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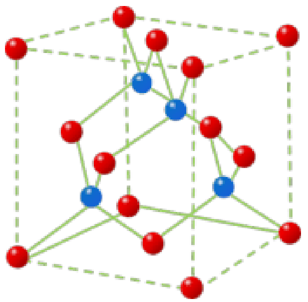
Numerical Device Modeling & Simulation of Infrared Detectors: Challenges & Techniques

October 30, 2023



II-VI Tutorial

U.S. Workshop on the Physics and Chemistry of II-IV Materials

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Acknowledgements & Contributors

Methodology & Requirements

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- Dr. Philip Perconti (** DEVCOM ARL)
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- Dr. Arvind D'Souza (Leonardo DRS)
- Dr. Andreu Glasmann (DEVCOM ARL)

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- DEVCOM ARL
  - Multiscale Modeling of Electronic Materials Collaborative Research Environment (MSME CRA)
    - **10-year numerical model development program**
  - Center for Semiconductor Modeling of Materials & Devices (CSM)

Analytical Modeling

- Dr. Roger E. DeWames (**DEVCOM C5ISR-RTI)

Model Development – Drift-Diffusion

- Dr. Danilo D'Orsogna (**Boston University)
- Dr. Craig Keasler (**Boston University)

Model Development – NEGF & SPDD

- Dr. Francesco Bertazzi (Politecnico di Torino)
- Dr. Alberto Tibaldi (Politecnico di Torino)

Model Development – FBMC3D

- Dr. Stefano Dominici (**Politecnico di Torino)
- Dr. Ilya Prigozhin (**Boston University)
- Mr. Mike Zhu (Boston University)
- Dr. Mateo Alasio (Boston University)

Model Development – MTF

- Dr. Benjamin Pinkie (**Boston University)

Simulations – T2SL Transport

- Prof. Enrico Bellotti (Boston University)

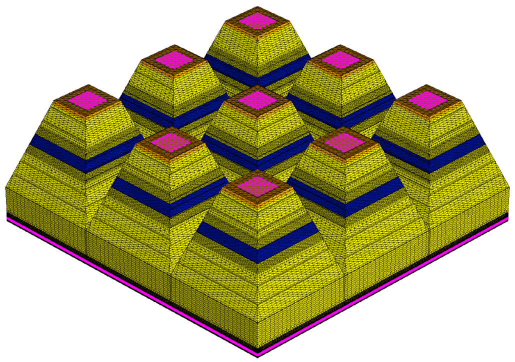
Simulations – HgCdTe APDs

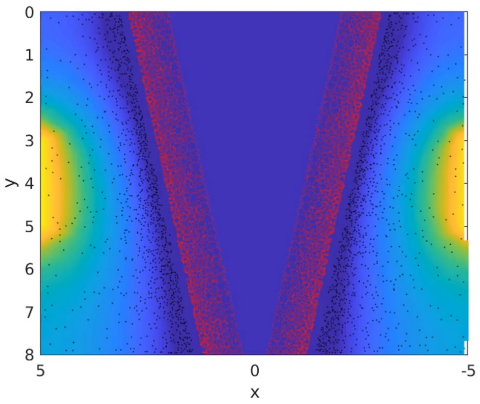
- Dr. Ilya Prigozhin (**Boston University)
- Mr. Mike Zhu (Boston University)

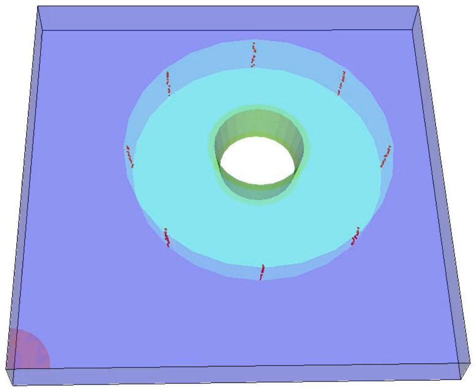
**Affiliation when contribution was made

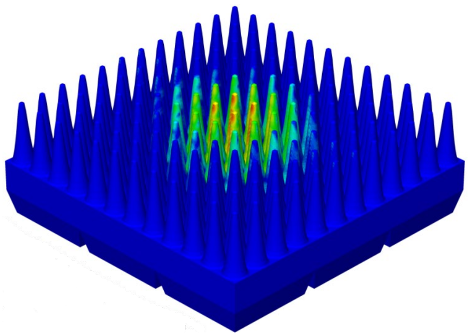
Outline

- ➢ Why Perform Modeling?
- ➢ Modeling Overview and Capabilities
  - What Numerical Modeling Buys You!
- ➢ Modeling Device Metrics – Single Devices & Arrays
  - Alloy Semiconductors (*e.g.*, HgCdTe, InGaAs, Alloy nBn, *etc.*)
  - Type II Superlattices (T2SL)
    - Nonequilibrium Green's Function (NEGF)
    - Quantum Corrected Drift Diffusion (QCDD)
  - Avalanche Photodiodes (APDs)
    - Full Band Monte Carlo (FBMC)
- ➢ Modeling Imaging Metrics – Modulation Transfer Function (MTF)
- ➢ Summary & Takeaways









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Why Perform Numerical Device Modeling?

The Challenge

- ➢ Characteristic time to transition from technology to product development is long and contains unknowns that impact risks/benefits ratio
  - Inadequate understanding of real device operation
- ➢ Bridging the gap between what we design and what we build

To Realize Benefits of Device Modeling – Predictive and Explanatory

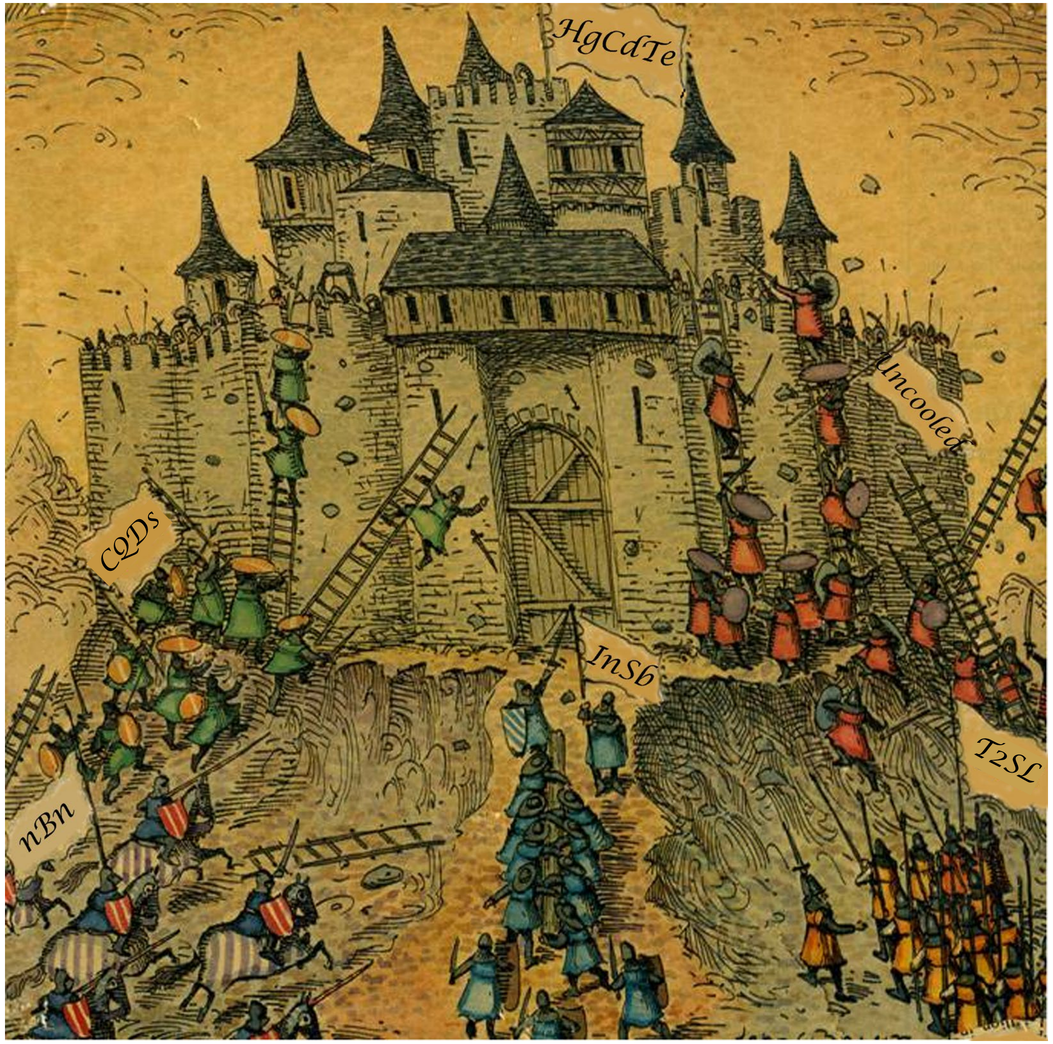
- ➢ Reliable material parameters – Accurate and *independently* validated
- ➢ Accurate device geometries, specifications & measured data
  - Layer dimensions & interfaces
  - Composition and doping profiles (ideally measured by SIMS)
  - Surface morphology & properties
- ➢ Coupled to experimental efforts
  - Device data (temperature & voltage dependence) → Essential to understand the operation of the final devices
  - Thorough data analysis

Impact: Successfully Accelerate Technology – Reduce Risks/Costs & Increase Performance

1) Understand current state-of-the-art devices – fundamental vs. technological limitations
2) Explore parameter space – design/formulate experiments → achieve optimal performance
3) Conceptualize new device architectures that may provide improvements over current SOA

New IR Detector Materials & Simulation Challenges

Recently Emerging IR Materials (*e.g.*, Superlattices & CQDs) and Device Architectures (*e.g.*, APDs) Cannot be Simulated With Semi-Classical Approaches (*e.g.*, Drift-Diffusion Solvers) → More Robust Models Developed



Cartoon originally produced by Dr. Gérard Destéfanis at CEA-LETI-Minatec. Provided by Dr. Paul Norton (Norton, 2013).

Widely Used Semi-Classical Drift-Diffusion Simulators Are Not Applicable to Newly Emerging IR Materials → Quantum Mechanical-based Simulators Required

Semiconductor Device Modeling

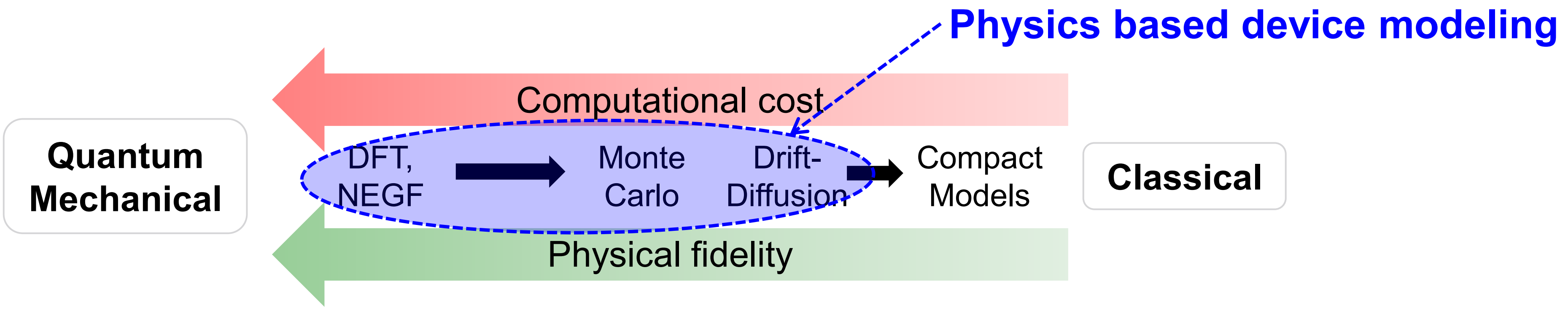
Fabrication Limitations

- Costly, time consuming
  - IR materials equipment are expensive
  - Fabrication cycles take months
  - Poor yield
- Design optimization requires several manufacturing/testing cycles

Semiconductor Modeling

- Helps explain measurements
  - What limits performance?
  - Decouples fabrication issues & testing limitations from device performance
- Effective & efficient design optimization

→ Must be predictive
→ Should be coupled to experiment



Device models solve Boltzmann Transport Equation (BTE) – describes time evolution of carriers

$$\frac{\partial f}{\partial t} + \frac{\boldsymbol{F}_{ext}}{m} \cdot \nabla_v f + \boldsymbol{v} \cdot \nabla_x f = \left(\frac{\partial f}{\partial t}\right)_{collisions}$$

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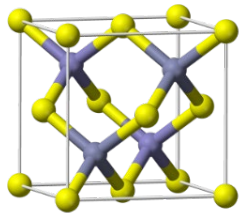
The Vision: From Atoms to MTF – Multi-Scale IR Detector Modeling

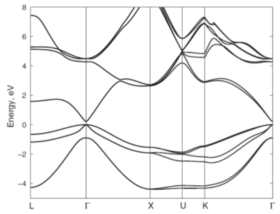
Material Modeling **Device Modeling** **System Modeling**

Increasing length scale from atoms-to-systems

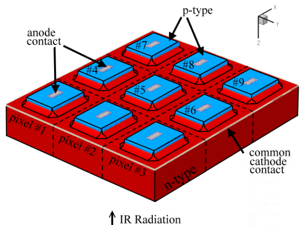
1 – 50 Å | 1 – 500 nm | 100 nm – 10 µm | 5 – 50 µm | 1 – 1000 mm

Feedback to earlier levels for validation

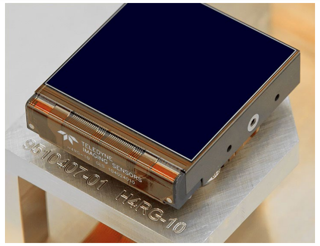




F. Bertazzi et al., J. of Electron. Mater. (2010)



D. D’Orsogna et al., J. of Electron. Mater. (2008)



http://www.teledyne-si.com/ps-h4rg.html

http://www.defensemedianetwork.com

Parameters extracted at each level become inputs for next level

Material Characteristics:
- Properties
- Carrier Recombination
- Transport Phenomena

Device/Array Performance:
- Geometrical effects
- J(V), SR, QE, MTF
- Crosstalk
- Array MTF

System Performance:
- Sensitivity
- Dynamic Range
- Resolution (MTF from detector/lenses, etc.)

