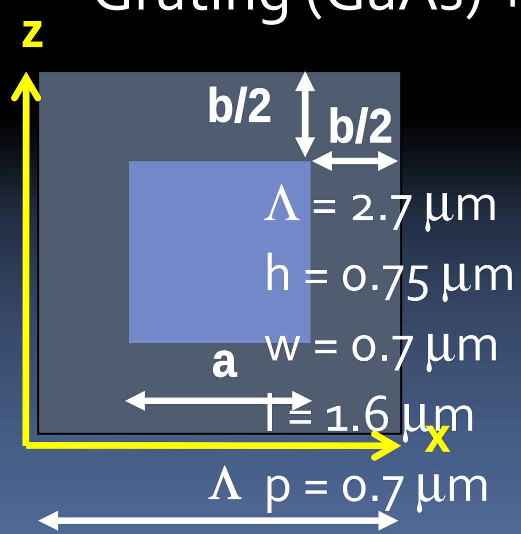
$$A(\lambda) = \frac{P_a(\lambda)}{P_0(\lambda)}$$

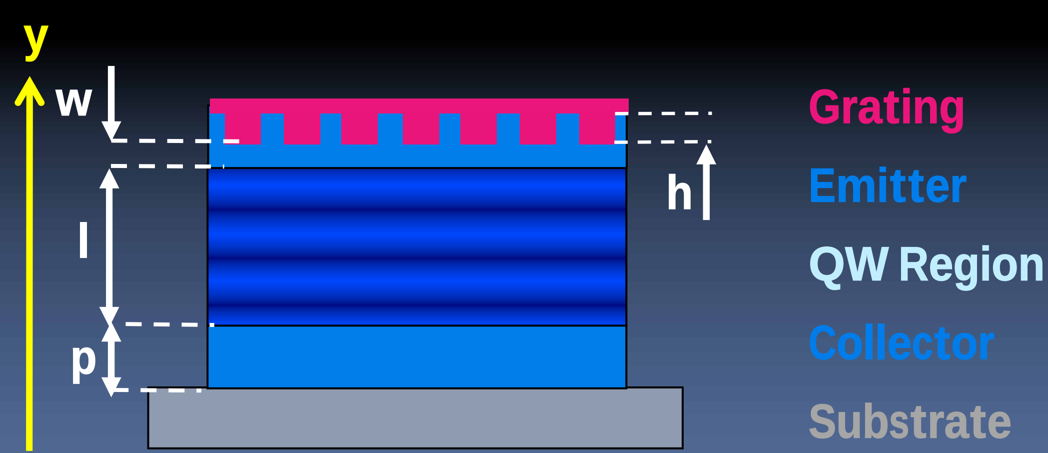


QWIP Parameters

- Complete simulated structure for a realistic QWIP
  - Substrate
  - GaAs:Si Collector
  - Active Zone: 40 QW (1.6µm)
  - GaAs:Si Emitter
  - Grating (GaAs) + metallic coat





