ACCURATE SIMULATION OF QUANTUM WELL INFRARED PHOTODETECTORS BY FDTD
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 (Breast Cancer Detection)
  - Military
Introduction: Image Formation

Lightened environment
Visible - Infrared

Reflection of Solar Radiation

Dark Environment
Thermal Infrared

Self Radiation

Reflected Light

$\lambda$

0.5 $\mu$m  3 $\mu$m  10 $\mu$m

Ultra-violet  Visible  Reflected IR  Thermal IR
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

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

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

- \( c = 310^{-8} \) m/s
- \( h = 6.62510^{-27} \) erg/s
- \( k = 1.3810^{-27} \) erg/°K
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 \( \propto \frac{1}{E_g} \) and EMt in the detector
- Absorbed \( \lambda \) depend on the semiconductor band-gap

\[ \Rightarrow \text{Only } \lambda: \ E_g > E_{g_0} \text{ can be absorbed} \]

\[ \therefore \text{Problems in obtaining detectors for long wave (} \lambda \approx 10 \ \mu m \text{ ) IR} \]
\[ \text{(small } E_g \text{ materials: } E_g \approx 0.1 \text{ eV)} \]

\[ \downarrow \text{‘Conventional Detection’ (with weak band-gap materials as } Hg_xCd_{1-x}Te \text{) is not efficient (exotic materials, not developed!)} \]

\[ \Rightarrow \text{‘Effective’ band-gap materials (} GaAs/AlGaAs \text{ heterostructures) which use InterSubBand transitions created by} \]
\[ \text{Quantum Wells in large-band-gap semiconductors} \]
Quantum Well Infrared Detectors

- **Photonic detectors with weak band-gap** \((\text{Hg}_x\text{Cd}_{1-x}\text{Te})\)
  (to have detection @ long wave IR)
  - Concentration adjusted for \(\lambda\) 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$_x$Ga$_{1-x}$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 $\Rightarrow$ 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)

- Photodetectors are assembled in Matrices
- Each Pixel is a QWIP

Matrices are then put in the detector system and installed inside the IR Camera.
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
Optics
Applications
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 $\lambda$ 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)

- Total PEs: 4 PEs × 3 PEs × 4 PEs = 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

Real Conductor

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

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

\[ \frac{\partial \vec{J}_p}{\partial t} = -\omega \vec{J}_p + \varepsilon_0 \omega_p^2 \vec{E} \]

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

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

\( \omega_p \): Plasma frequency
\( \nu \): Collision frequency

Parameters for Gold

\( \omega_p \): \( 2\pi \times 2.175 \times 10^{15} \) rad/s
\( \nu \): \( 2\pi \times 6.5 \times 10^{12} \) rad/s
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)

\[ \varepsilon_0 \frac{\partial \vec{E}}{\partial t} = \nabla \times \vec{H} - \vec{J}_p \]
\[ \frac{\partial \vec{J}_p}{\partial t} = -\nu_1 \vec{J}_p + (\varepsilon_s - \varepsilon_\infty)\varepsilon_0 \omega_1^2 \vec{P} \quad \frac{\partial \vec{P}}{\partial t} = \vec{J}_p \]
\[ \hat{\varepsilon} = \varepsilon_0 \varepsilon_\infty + \frac{(\varepsilon_s - \varepsilon_\infty)\varepsilon_0 \omega_1^2}{\omega_1^2 + j \omega \nu_1 - \omega^2} = \varepsilon_0 [1 + \hat{\chi}(\omega)] \]

- 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)

\( \omega_1 \): Resonant frequency
\( \nu_1 \): Damping frequency
\( \varepsilon_s \): Static relative permittivity
\( \varepsilon_\infty \): Infinite relative permittivity
Parameters for the Lorentz Model

The parameters $\omega_1$, $\psi_1$, $\varepsilon_\infty$ 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)

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

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

\[
P_i(\lambda) = \text{Re}\left\{ \int\int_{S_i} \frac{\tilde{E}_\parallel \times \tilde{H}^*_\parallel}{2} \, ds \right\}
\]

\[
A(\lambda) = \frac{P_a(\lambda)}{P_0(\lambda)}
\]
**QWIP Parameters**

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

- \[ \Lambda = 2.7 \, \mu m \]
- \[ h = 0.75 \, \mu m \]
- \[ w = 0.7 \, \mu m \]
- \[ l = 1.6 \, \mu m \]
- \[ p = 0.7 \, \mu m \]

- d.c. = \( a / (a+b) = a / \Lambda \)
FDTD Simulation Parameters

- **Discretization**
  - $\Delta_x = \Delta_y = \Delta_z = 75 \text{ nm (36 points}/\Lambda)$
  - $7\Lambda \times 7\Lambda \text{ QWIP: } 277 \times 63 \times 277 \text{ cells}$
  - PML Layer: 14 cells, $\rho = 1.0 \times 10^{-6}$ (8,465,275 overall mesh points)
  - Temporal Time Step: $7.22 \times 10^{-16} \text{ s}$

- **Input / Output Parameters**
  - TFSF Excitation: $f_0 = 35 \text{ THz (} \lambda = 8.5 \mu\text{m}); \text{ BW = 12THz}$
  - DFT Computation: frequency range $[25 \div 45] \text{ THz (50 samples)}$
  - Number of Time steps: 30000
  - Total Computation Time: $8600 \text{ s (~ 2.4 h on 6 PEs – PIV 3GHz)}$
FDTD Parallel Performance

- 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

*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*
FDTD Parallel Performance (II)

- **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

Ey Field Component @ $\lambda=8.28 \mu m$ for a 7 x 7 QWIP

$\Lambda = 2.7 \mu m$

$h = 0.75 \mu m$

$w = 0.7 \mu m$

$l = 1.6 \mu m$

$p = 0.7 \mu m$

d.c. = 0.6
QWIP Optimization

7 × 7 structure (20.5 × 20.5 μm)

Average Normalized Absorbed Flux $A_0$

$$A_0 = \frac{\int A(\lambda) d\lambda}{\Delta \lambda}$$

$\Lambda = 2.7 \mu m$
$h = 0.75 \mu m$
$w = 0.7 \mu m$
$l = 1.6 \mu m$
$p = 0.7 \mu m$
$d.c. = 0.6$

PEC good approximation for the metallic coating (Au)
QWIP Optimization (II)

7 × 7 structure (20.5 × 20.5 μm)

\[ \lambda = 2.7 \text{ μm} \]
\[ h = 0.75 \text{ μm} \]
\[ w = 0.7 \text{ μm} \]
\[ l = 1.6 \text{ μm} \]
\[ p = 0.7 \text{ μm} \]
\[ d.c. = 0.6 \]

\[ A_0 = \frac{\int A(\lambda) \, d\lambda}{\Delta \lambda} \]

Average Normalized Absorbed Flux \( A_0 \)

Ey Field Component @ \( \lambda \) of the maximum absorption

Metallic grating is fundamental for optimum performance of the QWIP device

No Grating \( \lambda = 8.59 \text{ μm} \)
Grating \( \lambda = 8.28 \text{ μm} \)

1, 2 .... 7 periods
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 × 20.5 μm)

- \( \Lambda = 2.7 \, \mu m \)
- \( h = 0.75 \, \mu m \)
- \( w = 0.7 \, \mu m \)
- \( l = 1.6 \, \mu m \)
- \( p = 0.7 \, \mu m \)
- \( d.c. = 0.5 \)

Ey Field Component @ \( \lambda \) of the maximum absorption (8.68 μm)
1D Coupling Grating - Results
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