Modeling Applied from Both Directions

Working from the Material Up

- Material Modeling and Validation
- Device Analysis and Modeling
- Disruptive Innovations

Working from the System Down

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What is the Impact of 1D Analytical to 3D Numerical Device Modeling?

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1D Analytical Modeling

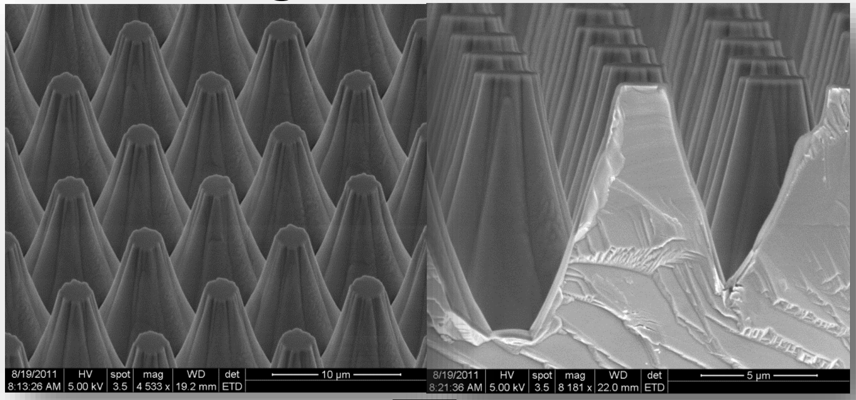
- Closed form solutions to analytical semiconductor equations
- Usually 1D
- Used at numerous institutions (ARL, Teledyne, *etc.*)
- Very useful tool to predict device parameters & performance (quick feedback but limited information)

2D & 3D Numerical Device Modeling

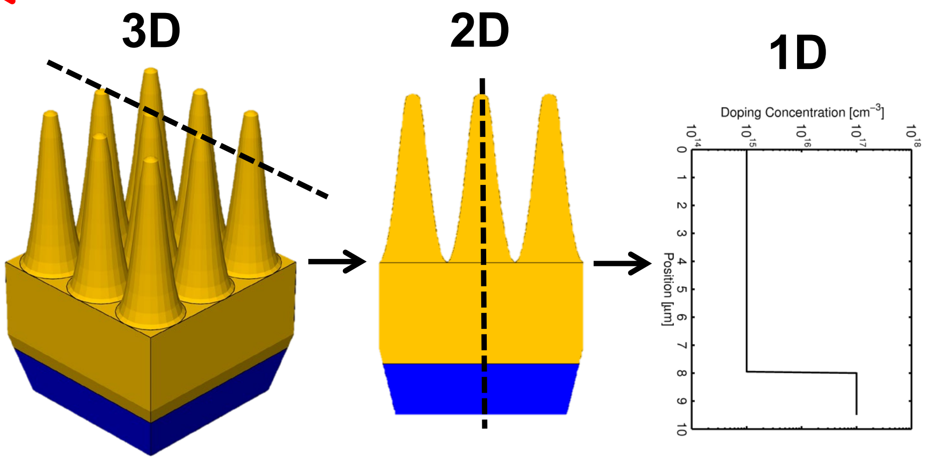
What are we gaining?

Device Architecture / Design Optimization		Analytical 1D	Numerical 1D	Numerical 2D	Numerical 3D
Homojunction		1D-3D	✓	✓	✓
Heterojunction		✗	✓	✓	✓
Junction Location Opt.		✗	✓	✓	✓
Large Area Devices		✓	✓	✓	✓
Dual Band Devices		Limited (LM)	✓	✓	✓
Pixel Arrays ($L_p \geq$ pitch)	Dark Current	✗	✗	LM	✓
	QE	✗	✗	LM	✓
	Crosstalk	✗	✗	LM	✓
	MTF	✗	✗	LM	✓
Photonic Structures		✗	✗	✗	✓

SEM Image of Devices



Increasing Computational Complexity



Decreasing Dimensionality = Loss of Information

Sophisticated IR Materials & Device Architectures Required High Fidelity Numerical Models

Optical Excitation Approaches

1) Beer's Law

- FEM Absorption Model (others exist)

$$G_{opt}(z) = P_0\left(\frac{\lambda}{hc}\right)F_t(t)F_{xy}\alpha(\lambda,z)\exp\left(-\left|\int_{z_0}^{z}\alpha(\lambda,z')dz'\right|\right)$$

Consider
- Quasi-static
- Growth (z-direction) only

$$G_{opt}(z) = \phi\alpha(\lambda,z)\exp(-\alpha(\lambda,z)\times z) \approx \phi\alpha\exp(-\alpha z)$$

- Simple & computationally efficient
- Omits reflections off interfaces & time-dependence
- Inappropriate for complex geometries

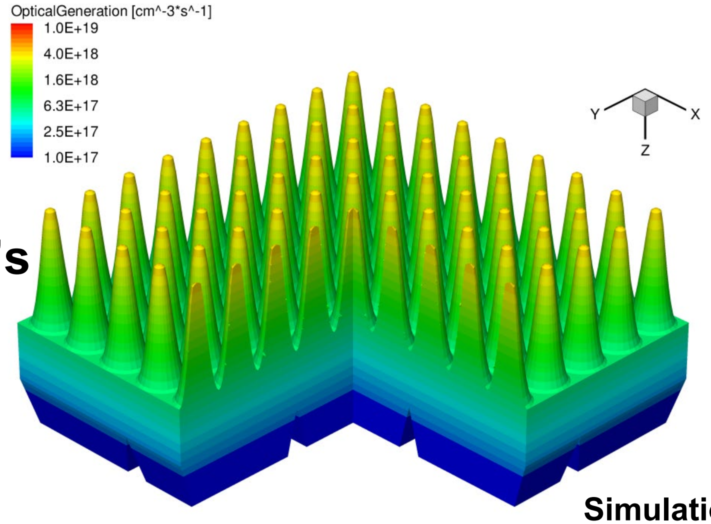
2) Ray Tracing

- All the benefits to Beer's Law approach, but includes reflections off of interfaces

3) Full Solution of Maxwell's Equations

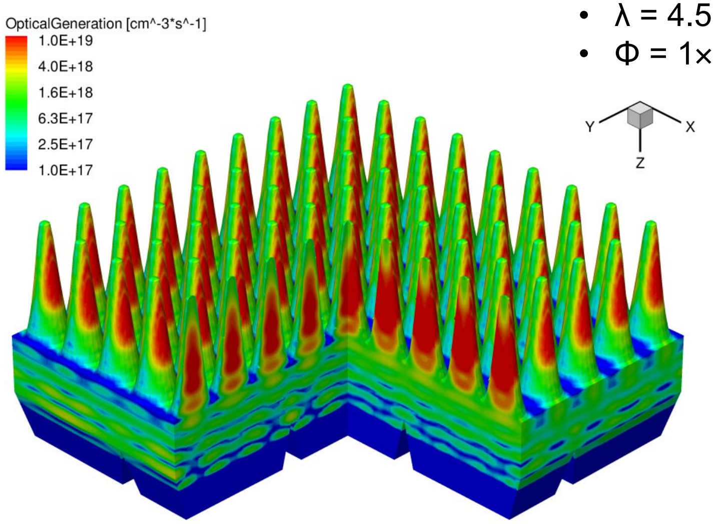
- Most verbose solution (suitable for complex geometries), but computationally expensive

1) Beer's Law



Simulation Conditions:
- 6×6 μm^2 pixel
- T = 140 K
- λ = 4.5 μm
- Φ = 1×10^{15} ph/cm^2-s

3) FDTD Solution of Maxwell's Equations



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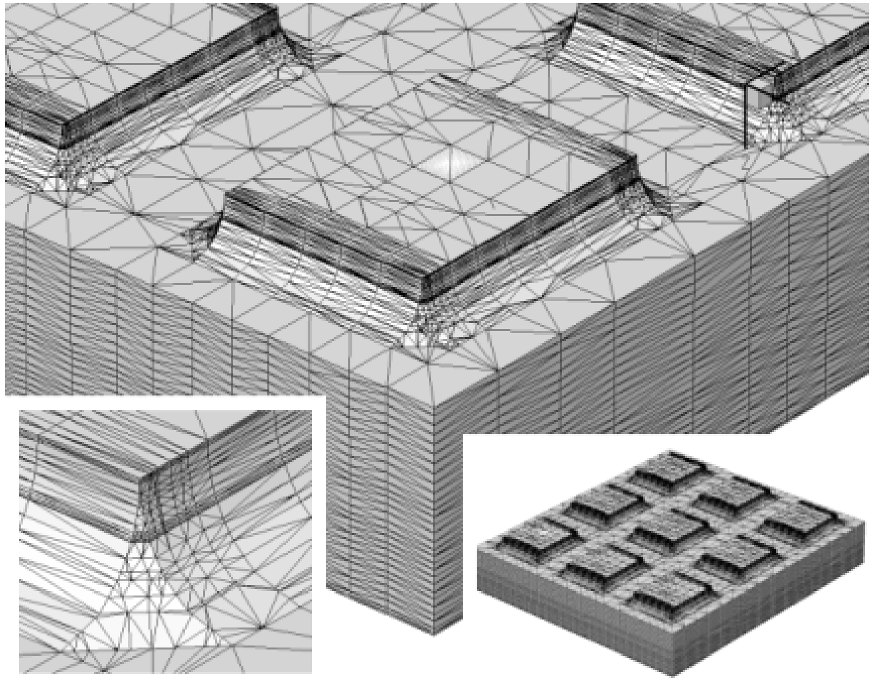
Drift-Diffusion Model & Finite Element Method

$$\nabla^2\phi = -\frac{q}{\epsilon}(p - n + N_D^+ - N_A^-) + \rho_{trap}$$

$$\frac{\partial n}{\partial t} = \frac{1}{q}\nabla\cdot \boldsymbol{J}_n + G_n - R_n \qquad \boldsymbol{J}_n = qD_n\nabla \mathrm{n} + q\mu_n n\nabla\phi$$

$$\frac{\partial p}{\partial t} = -\frac{1}{q}\nabla\cdot \boldsymbol{J}_p + G_p - R_p \qquad \boldsymbol{J}_p = -qD_p\nabla p - q\mu_p p\nabla\phi$$

Numerically solve this system of differential equations to yield $\phi(x,y,z,t)$, $n(x,y,z,t)$, and $p(x,y,z,t)$



D. D'Orsogna *et al.* , *J. Electron. Mater*. Vol. 37, (2008)

Material Model

Electrical Parameters

- ✓ Energy Gap
- ✓ Affinity
- ✓ Effective Mass
- ✓ Mobility
- ✓ Dielectric constant
- ✓ Radiative Lifetime
- ✓ Auger Lifetime
- ✓ SRH Lifetime

Recombination Rates

$$R_{Aug} = (C_n n + C_p p)(np - n_i^2) \approx N_D/\tau_{Aug}$$

$B, C_{n,p}$ calculated externally

$$R_{Rad} = B(np - n_i^2) \approx N_D/\tau_{Rad}$$

$$R_{SRH} = \frac{np - n_i^2}{\tau_p(n+n_1) + \tau_n(p+p_1)}$$

$\tau_{n,p}, E_{trap}$ extracted from data

$$n_1 = n_i \exp(+E_{trap}/(kT))$$

$$p_1 = n_i \exp(+E_{trap}/(kT))$$

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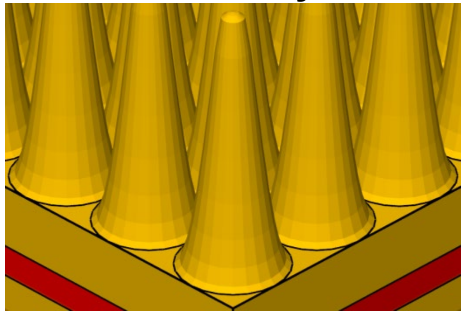
Proper Mesh Design Critical for Accurate Results

Numerical Device Modeling 2D & 3D Numerical Approach

Numerical model validated by comparing results to experimental data provided by BAE, DRS, RVS, and data available in literature

Geometry



- J. Schuster, *et al*., “Numerical simulation of third-generation HgCdTe detector pixel arrays,” *IEEE* J. Sel. Top. Quant. Electron., Vol. 19, 3800415 (2013)
- J. Schuster and E. Bellotti, “Evaluation of Quantum Efficiency, Crosstalk, and Surface Recombination in HgCdTe Photon-Trapping Structures,” J. Electron. Mater., Vol. 43, pp. 2808 (2014)

Numerical Device Modeling 2D & 3D Numerical Approach

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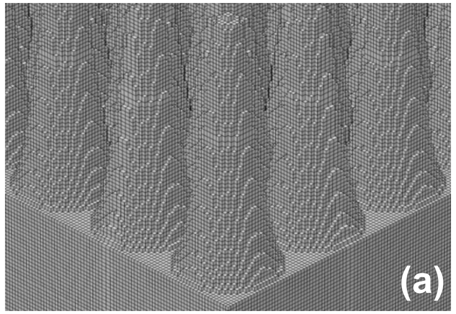
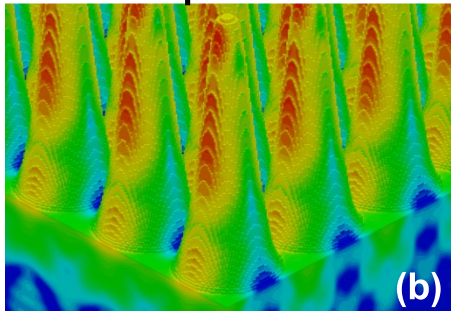
FDTD Mesh