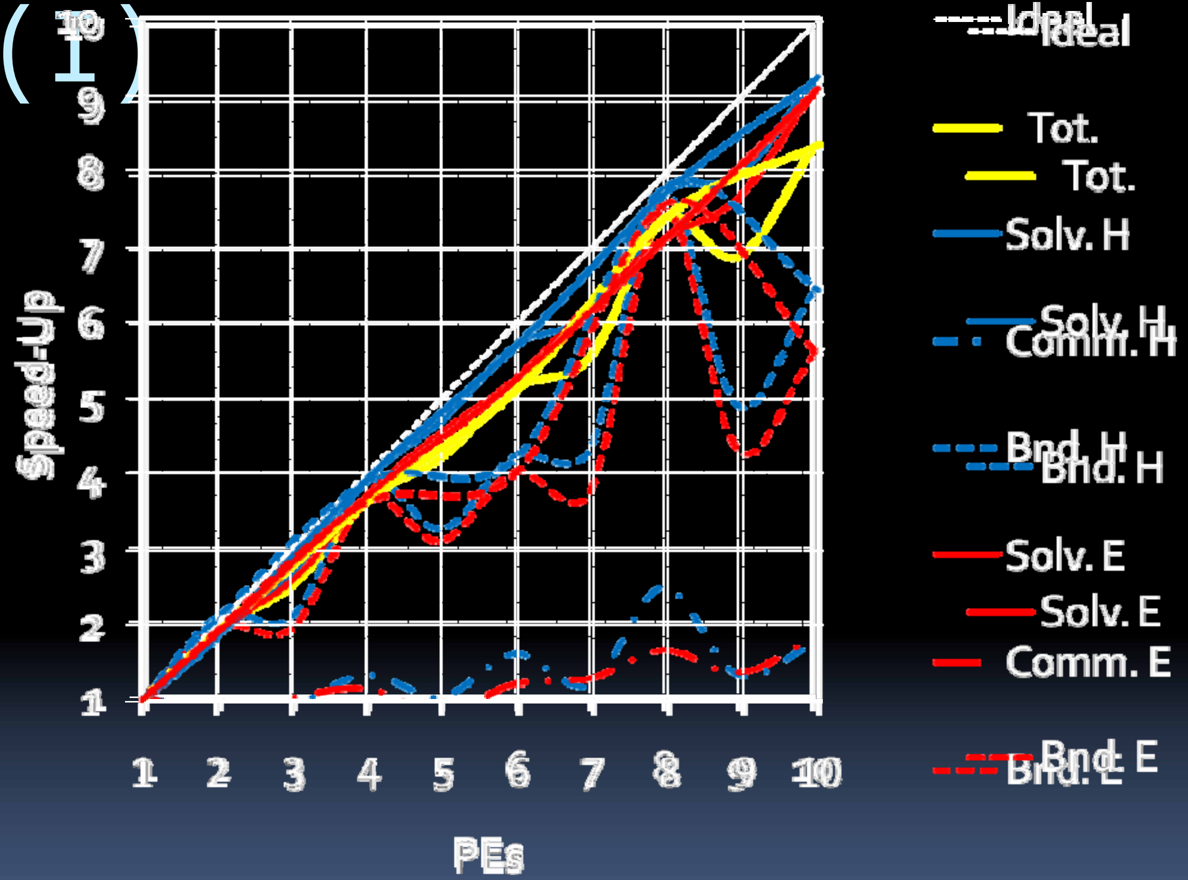


d.c. = a / (a+b) = a / Λ

FDTD Simulation Parameters

- Discretization
  - $\Delta_x = \Delta_y = \Delta_z = 75$ nm (36 points/Λ)
  - $7\Lambda \times 7\Lambda$ QWIP: 277 x 63 x 277 cells
  - PML Layer: 14 cells, $\rho = 1.0\ e^{-6}$ (8,465,275 overall mesh points)
  - Temporal Time Step: $7.22\ e^{-16}$ s
- Input / Output Parameters
  - TFSF Excitation: $f_o = 35$ THz ($\lambda = 8.5\ \mu$m); BW = 12THz
  - DFT Computation: frequency range [25÷45] THz (50 samples)
  - Number of Time steps: 30000
  - Total Computation Time: 8600 s (~ 2.4 h on 6 PEs – PIV 3GHz)

FDTD Parallel Performance (1)

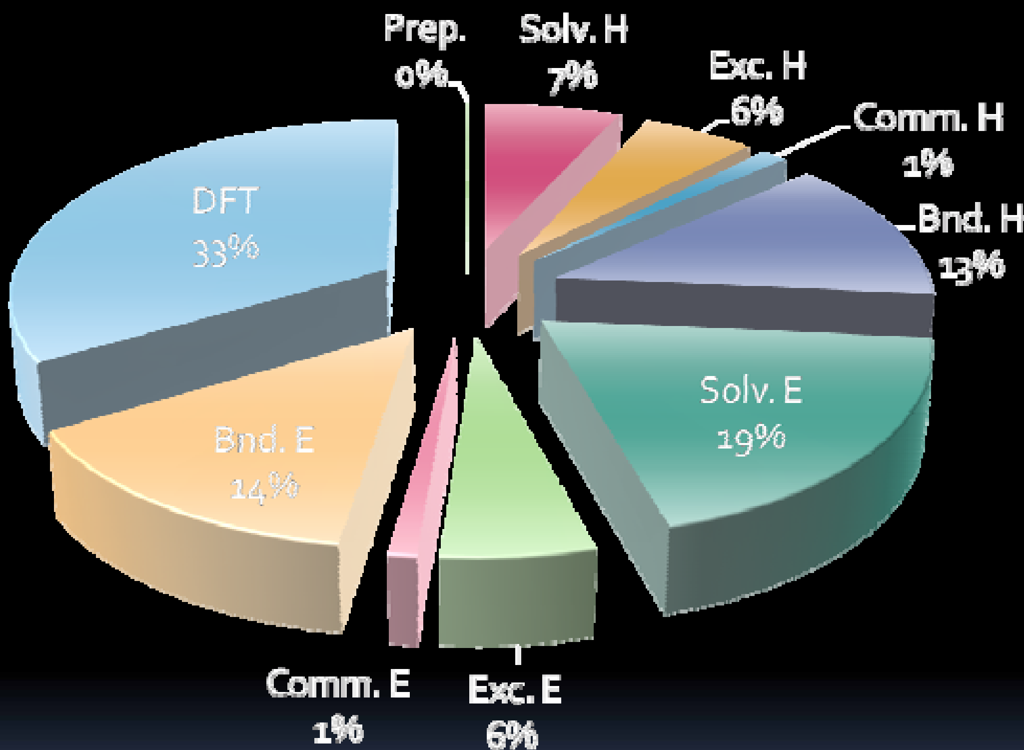


- Good scaling of 'pure computations' (Yee's Solver: Solv. H, Solv. E)
- Boundary Conditions don't scale as good as the Yee's Solver
- No good performance with an odd number of PEs

- Good performance with an even number of PEs
- Optimum Number of PEs exists
- Speed-Up (Overall Computations): 7.4 with 8 PEs; 8.3 with 10 PEs