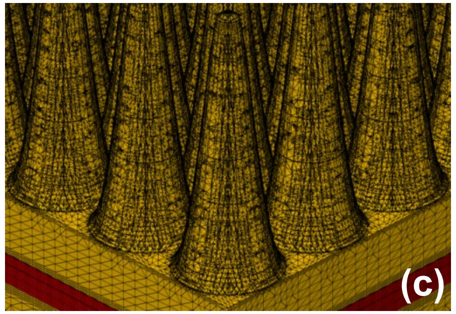


Perform FDTD Simulations

FDTD Opt. Gen. Rate

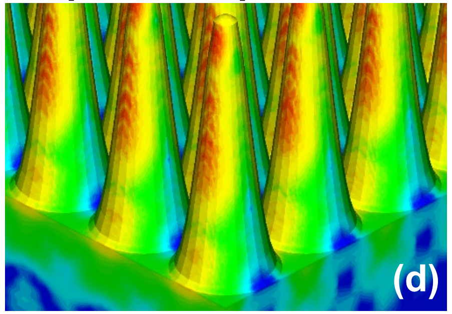


FEM Mesh



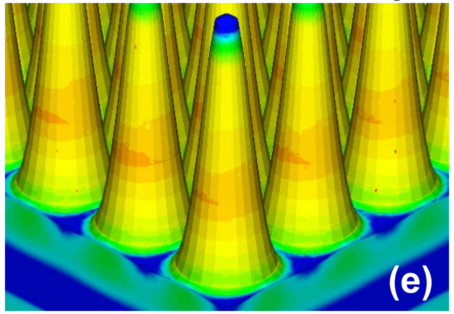
Interpolate Opt. Gen. Rate Onto FEM Mesh

Interpolated Opt. Gen. Rate



Perform FEM Simulations

Hole Current Density



Performance and Figures Of Merit

(I)
- Reflectance
- Optical Crosstalk

(II)
- Dark Current
- Photo Current

- Quantum Efficiency
- Diffusion Crosstalk
- MTF

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Material Libraries

Paramount to have library of material parameters that are

- Complete
- Impartial
- Independent

Status

- HgCdTe – mostly completed
- InAsSb – relatively good
- InGaAs – relatively good
- T2SL – significantly lacking, especially LW

Parameters		Alloy Material Systems		
		$Hg_{1-x}Cd_xTe$	$InAs_{1-x}Sb_x$	$In_{1-x}Ga_xAs$
Energy Gap		✓	✓	✓
Affinity		✓	✓	✓
Effective Mass		✓	✓	✓
Mobility		✓	✓	✓
Dielectric Constant		✓	✓	✓
Recombination	Radiative	✓	✓	✓
	Auger	✓	✓	✓
	SRH	✓	✓	✓
Refractive Index		✓	✓	✓
Absorption Coefficient		✓	✓	✓

↑ Most x values ↑ $x = \begin{cases} 0.09 \\ 0.21 \end{cases}$ ↑ $x = 0.53$

Type II Superlattices (T2SL)

- Specific structure (individual InAs & InAsSb layer thicknesses, # periods, mole fraction, *etc.*) must be known → directly impacts parameters
- Turn-on bias highly dependent on barrier affinity & doping w.r.t. T2SL absorber
- Parameters change every time individual layer thicknesses, periods, or mole fraction is altered
- Lifetimes, diffusion lengths, carrier concentration fairly well known for the best MWIR materials
- Measured lifetimes/mobilities are notably scattered!

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Accurate, Robust, Temperature-Dependent & Independently Verified Material Parameters Required For Predictive Simulations

Bottom line up front (BLUF) → What Numerical Modeling Buys You!

Two & Three Dimensional Numerical Models

Inputs

Material Parameters
- Measurement
- Modeling

Layer Specifications
- Thicknesses
- Mole Fraction
- Doping
- SIMS Profiles

No Approximations
No Fitting Parameters
(except SRH lifetime)

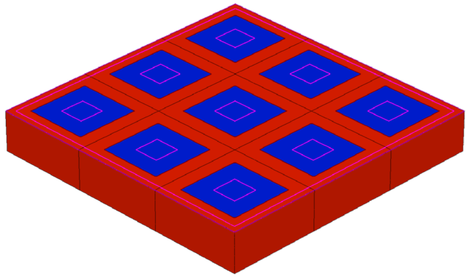
Outputs

Device Understanding
- Band Diagrams
- Carrier Distributions
- Electric Fields
- Surface Behavior
- Interface Behavior

Device Performance
- Reflectance
- Dark Current
- Quantum Efficiency
- Crosstalk
- Modulation Transfer Function

Analytical vs Numerical Model Capabilities

Device Architecture / Design Optimization		Analytical	Numerical		
		1D	1D	2D	3D
Homojunction		1D-3D	✓	✓	✓
Heterojunction		✗	✓	✓	✓
Junction Location Opt.		✗	✓	✓	✓
Large Area Devices		✓	✓	✓	✓
Dual Band Devices		Limited (LM)	✓	✓	✓
Pixel Arrays ($L_p \geq$ pitch)	Dark Current	✗	✗	LM	✓
	QE	✗	✗	LM	✓
	Crosstalk	✗	✗	LM	✓
	MTF	✗	✗	LM	✓
Photonic Structures		✗	✗	LM	✓



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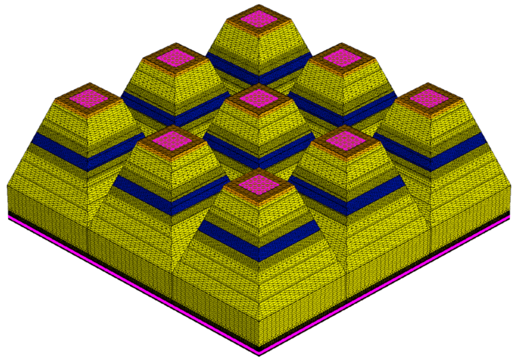
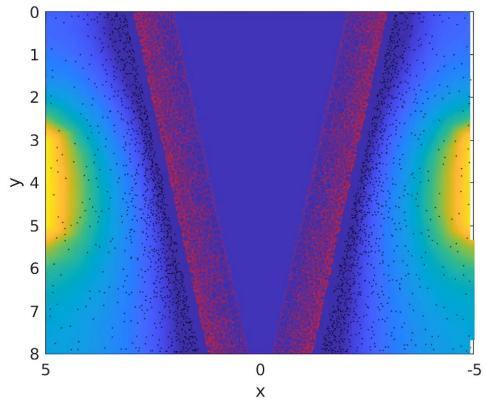
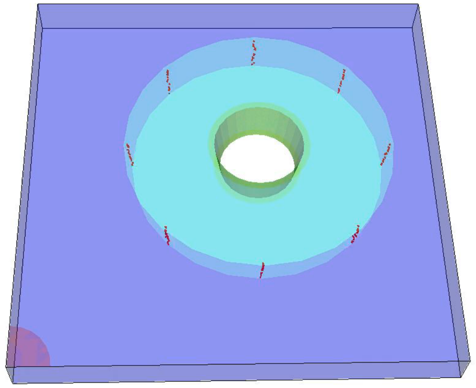
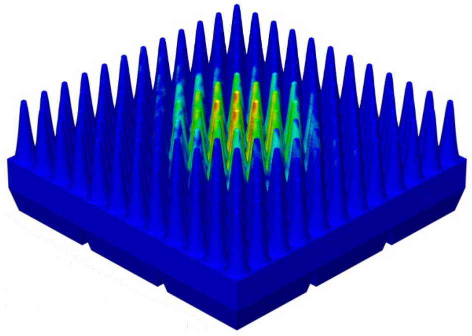
- Summary & Takeaways









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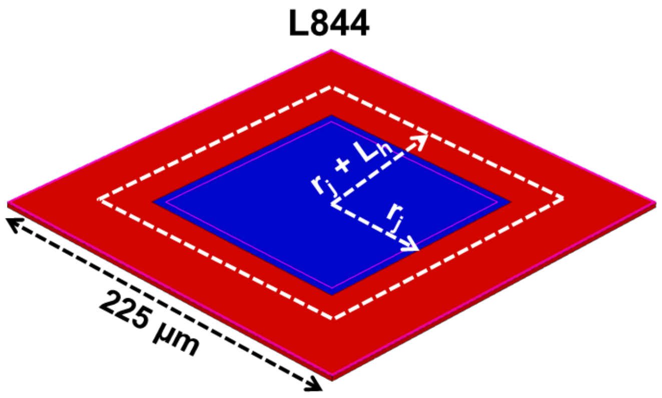
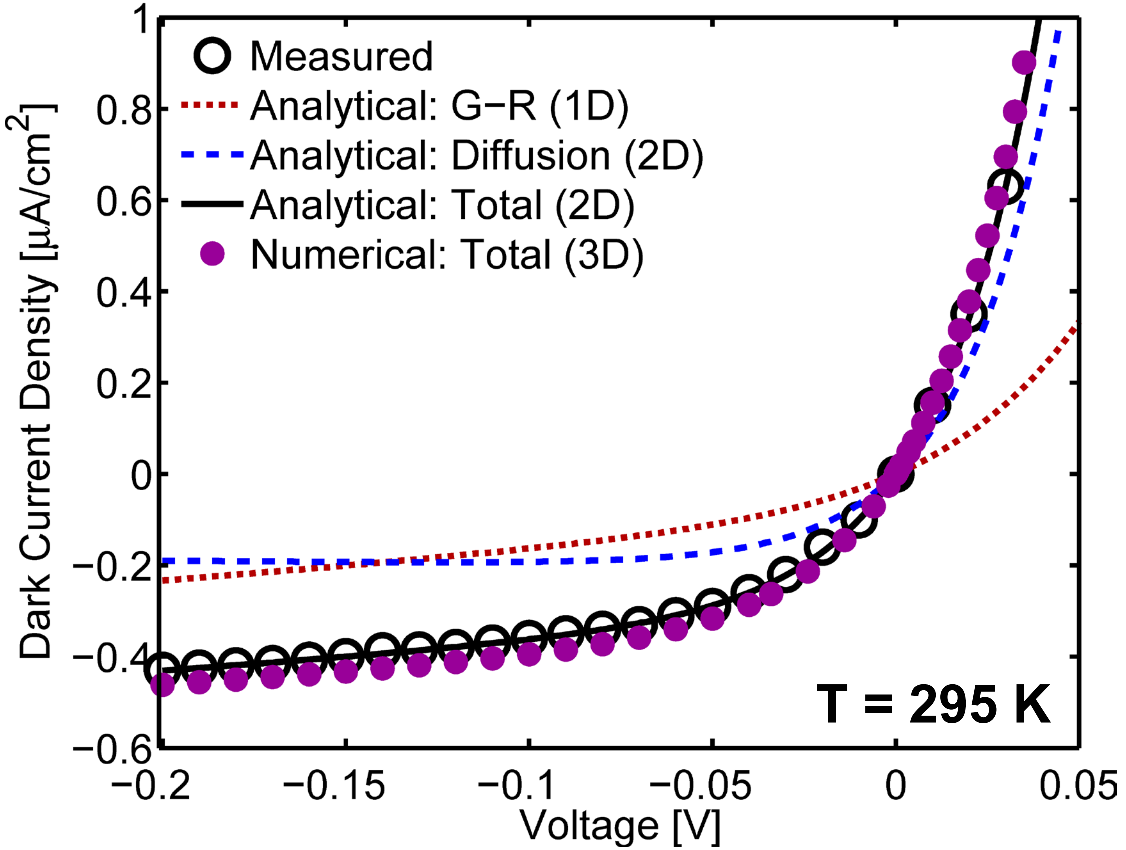
Semi-Classical Drift-Diffusion: $Hg_{1-x}Cd_xTe$ SWIR DLPH Photodiodes – I(V) Characteristics



	L844
x	0.564
N_d (cm^{-3})	1.5×10^{15}
d (µm)	2.8
Size (µm)	125 (sq.)
A_j (cm^2)	1.56×10^{-4}

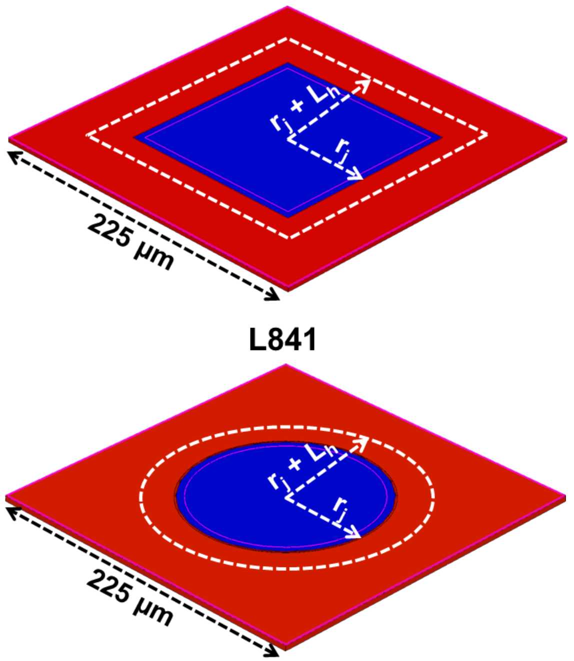


SRH Lifetime

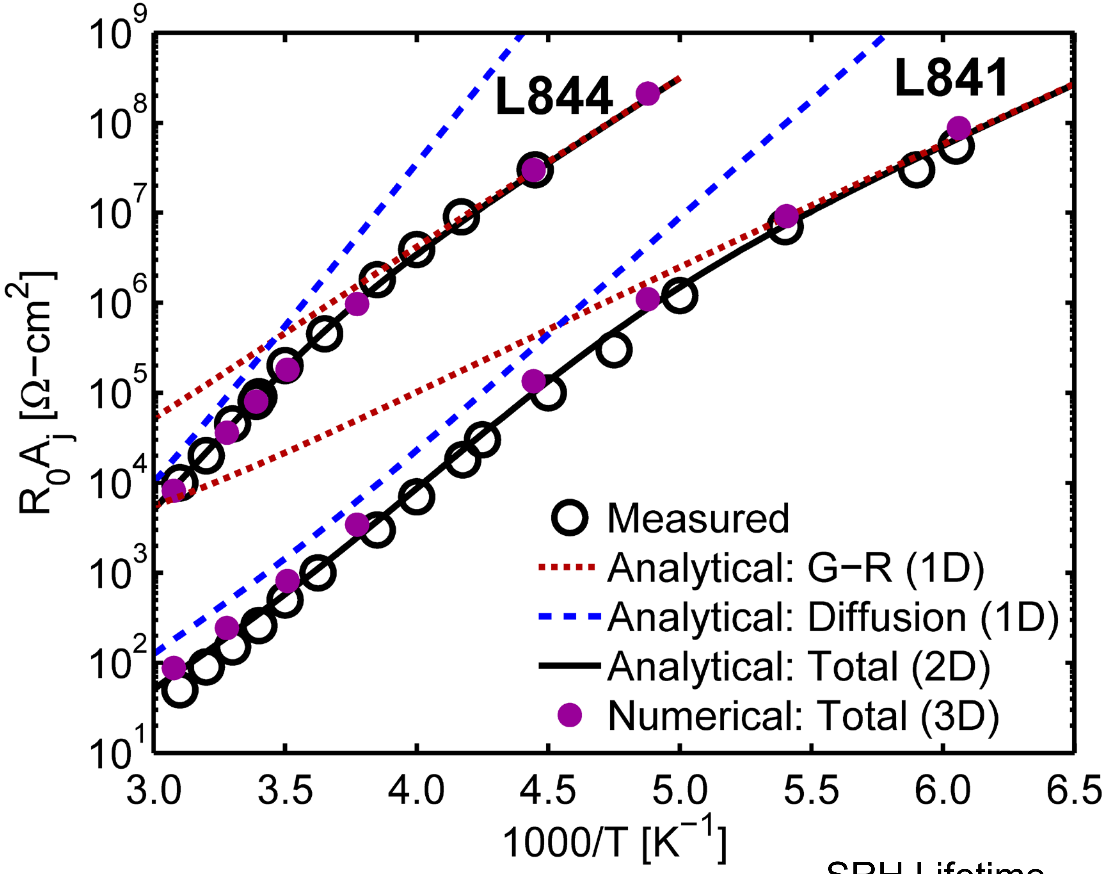
- $\tau_{n0} = 80.0$ µs
- $\tau_{p0} = 2.5$ µs
- $E_t = E_F$