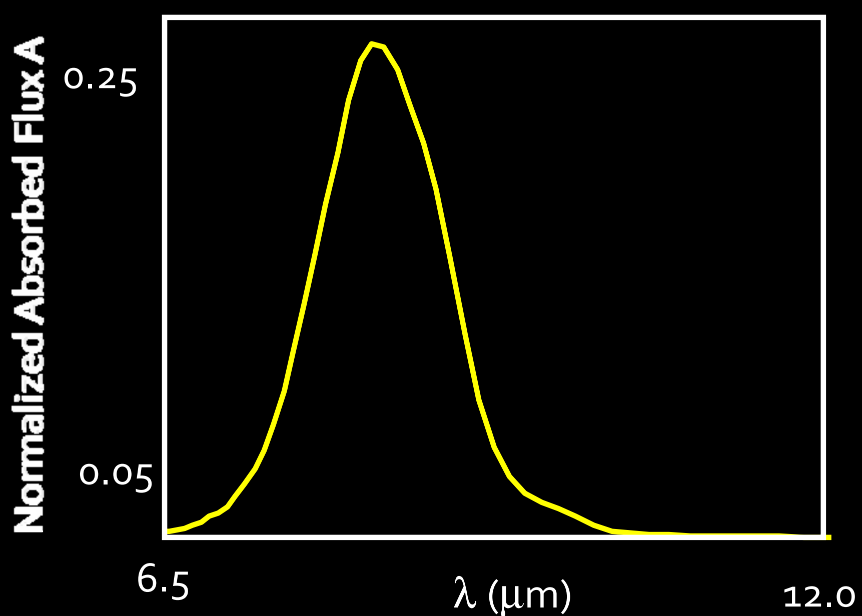
FDTD Parallel Performance (II)

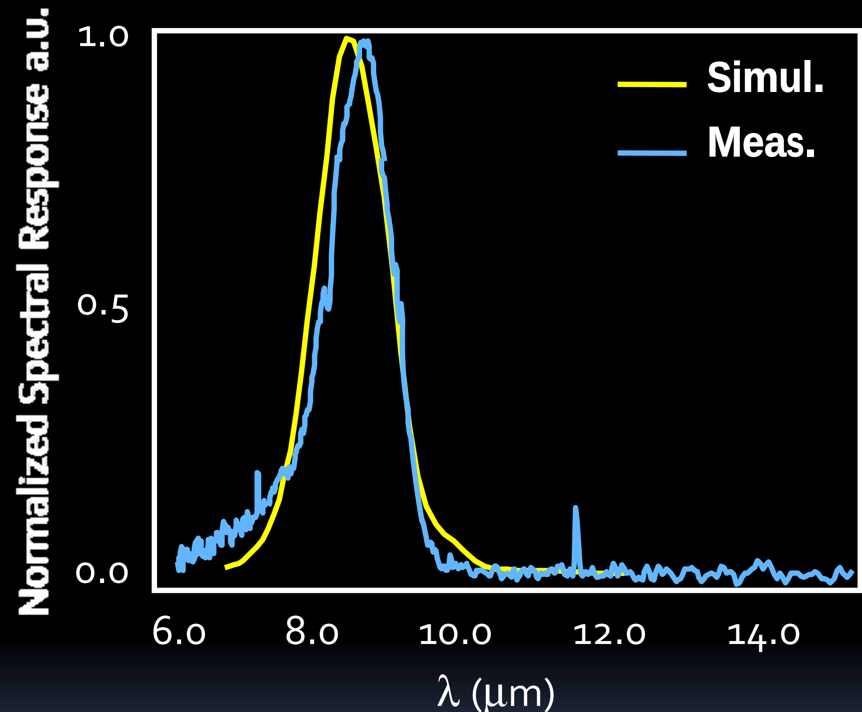
8 PEs



- **E Solver** more time consuming than **H Solver** because of **J** and **P** computations (Dispersive Materials in the QW region)
- Good work balance between **E** and **H** in Communication, Excitation and Boundary Computation
- DFT computationally intensive

Spectral Response of a QWIP





Λ = 2.7 μm

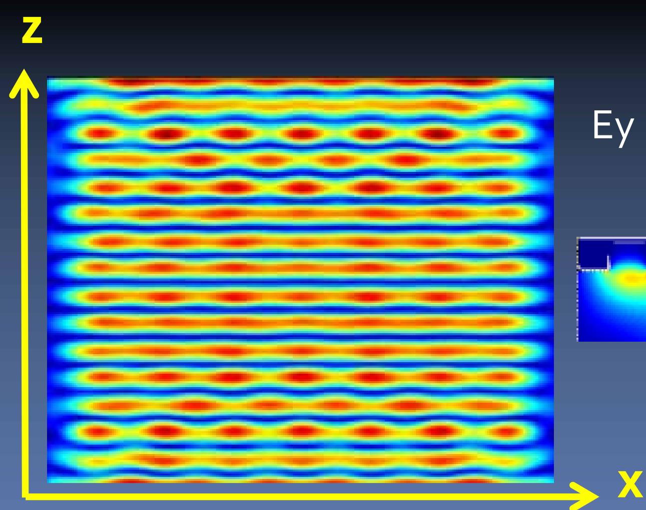
h = 0.75 μm

w = 0.7 μm

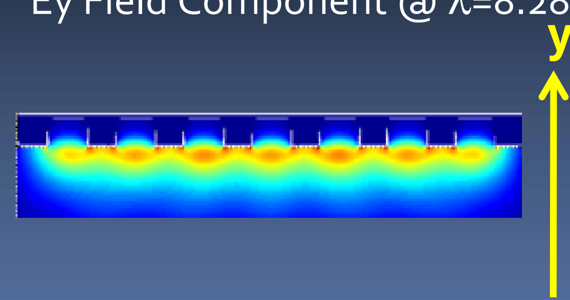
l = 1.6 μm

p = 0.7 μm

d.c. = 0.6



Ey Field Component @ λ=8.28 μm for a 7 x 7 QWIP



QWIP Optimization

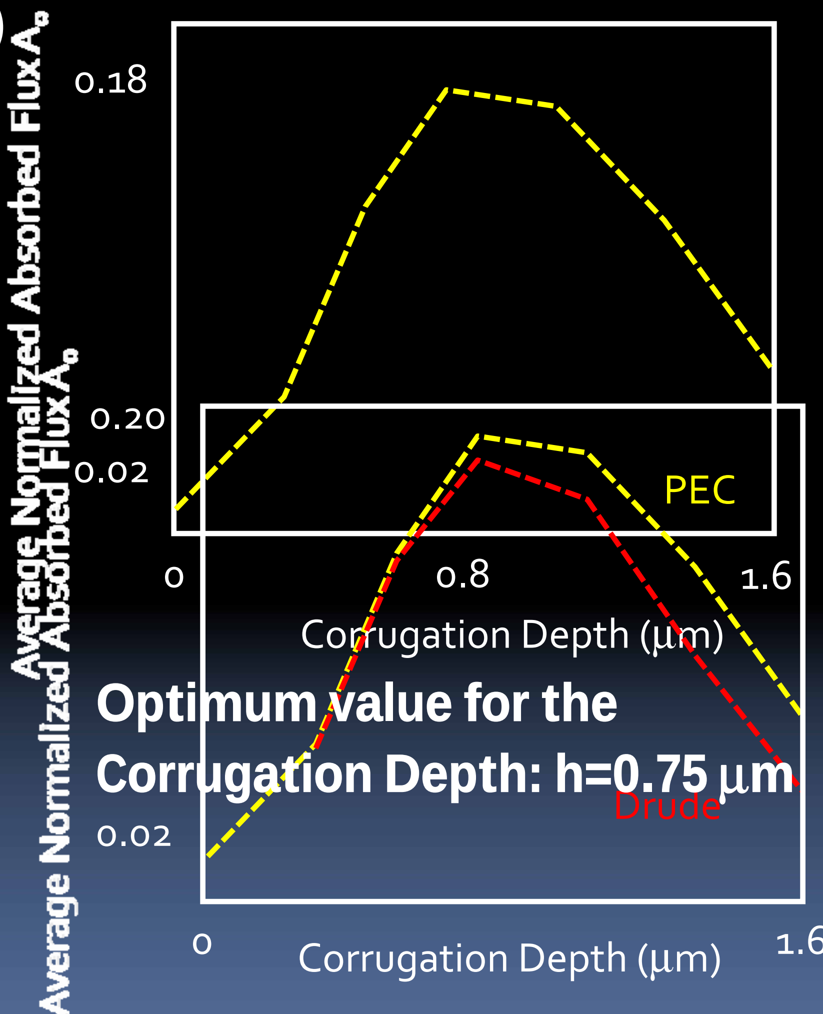
7 × 7 structure (20.5 × 20.5 µm)

- Λ = 2.7 µm
- h = 0.75 µm 1.6 µm
- w = 0.7 µm
- l = 1.6 µm
- p = 0.7 µm
- d.c. = 0.6

Average Normalized Absorbed Flux A_0

$$A_0 = \frac{\int_{7.5\,\mu m}^{9.5\,\mu m} A(\lambda)\, d\lambda}{\Delta\lambda}$$

PEC good approximation for the metallic coating (Au)



Optimum value for the Corrugation Depth: h=0.75 µm

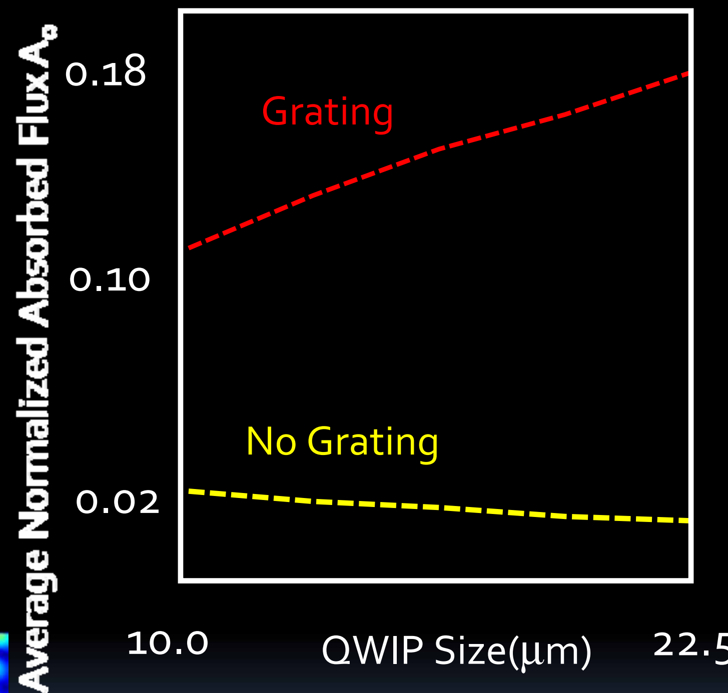
QWIP Optimization (II)