J. Schuster et al., "Numerical Device Modeling, Analysis, and Optimization of Extended-SWIR HgCdTe Infrared Detectors," J. Electron. Mater., Vol. 45, pp. 4654 (2016)

Semi-Classical Drift-Diffusion: $Hg_{1-x}Cd_xTe$ SWIR DLPH Photodiodes – R_0A_j Product vs. Inv. Temperature



	L844	L841
x	0.564	0.455
N_d (cm^{-3})	1.5×10^{15}	2.0×10^{15}
d (µm)	2.8	3.6
Size (µm)	125 (sq.)	125 (c.)
A_j (cm^2)	1.56×10^{-4}	1.23×10^{-4}



SRH Lifetime
- $\tau_{n0} = 80.0$ µs
- $\tau_{p0} = 2.5$ µs
- $E_t = E_F$

J. Schuster et al., "Numerical Device Modeling, Analysis, and Optimization of Extended-SWIR HgCdTe Infrared Detectors," J. Electron. Mater., Vol. 45, pp. 4654 (2016)

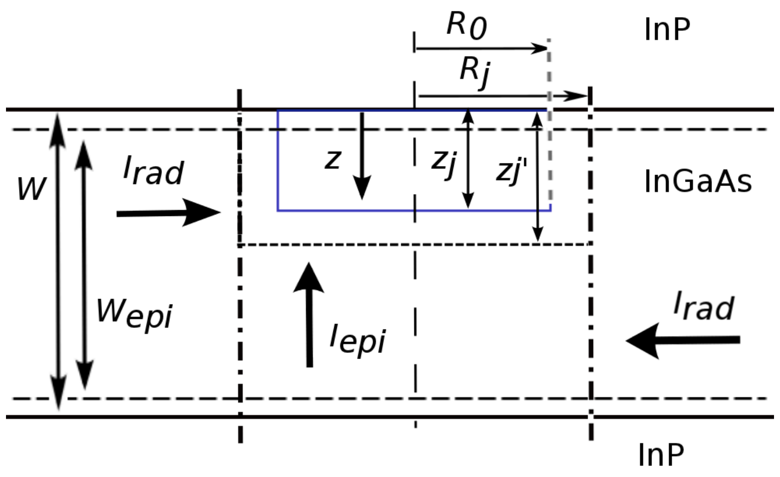
Semi-Classical Drift-Diffusion: 3×3 Mini-Array and Axial geometry – "Pixel Diode"

- ❑ Thin epitaxial diode
- ❑ Case:

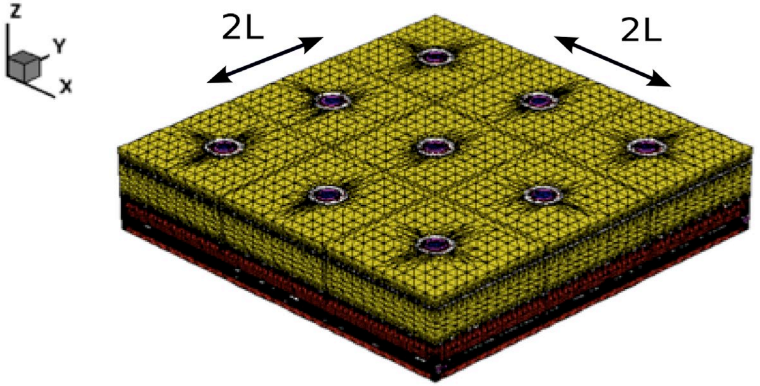
  R_0 < pitch (2L) << L_p

  W << L_p

- ❑ Neighboring diodes limit lateral diffusion



"pixel diode"



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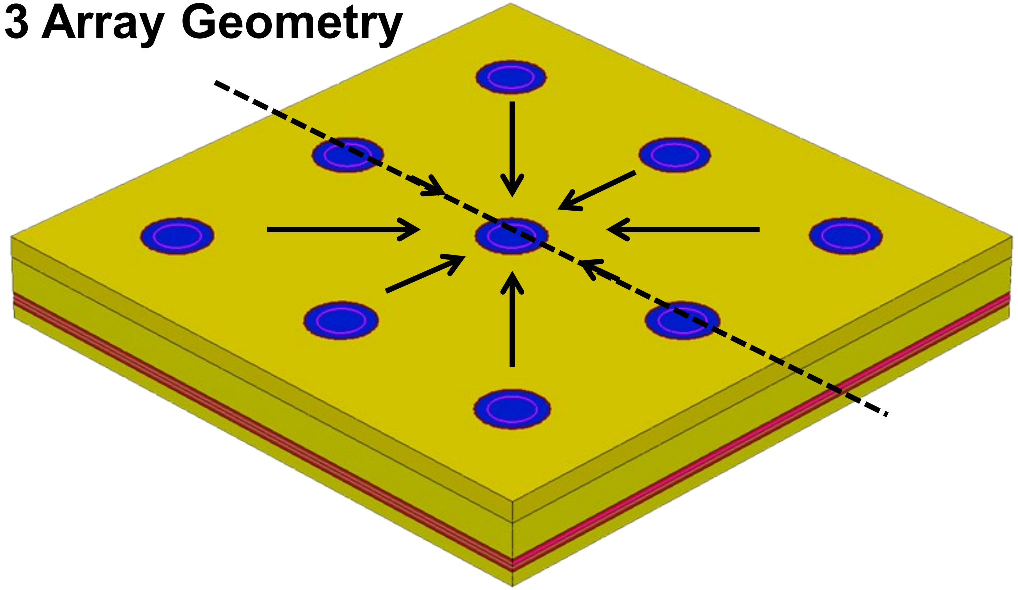
Semi-Classical Drift-Diffusion: HgCdTe Planar Hetero-junction Pixel Arrays

3 × 3 Array Geometry

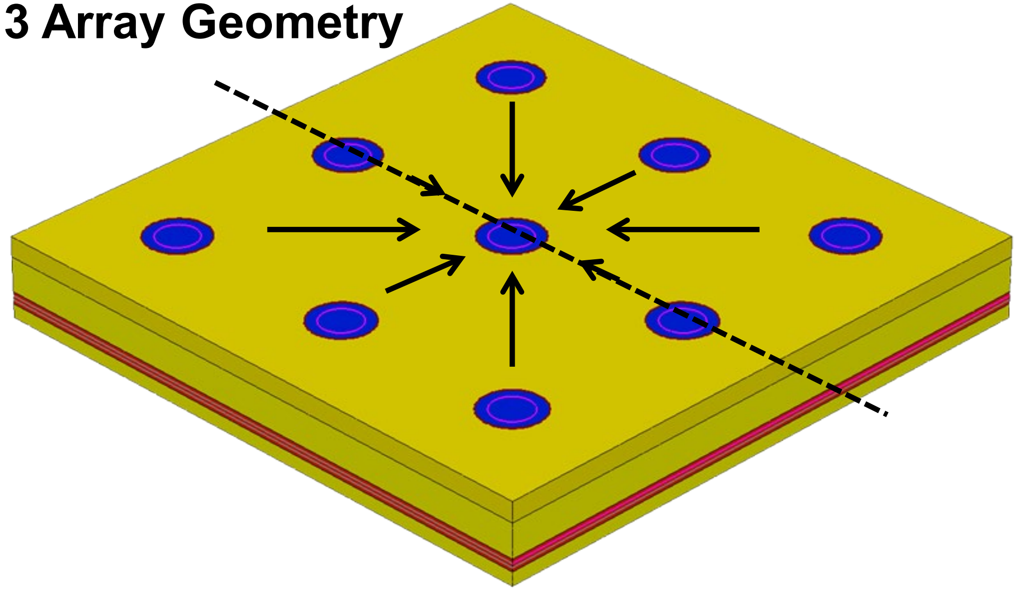


Three-Dimensional Model
- Impact of neighboring pixels (effects boundary conditions)
- Lateral Diffusion Current
- Interface Current
- Area G-R Current
- Surface G-R Current

Semi-Classical Drift-Diffusion: HgCdTe Planar Hetero-junction Pixel Arrays

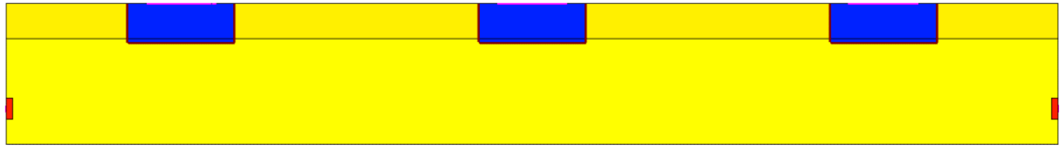
DEVCOM ARMY RESEARCH LABORATORY

3 × 3 Array Geometry

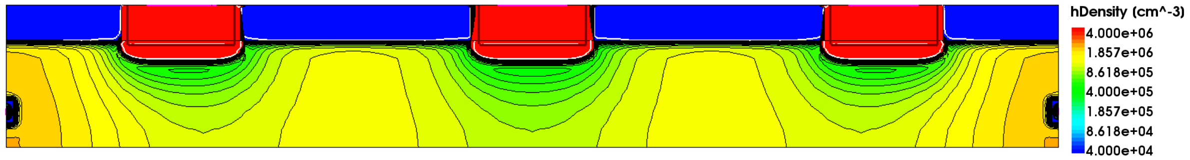


(Taken Along Dashed Line)

Doping

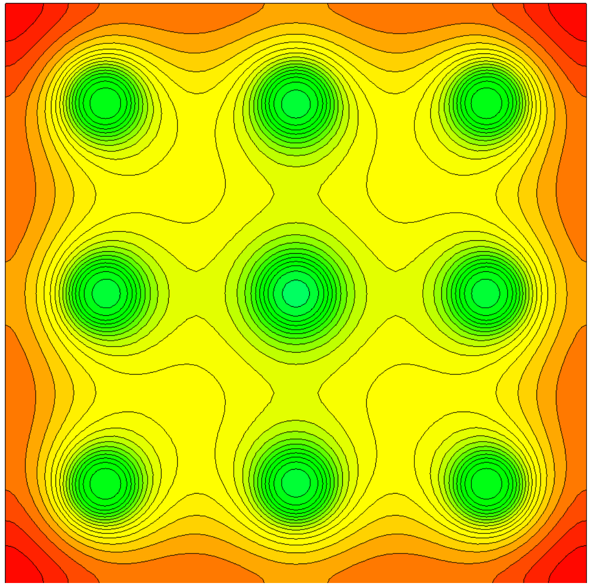


Hole Distribution



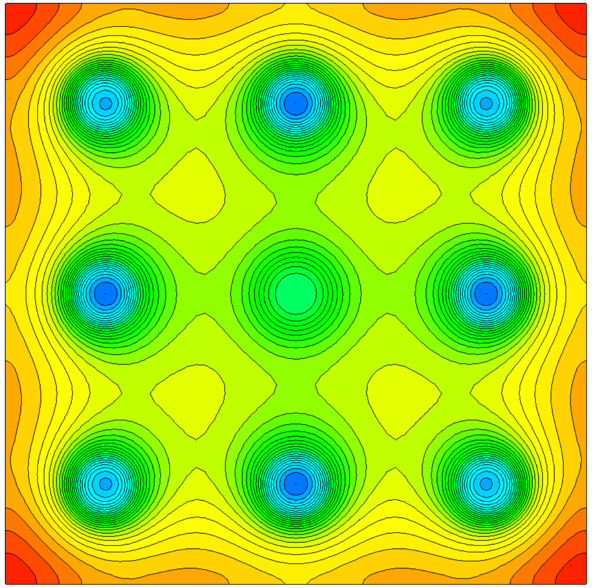
Hole Distribution
(absorber layer beneath junction)