7 × 7 structure (20.5 × 20.5 μm)

Λ = 2.7 μm
h = 0.75 μm
w = 0.7 μm
l = 1.6 μm
p = 0.7 μm
d.c. = 0.6

Average Normalized Absorbed Flux A_0

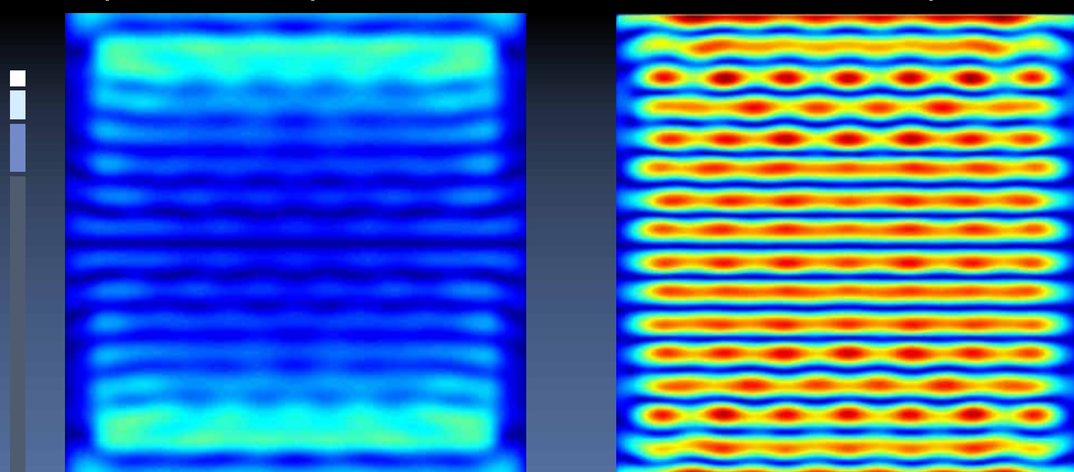
$$A_0 = \frac{\int_{7.5\,\mu m}^{9.5\,\mu m} A(\lambda)\,d\lambda}{\Delta\lambda}$$