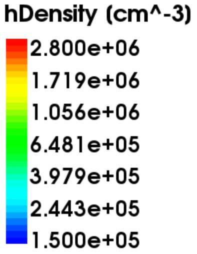
All Pixels:
- **V = -0.10 V**



Center Pixel:
- **V = -0.10 V**

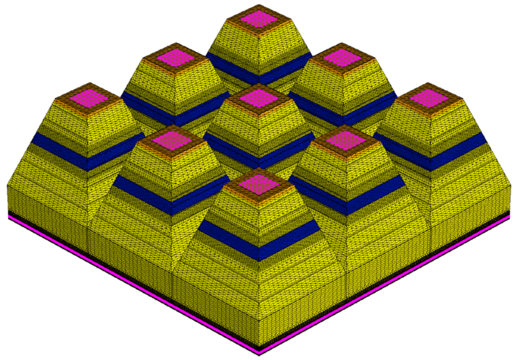
Other Pixels:
- **V = -0.15 V**

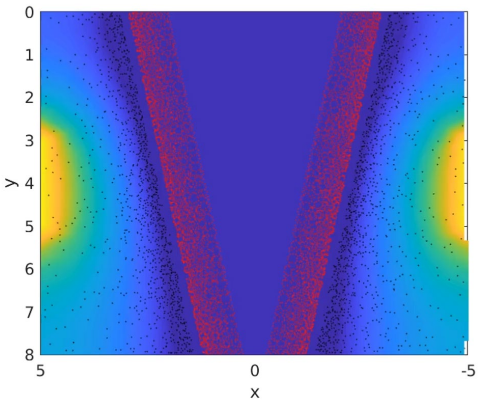


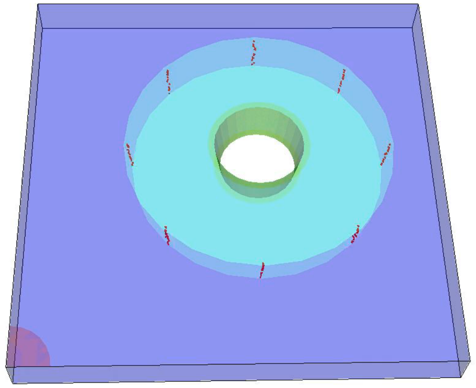


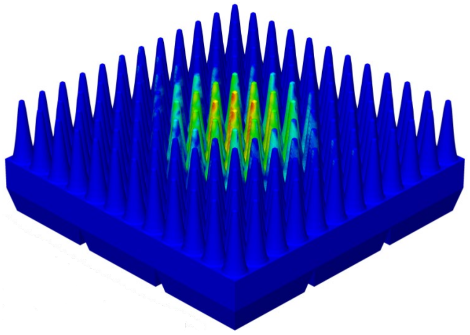
Outline

- ➢ Why Perform Modeling?
- ➢ Modeling Overview and Capabilities
  - What Numerical Modeling Buys You!
- ➢ Modeling Device Metrics – Single Devices & Arrays
  - Alloy Semiconductors (*e.g.*, HgCdTe, InGaAs, Alloy nBn, *etc.*)
  - Type II Superlattices (T2SL)
    - Nonequilibrium Green's Function (NEGF)
    - Quantum Corrected Drift Diffusion (QCDD)
  - Avalanche Photodiodes (APDs)
    - Full Band Monte Carlo (FBMC)
- ➢ Modeling Imaging Metrics – Modulation Transfer Function (MTF)
- ➢ Summary & Takeaways









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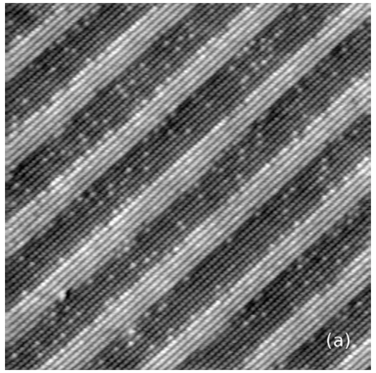
Motivation for III-V InAs/InAsSb Type II Superlattices (T2SL)

- Theoretically, “defect free” III-V T2SL possess several potential advantages over HgCdTe alloy*,†
  - Reduced dark current → Higher SNR (actually material tends to be SRH limited)
  - Reduced cost
  - Greater uniformity
  - Reduced cluster defects

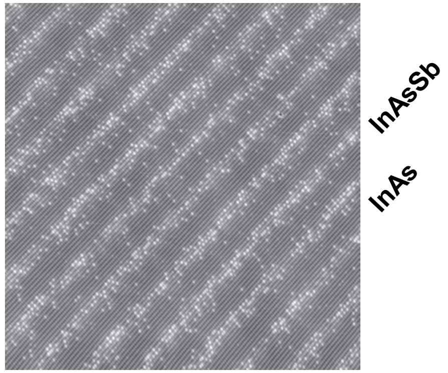
  (Reduced cost, Greater uniformity, Reduced cluster defects:) **From leveraging III-V industrial base**
- Significant progress made to date during VISTA program ($100 million over 5 years)
  - T2SL’s camera demonstrations
  - MWIR products (tactical)
- Challenges persist limiting strategic MWIR & LWIR
  - Ga-free III-V T2SLs exhibits low absorption coefficient
  - Fundamental understanding of key material characteristics still lacking
  - n-type $InAs/InAs_{1-x}Sb_x$ T2SL vertical hole mobility very low
    - Localized hole states and hopping transport
  - Anisotropic effective masses & mobilities ($\mu_{||} \gg \mu_{\perp}$)

$InAs/Ga_{0.91}In_{0.09}Sb$

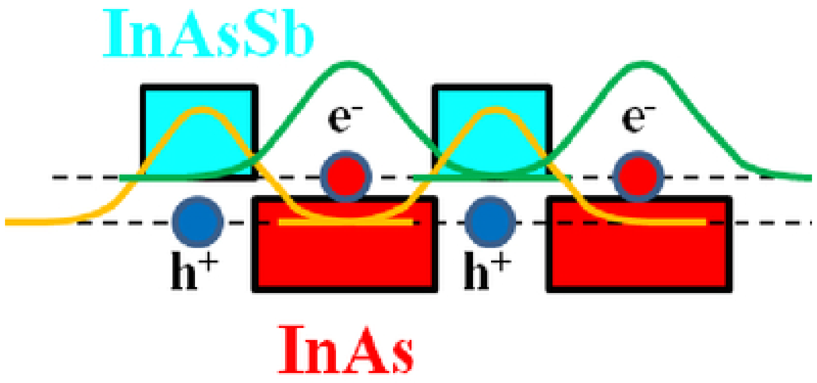


M. K. Yakes *et al*., Appl. Phys. Lett. 101, 241908 (2012)

$InAs/InAs_{0.67}Sb_{0.33}$



M.R. Wood *et al*., J. Cryst. Growth 425, pp. 110–114 (2015)



M. Razeghi *et al*., Proc. SPIE 9819, 981909 (2016)

*M. Z. Tidrow, Infr. Phys. Tech., vol. 52, no. 6, pp. 322–325 (2009)
†P.-Y. Delaunay et al.,Proc. SPIE, vol. 10177, 101770T (2017)

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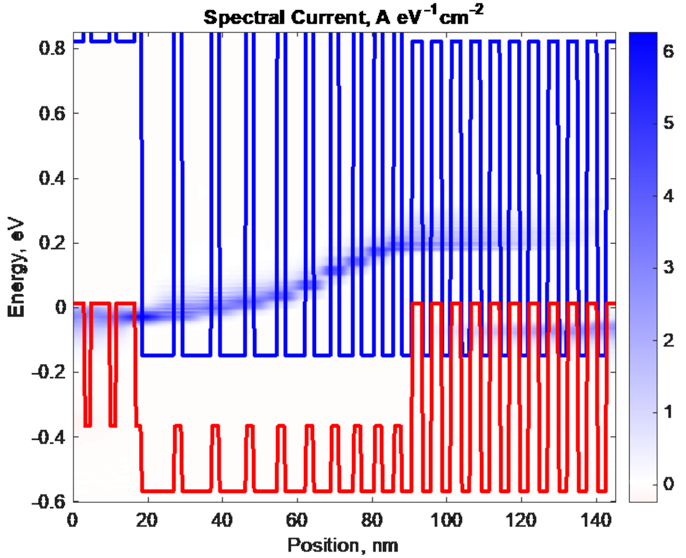
T2SL Modeling Approaches

Non-Quantum Mechanical Methods – Uses Approximated Structure to Solve for Device Performance)

- Semi-Classical Drift-Diffusion Simulator
  - Material Parameters
    - $k \cdot P$ solver yields band structure / material parameters
    - Measurements of identical superlattice material (vertical minority carrier mobility very difficult to measure)
  - Device Simulations
    - Approximate T2SL layers as “bulk”-like layers with “global” material properties
    - Perform drift-diffusion simulations on “approximated” device
    - Accounts for effects related to mesa, neighboring pixel interactions, crosstalk, etc.)
    - Omits underlying superlattice structure
    - Completely omits quantum mechanical transport mechanism (hopping, sequential tunneling) that dictate TSL device performance
  - Examples: NRL MULTIBANDS (Trademark Serial Number: 85883321)

Quantum Mechanical Methods – Uses Exact Structure & Makes No Prior Assumptions to Transport Mechanisms

- Method: Non-equilibrium Green’s function formalism
- Uses actual superlattice structure
- Extremely computationally expensive



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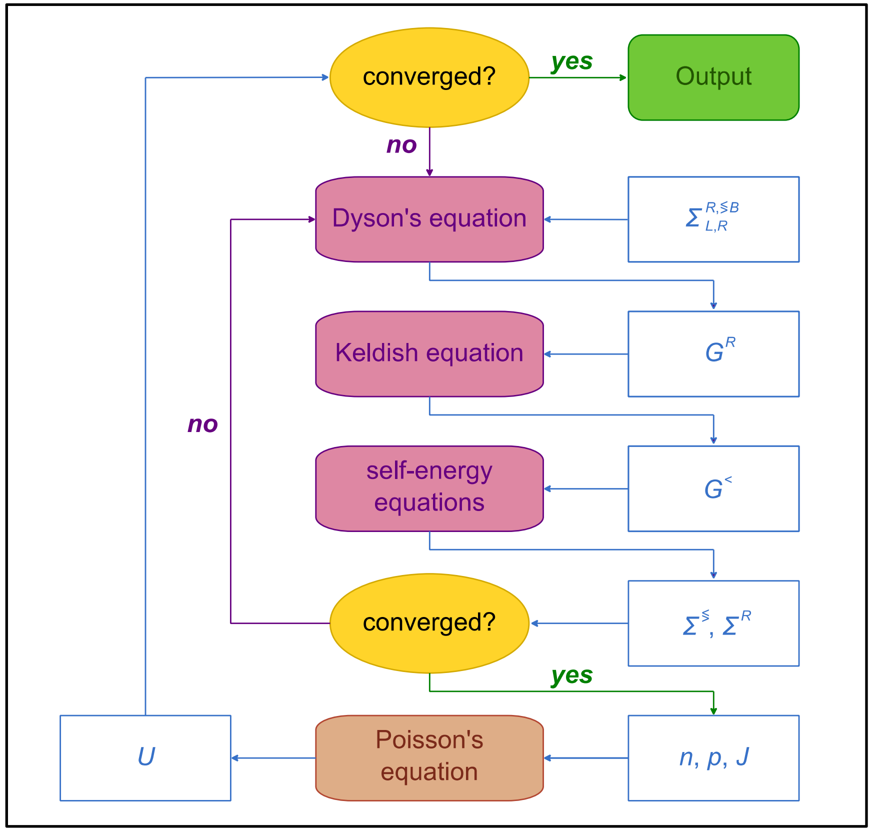
NEGF Transport Model for T2SL

A quantum mechanical transport simulation tool including full carrier-photon and -phonon interactions

Non-equilibrium Green's Function Model

- Quantum mechanical transport model
- $k \cdot P$ Hamiltonian for band structure
- No prior assumptions to transport mechanisms (e.g., drift or diffusion)
- Natively includes non-ideal transport mechanisms
  - Hopping, sequential tunneling, etc.
- Model is extraordinary computational expensive
  - Limited to relatively small structures
  - Limited to 1D
  - Results must be incorporated into lower fidelity models for 3D simulations



F. Bertazzi, et. Al, Phys. Rev. Appl. 14, 014083 (2020)
A. Tibaldi, et al, Phys. Rev. Appl. 14, 024037 (2020)
A. Tibaldi et al., Phys. Rev. Appl. 16, 044024 (2021)

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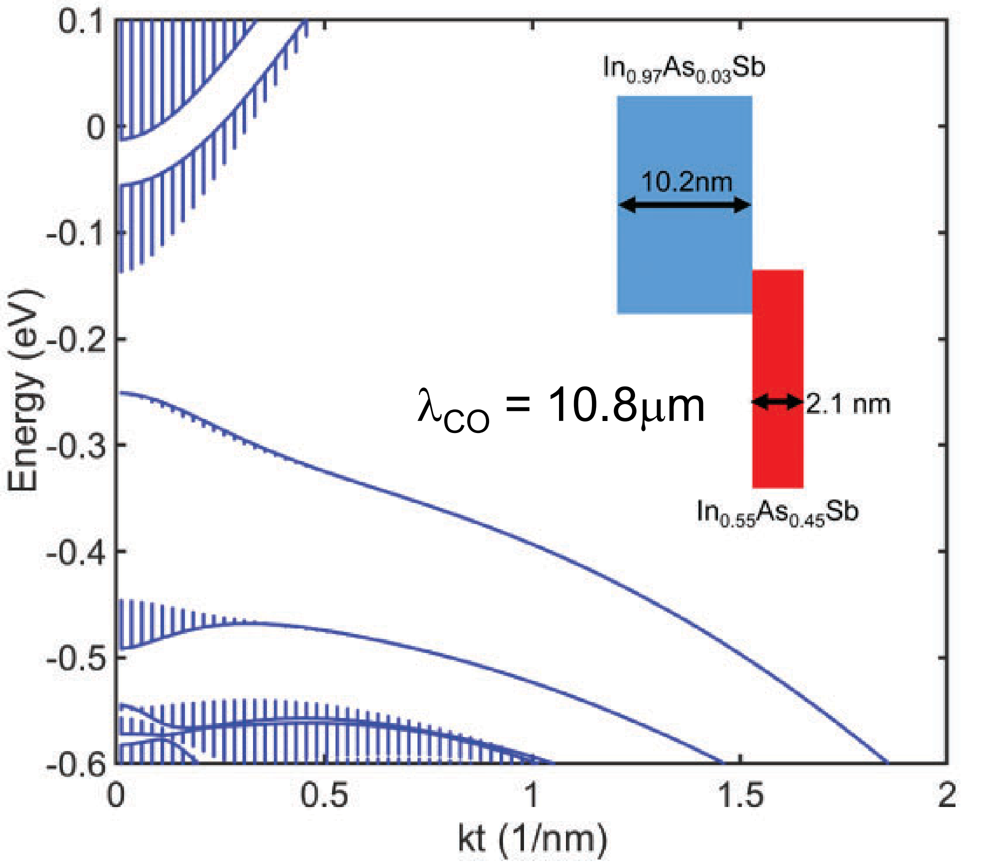
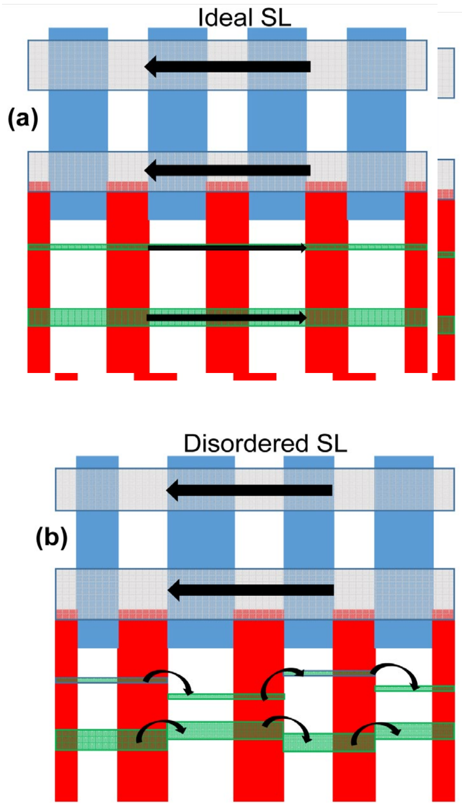
Model Development was Performed under ARL MSME CRA Funding at Politecnico di Torino

Superlattice Electronic Structure



Energy bands as a function of the in-plane (solid lines) and perpendicular (vertical lines) wavevector

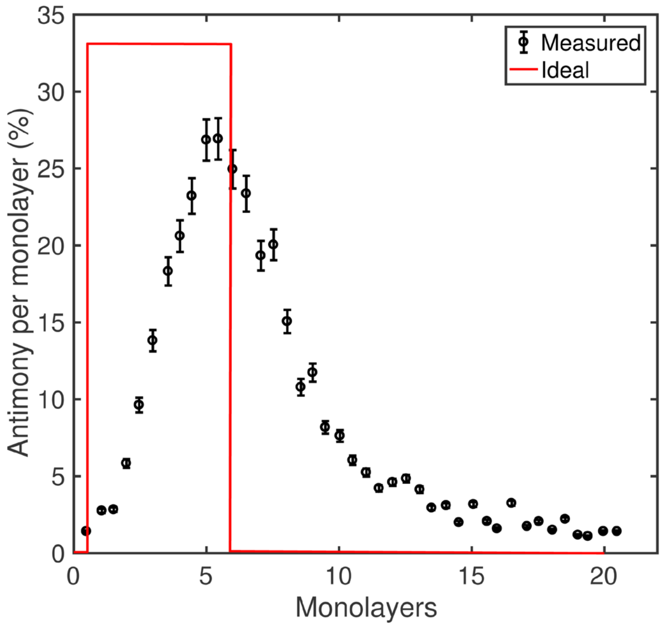


The electronic structure of the ideal superlattice is characterized by extended states (minibands)

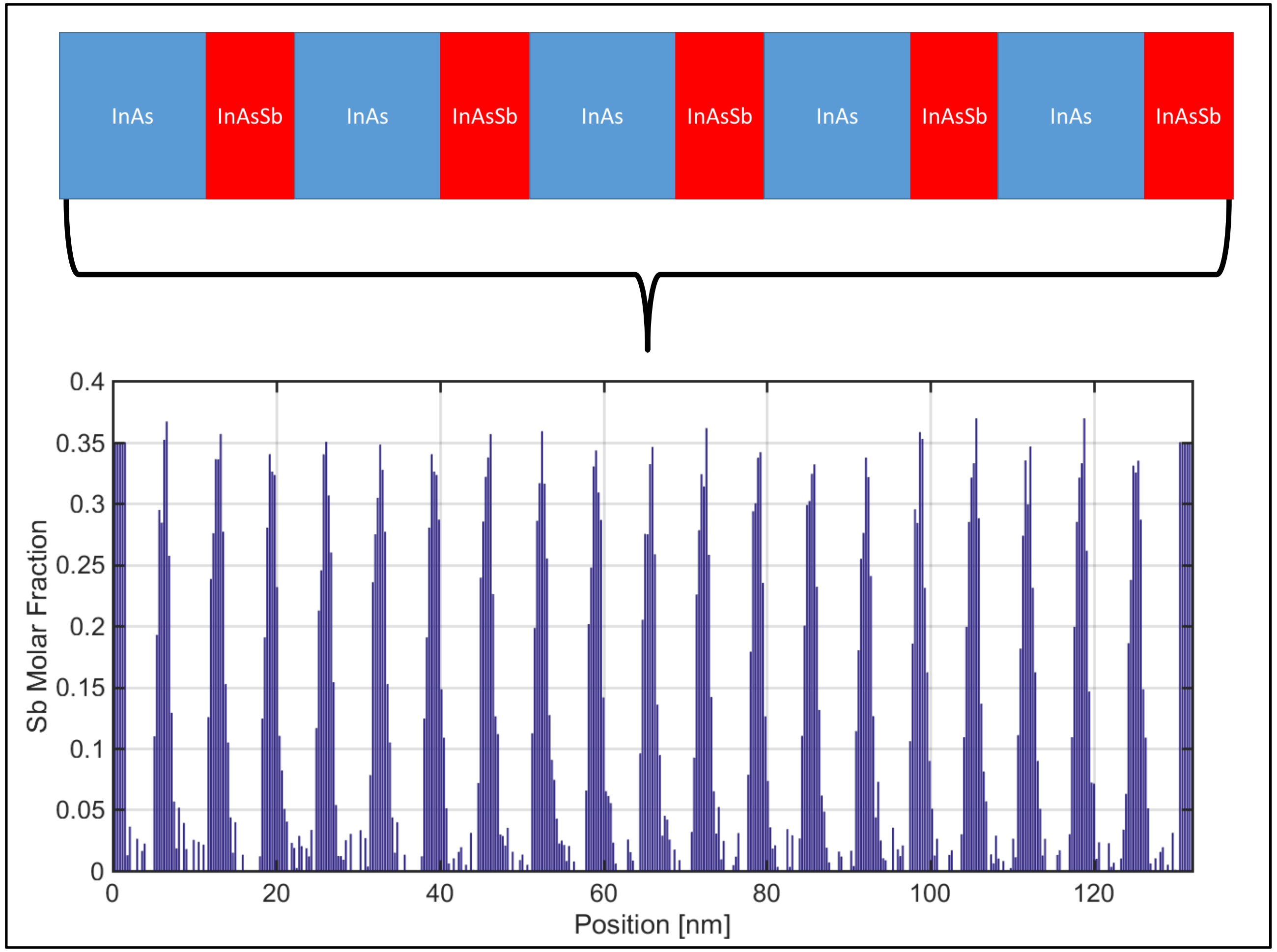
In a non-ideal SL, narrow minibands are disrupted and transport may occur by hopping between different weakly-coupled states

E. Bellotti *et al.*, "Disorder-Induced Degradation of Vertical Carrier Transport in Strain-Balanced Antimony-Based Superlattices," Phys. Rev. Applied 16, 054028 (2021)

InAsSb/InAs Superlattice Model: Compositional Disorder



M.R. Wood PhD Thesis. UTA



- Of all the N randomly generated unit cells, we pick M<N to create a T2SL to simulate
- Several T2SL are generated in the same way

- Final simulated T2SL, based on 21 barrier/well pairs

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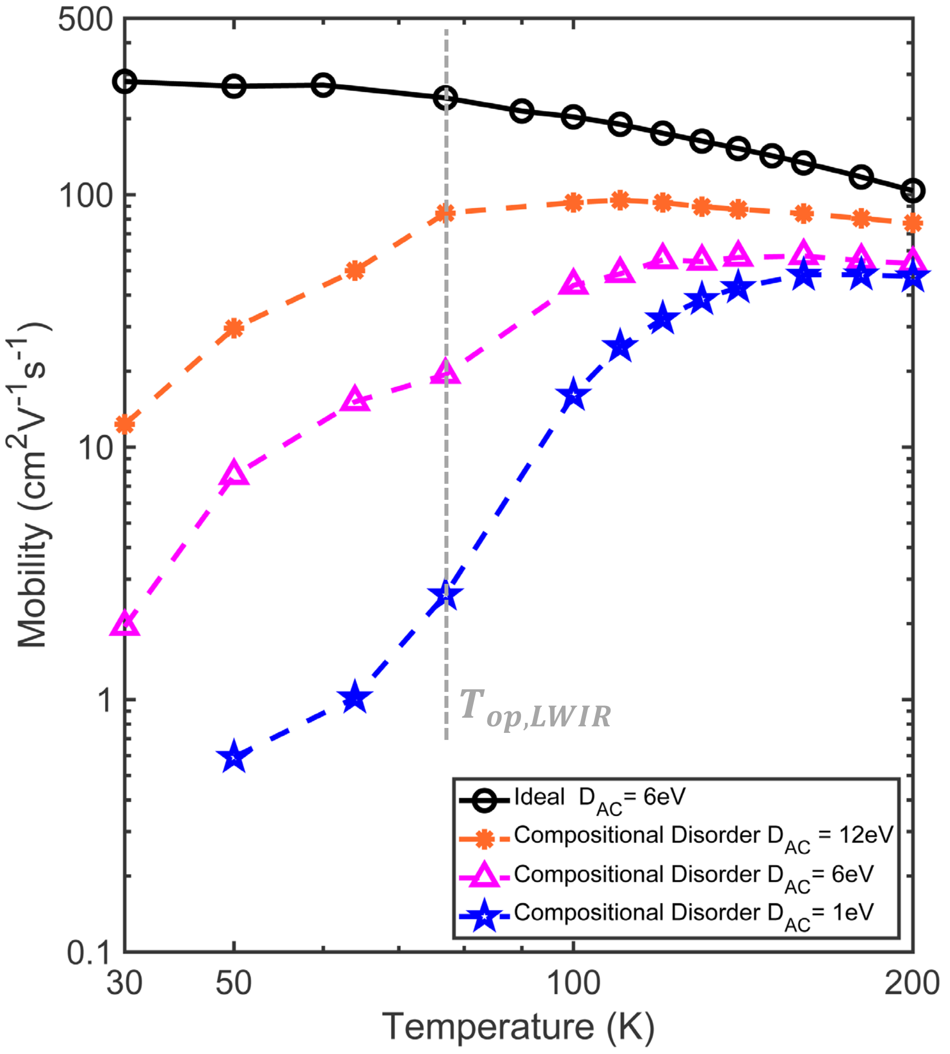
E. Bellotti *et al.*, "Disorder-Induced Degradation of Vertical Carrier Transport in Strain-Balanced Antimony-Based Superlattices," Phys. Rev. Applied 16, 054028 (2021)

Effect of Compositional Disorder: Holes Mobility



- T2SL generated using 21 randomly selected unit cells
- Different strength of the acoustic scattering: changes broadening
- Ideal: mobility decreases with temperature – coherent transport or phonon limited
- Disordered: mobility increases with temperature > localization and hopping
- Disorder reduces the absolute mobility
- Disorder changes the temperature dependence

Vertical hole mobility < 50 $cm^2V^{-1}s^{-1}$

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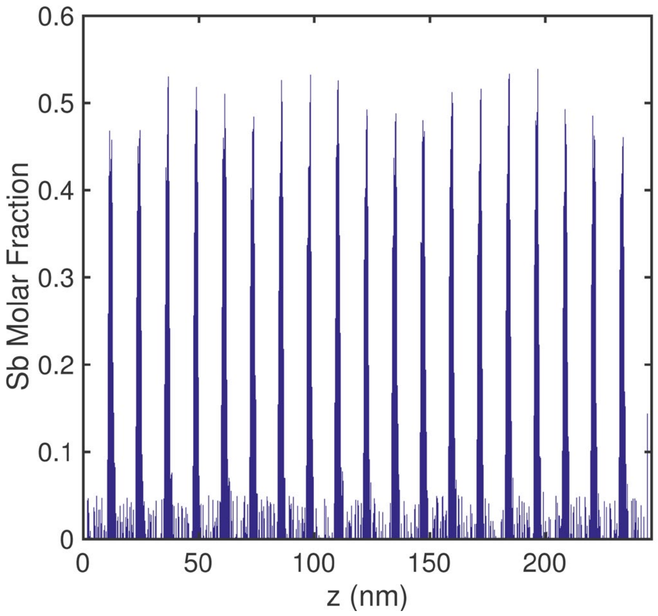
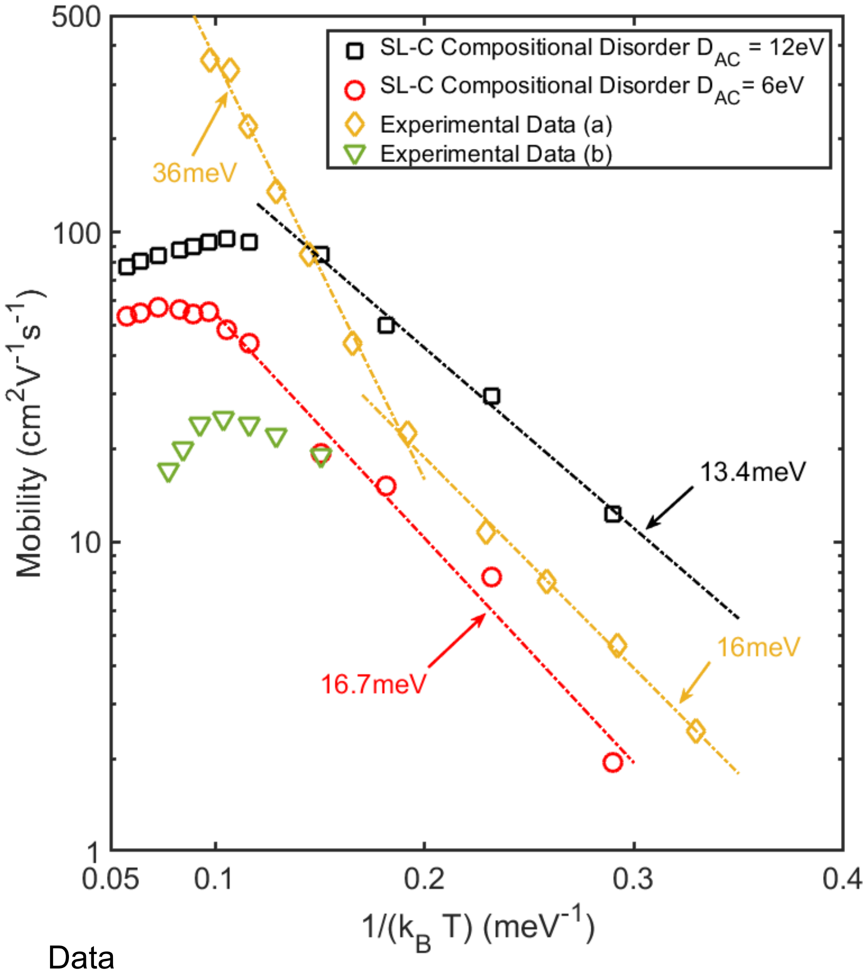
E. Bellotti *et al.*, "Disorder-Induced Degradation of Vertical Carrier Transport in Strain-Balanced Antimony-Based Superlattices," Phys. Rev. Applied 16, 054028 (2021)