1,2 .... 7 periods

Metallic grating is fundamental for optimum performance of the QWIP device

Ey Field Component @ λ of the maximum absorption

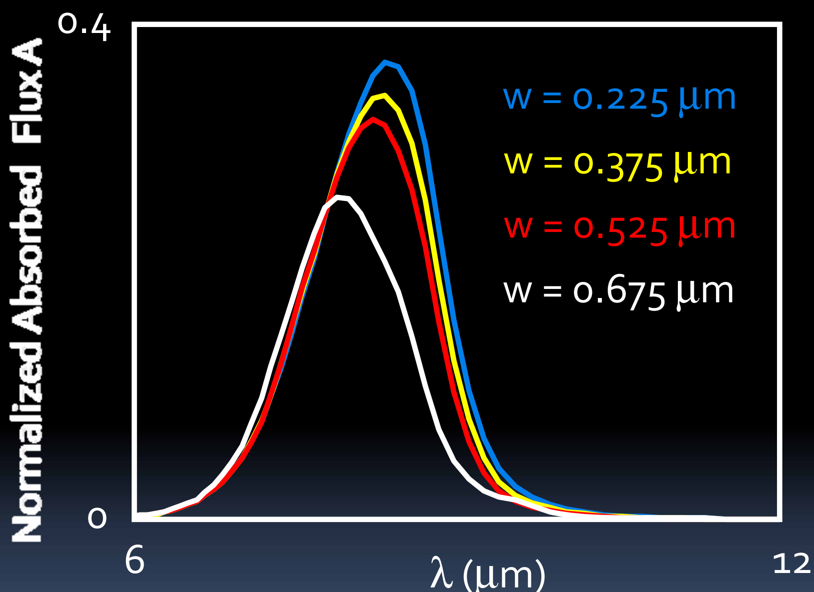


No Grating λ=8.59 μm **Grating λ=8.28 μm**

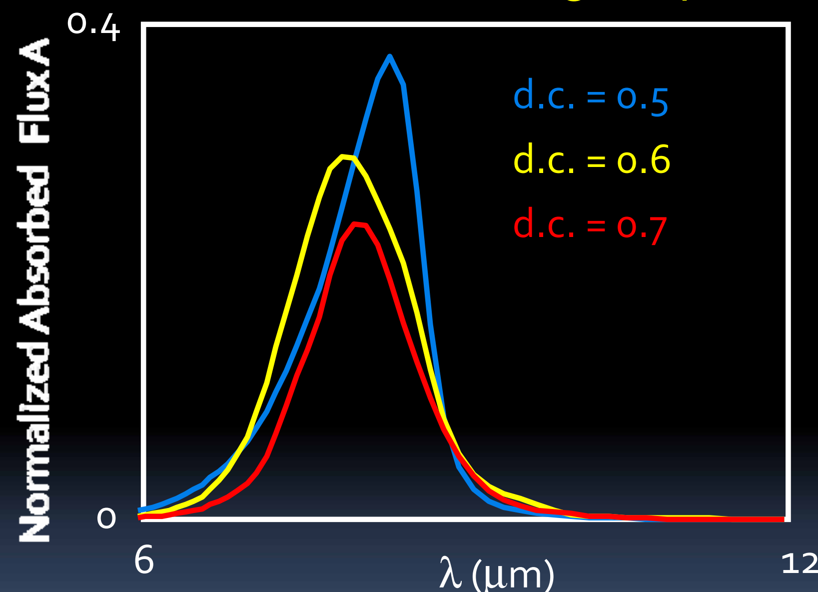
QWIP Optimization (III)

Λ = 2.7 µm
h = 0.75 µm
w = 0.225 ÷ 0.675 µm
l = 1.6 µm
p = 0.7 µm
d.c. = 0.5 ÷ 0.7

7 × 7 structure (20.5 × 20.5 µm)



w - Thickness of the Emitter

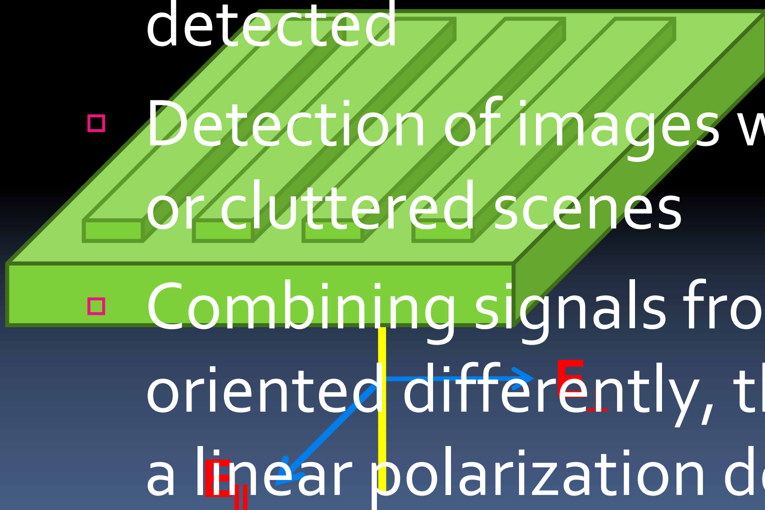


d.c. - Duty Cycle

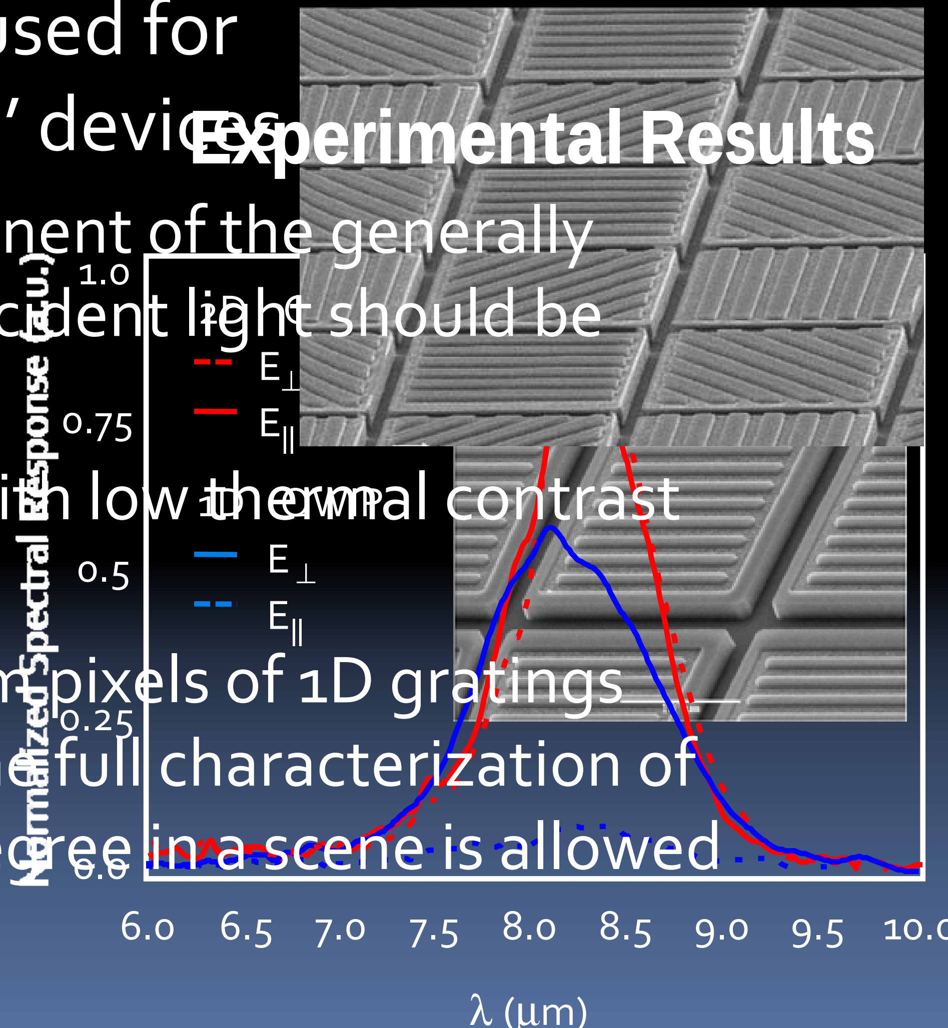
- Reducing the thickness of the emitters w, the distance between the grating and the active zone decreases, thus increasing the E_y field in the QW zone
- d.c. = 0.5 allows the best performance of the QWIP