Comparison with Experiments

Hole Mobility In LWIR T2SL Is Low and Indicative of Hopping

- We have simulated a realistic T2SL with compositional disorder
- Both theory and experiment show similar temperature dependence (**mobility decreases with temperature**)





- Clear indication of hopping and localization below 100 K
- "The unknown characteristics of the device may explain the difference between experiment and theory
- **Modeling results explain the physics and limitations of carrier transport in real T2SLs at low temperatures!**

Data
a) B. V. Olson, et al. Phys. Rev. Appl. 7, 024016 (2017)
b) D. Donetski, Personal Communication (2020)

E. Bellotti *et al.*, "Disorder-Induced Degradation of Vertical Carrier Transport in Strain-Balanced Antimony-Based Superlattices," Phys. Rev. Applied 16, 054028 (2021)

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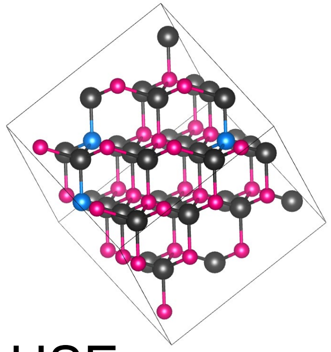
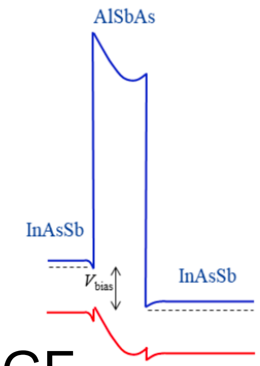
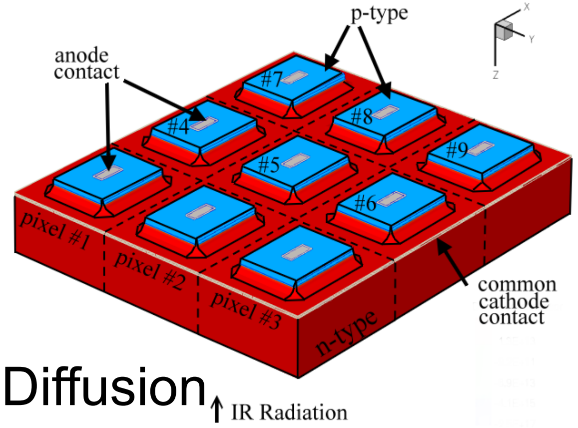
T2SL nBn – A Path to Full Device Simulation



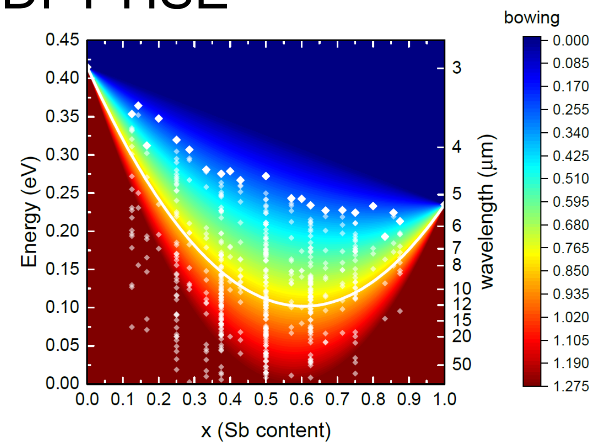
DFT-HSE

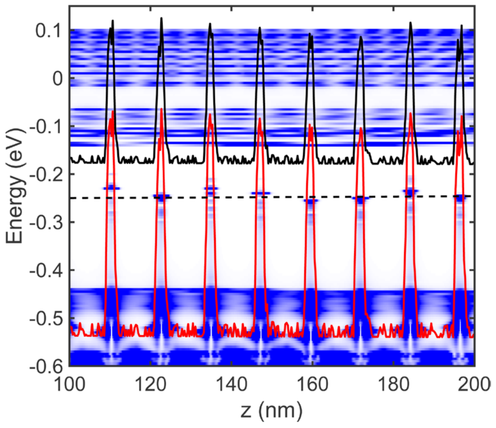


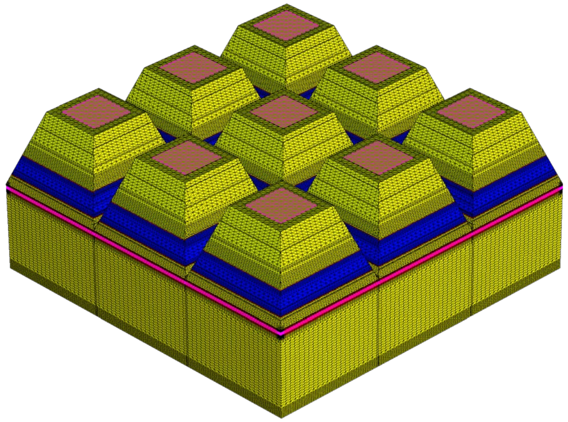
NEGF



Drift-Diffusion







Fundamental Physics

Device Design (2D,3D)

Fidelity of a Quantum Mechanical Description at the Cost of a Drift-Diffusion (DD) Model

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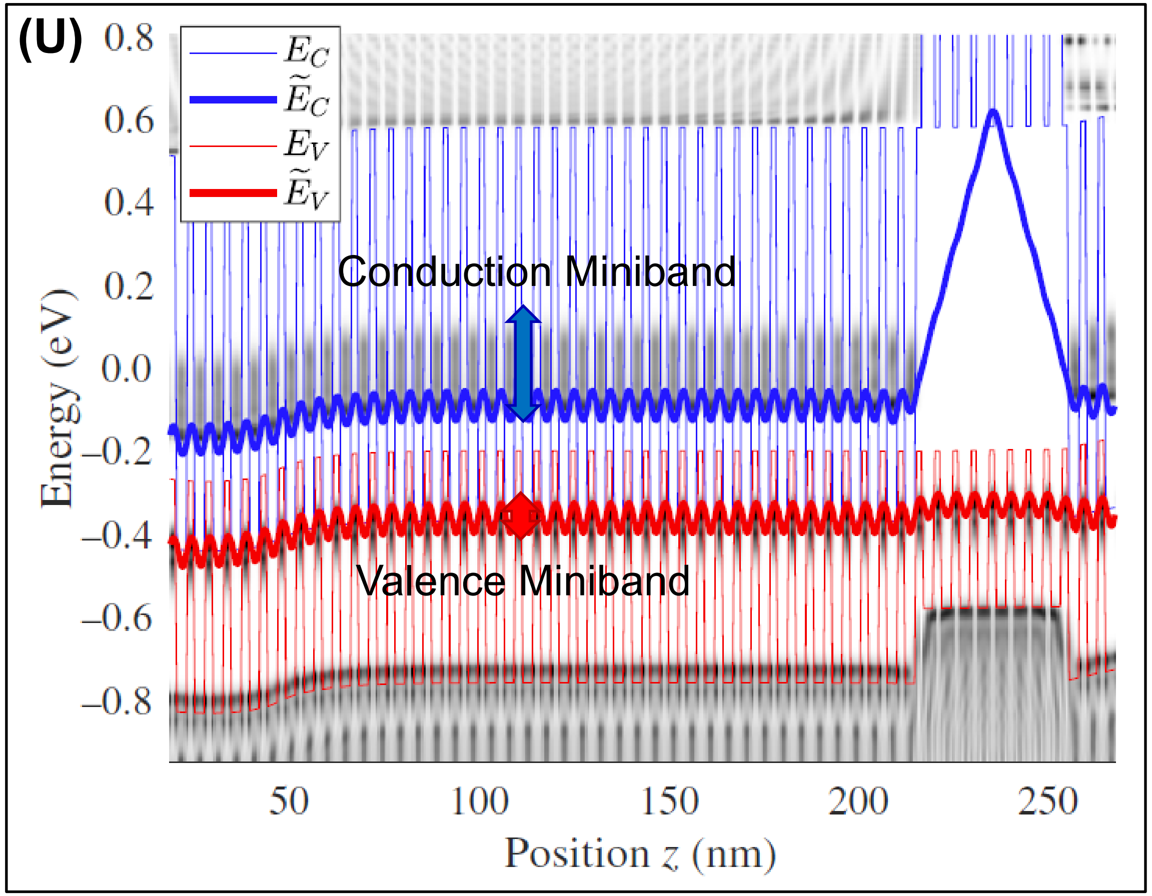
T2SL Device Simulations: InAs/GaSb MWIR T2SL

NEGF → Quantum-Corrected Schrödinger Poisson Drift-Diffusion (SPDD)



Device Specifications

- 200 nm InAs/GaSb absorber (1.8/2.4 nm)
- 50 nm GaSb/AlSb Barrier, (1.8/2.4 nm) un-doped
- 4.8 µm cutoff
- 10 ns lifetime (SRH only)

Figure

- Grey areas are NEGF LDOS
- Thin lines (blue and red) Ec and Ev computed using NEGF
- Thick lines (blue and red) Ec and Ev effective conduction bands From SPDD

NEGF Computation Requirements Make it Intractable for Large Devices → SPDD Provides Computational Compromise Enabling Larger Devices

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A. Tibaldi *et al.*, "Modeling Infrared Superlattice Photodetectors: From Nonequilibrium Green's Functions to Quantum-Corrected Drift Diffusion," Phys. Rev. Applied 16, 044024 (2021)

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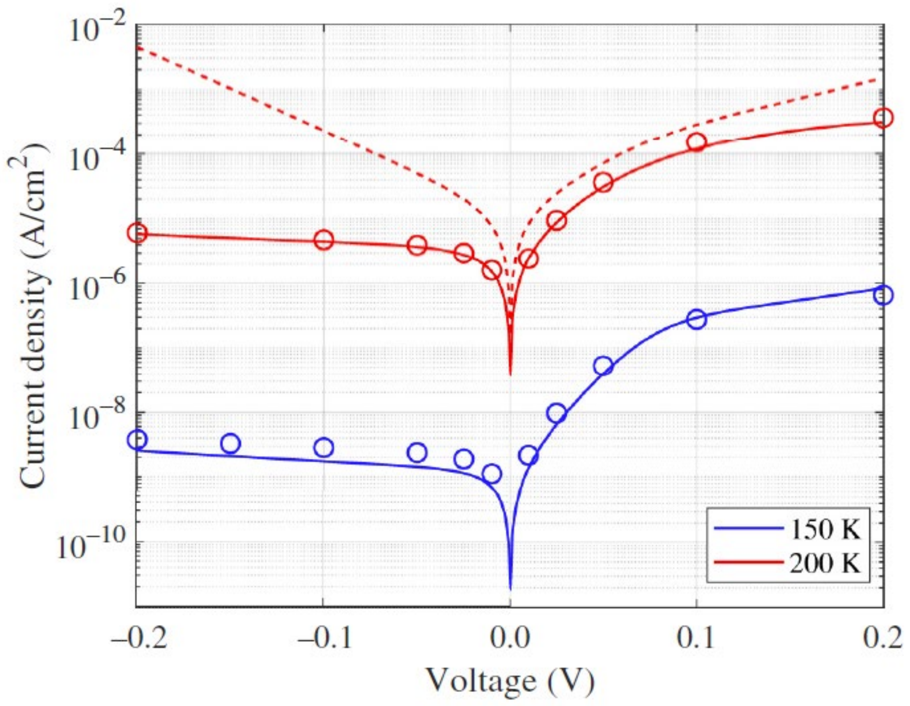

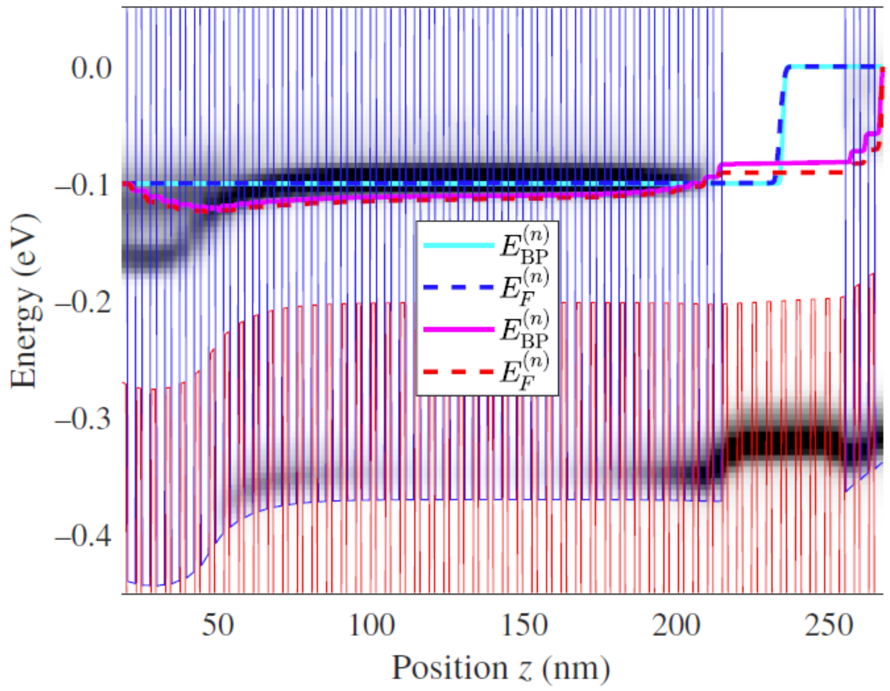

- ➢ Open circles NEGF
- ➢ Solid Lines SPDD lines
- ➢ Extracted apparent carrier mobility:
  - $\mu_n = 1000\ \mathrm{cm^2V^{-1}s^{-1}}$
  - $\mu_p = 1\ \mathrm{cm^2V^{-1}s^{-1}}$

- ➢ Spectrally & spatially resolved current densities
- ➢ Solid lines Fermi energies from NEGF
- ➢ Dashed lines - Fermi energies from SPDD

For thicker barrier layers SPDD agrees well with NEGF → Enabling Simulations of Larger Devices

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A. Tibaldi *et al.*, "Modeling Infrared Superlattice Photodetectors: From Nonequilibrium Green's Functions to Quantum-Corrected Drift Diffusion," Phys. Rev. Applied 16, 044024 (2021)