1D Coupling Grating QWIP

- 1D Coupling Grating used for ‘polarization sensitive’ devices
  - Only one linear component of the generally elliptically polarized incident light should be detected
  - Detection of images with low thermal contrast or cluttered scenes
  - Combining signals from pixels of 1D gratings oriented differently, the full characterization of a linear polarization degree in a scene is allowed

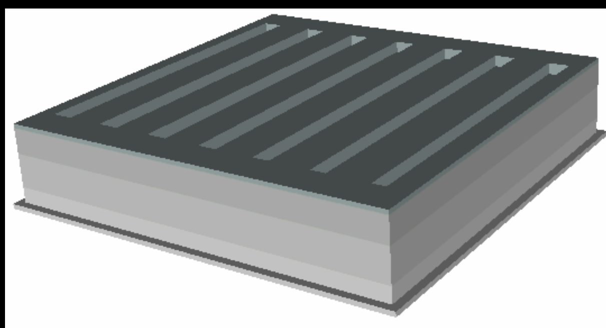


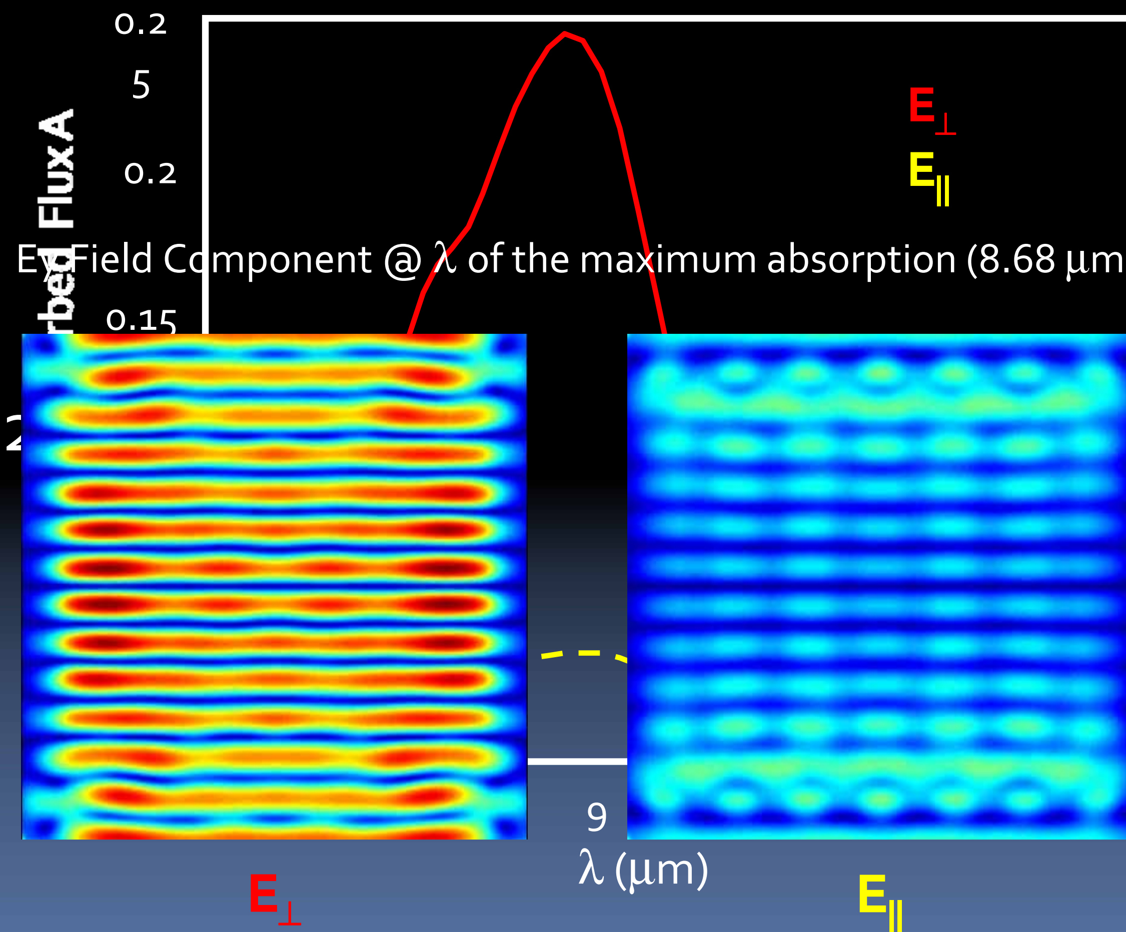
Experimental Results



1D Coupling Grating - Results

FDTD Model



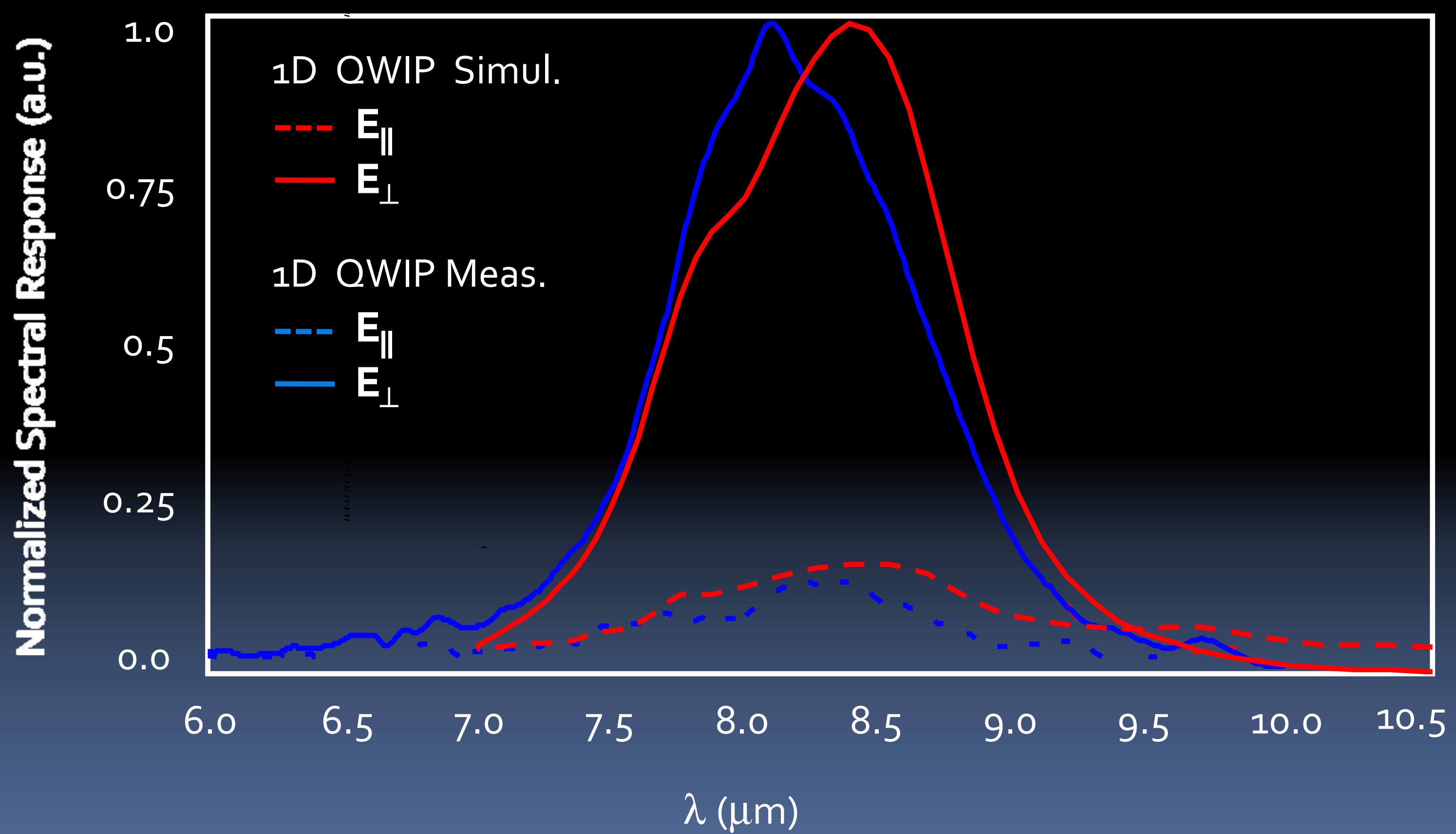


7 × 1 structure (20.5 × 2

- Λ = 2.7 μm
- h = 0.75 μm
- w = 0.7 μm
- l = 1.6 μm
- p = 0.7 μm
- d.c. = 0.5

1D Coupling Grating - Results

Simulation vs Measurement



Conclusions

- FDTD technique used as a design and optimization tool for QWIP devices
  - Design and Optimization of the Grating Surface
  - Investigations on the influence of the different parameters on the absorption of a QWIP
  - 2D and 1D coupling grating investigated
  - Good agreement between simulations and measurements