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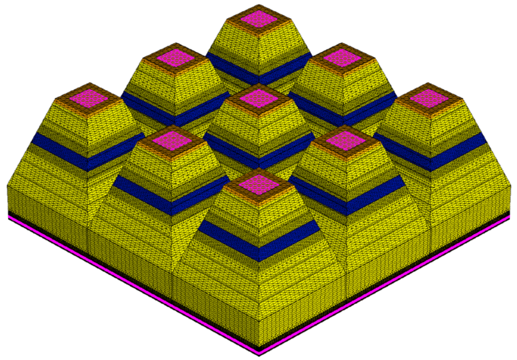

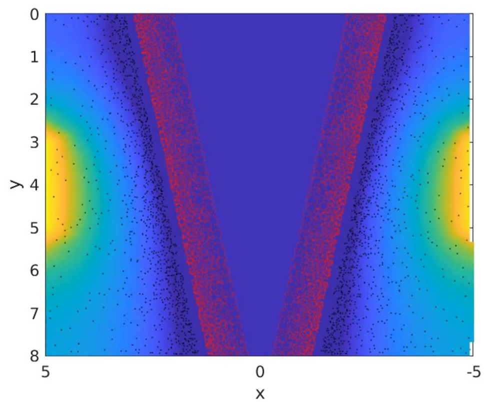

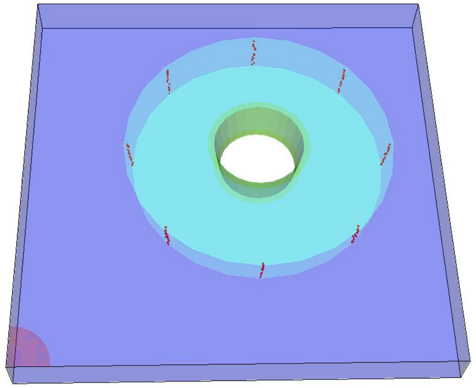

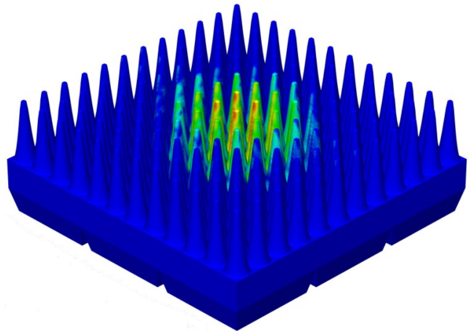

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Numerical Methods for Simulations of APDs

Drift Diffusion Solvers

- ➢ BTE distilled to set of purely classical equations (continuity equations)
- ➢ Solve for self-consistent, steady-state solution to electrostatics
  - Potential, current/carrier densities, electric field, *etc.*
- ✓ Computationally inexpensive
- ✓ Shown to be extremely successful for wide range of devices
- × Assumptions on reciprocal space distribution
- × Poor predictor of non-equilibrium transport, transient effects
- × Validity: $\tau_{transit} \gg \tau_{relaxation}$

BTE = Boltzmann Transport Equation

Monte Carlo (MC) Models

- ➢ Simulate the microscopic processes described in the BTE (free flight, scattering) to realize distribution function
  - Collisions **computed quantum mechanically**, chosen probabilistically
  - Particles bound to crystal's quantum mechanical energy dispersion
- ➢ Not a direct solution of BTE
  - Statistical representation of distribution function
- ➢ **No assumptions on distribution**: "exactness" of solution depends only implemented physics
- ✓ Predictive of non-equilibrium transport (impact ionization, carrier heating, ballistic transport, *etc.*)
- ✓ Captures time-dependent phenomena
- × Computationally expensive
- × Implementation difficulties
- × Obstacles for efficient discretization schemes

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Complexity & Computational Burden of Monte Carlo Models has Hindered 3D Simulations of Large Devices

FBMC3D – A 3D Full Band Monte Carlo Simulator

Developed a 3D full-band Monte Carlo (FBMC3D) simulator for simulations of high electric field carrier transport dynamics

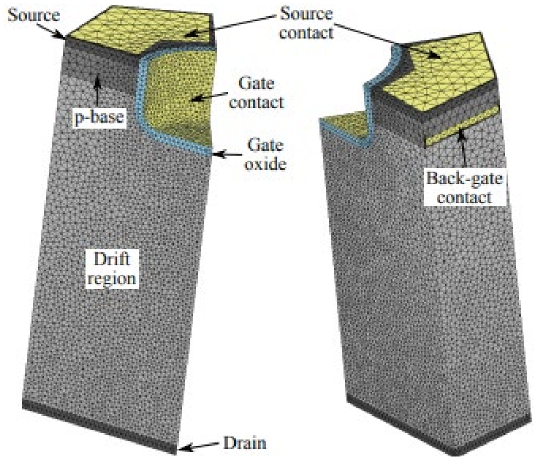
- Ideal for APDs, SPADs, RF/power devices

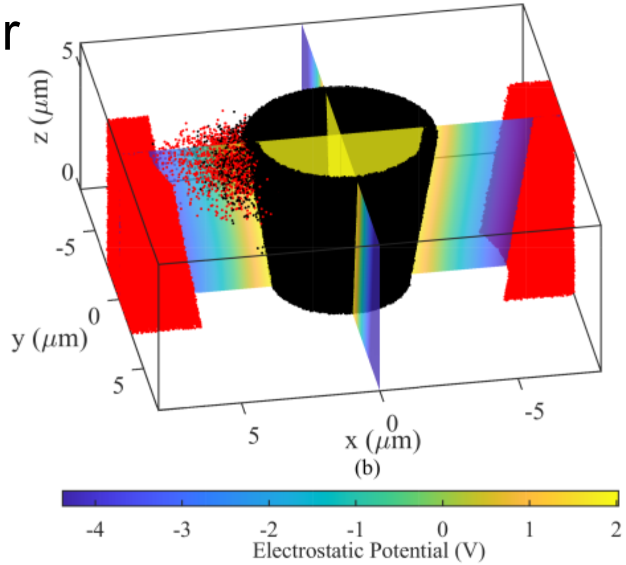
Written in C, parallelized where possible with OpenMP

- Designed to be material and application agnostic for general purpose use

Important features and capabilities

- Ability to simultaneously simulate analytic and numerical band structures in different regions of device
- Numerical band scattering rate calculator with enhanced coverage near band edges (unstructured mesh)
- Flexible, 1D+**3D** device simulation with **tetrahedral** grid
  - Self-forces correction
  - FEM Poisson solver
  - Arbitrary doping, compositional profiles





FBMC3D Simulator Developed as Open Platform for DoD Applications – Available to DoD Agencies & CSM Members

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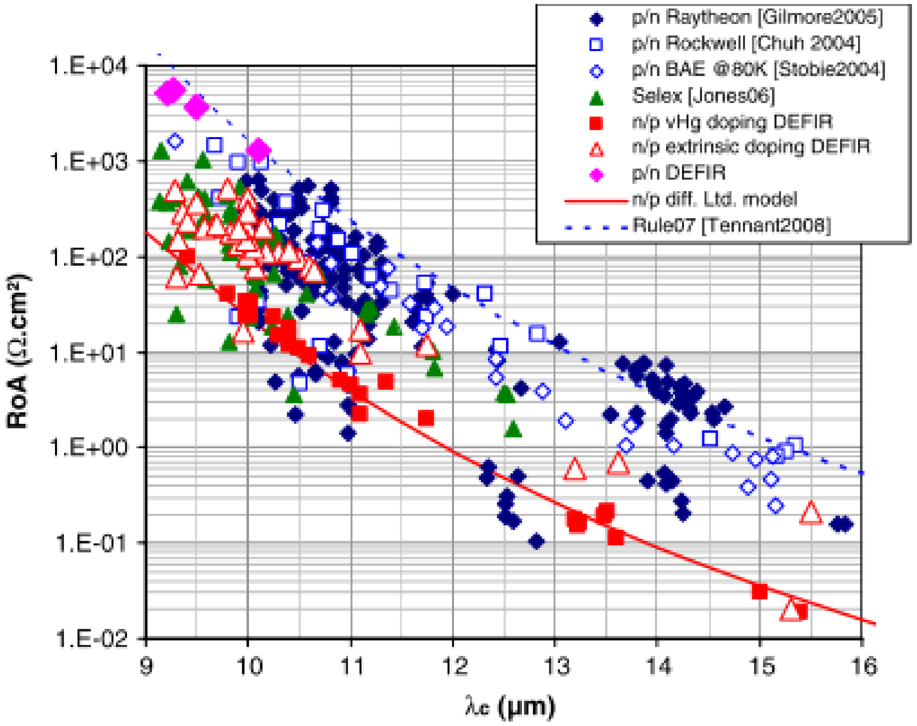
I. Prigozhin *et al.*, *IEEE TED*, Vol. 68(1), pp. 279-287 (2021)
I. Prigozhin, Doctoral Dissertation, Boston University (2022)

HgCdTe APD Trade-Offs

Relevant Metrics

- ➢ Quantum Efficiency
  - Better APD performance if absorption restricted to absorber
  - Potential barrier restricts molar grading impact
- ➢ Dark current
  - electron APD (eAPD) necessitates p-type absorber: n-on-p design rather than traditional low dark current p-on-n
- ➢ Multiplication Gain
  - Limited by design, band-to-band tunneling onset
  - Photocarriers generated in multiplication region experience lower gain
- ➢ Excess noise
  - Single carrier multiplication results in low excess noise, but absorption in multiplication region raises

O. Gravrand *et al.*, *J. Electron. Mater.*, 38, pp. 1733–1740 (2009)



Molar grading profile must balance pros/cons

- Reduce diffusion dark current
- Reduce SRH generation
- Delayed B2BT onset
- Avoid excess noise from absorption in multiplication region

- Can introduce barrier which lowers QE
- Lower gain

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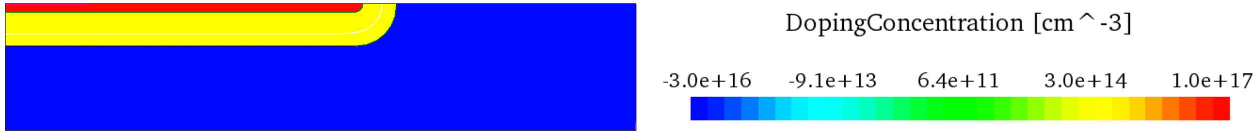
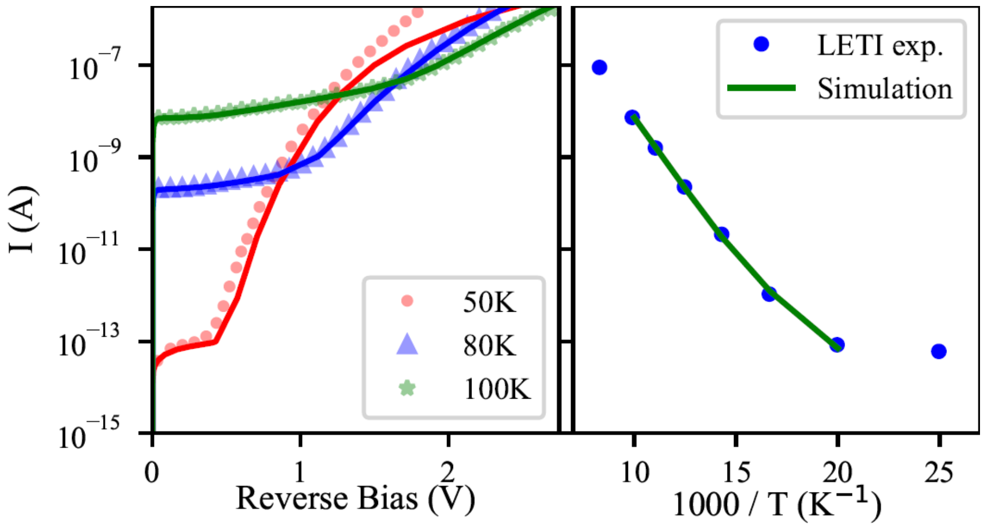
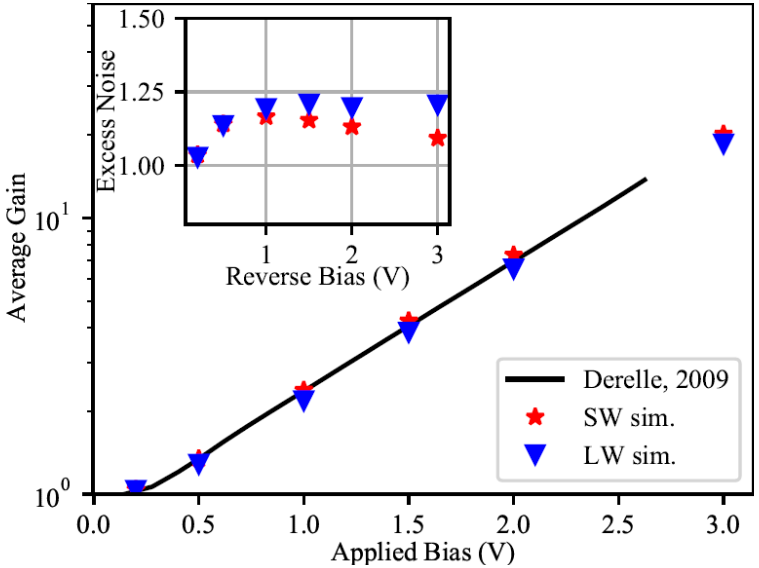
I. Prigozhin *et al.*, *IEEE TED*, 69(7), pp. 3791-3797 (2022)

HgCdTe APDs for LWIR Imaging – Model calibration

- LETI $x = 0.235$ (λ_c @ $80K \approx 9\ \mu m$) device used for model calibration and verification
  - MBE grown material
  - Planar device, high fields due to short n^- region
    ($N_D^- = 5 \times 10^{14}\ \text{cm}^{-3}$, $t_{n^-} = 0.8\ \mu m$)
  - $\tau_{SRH}^e = 1.9 \times 10^{-9}$ s: likely lower than extrinsically doped material
- Dark current modeled in 2D with cylindrical symmetry (drift-diffusion)
  - Lateral pixel, junction dimensions tuned to match low bias, high temp diffusion dominated dark current
  - Dark current behavior tuned with avalanche, B2BT models
- Multiplication properties modeled in 1D (Monte Carlo)







O. Gravrand *et al.*, *J. Electron. Mater.*, 38, pp. 1733–1740 (2009)

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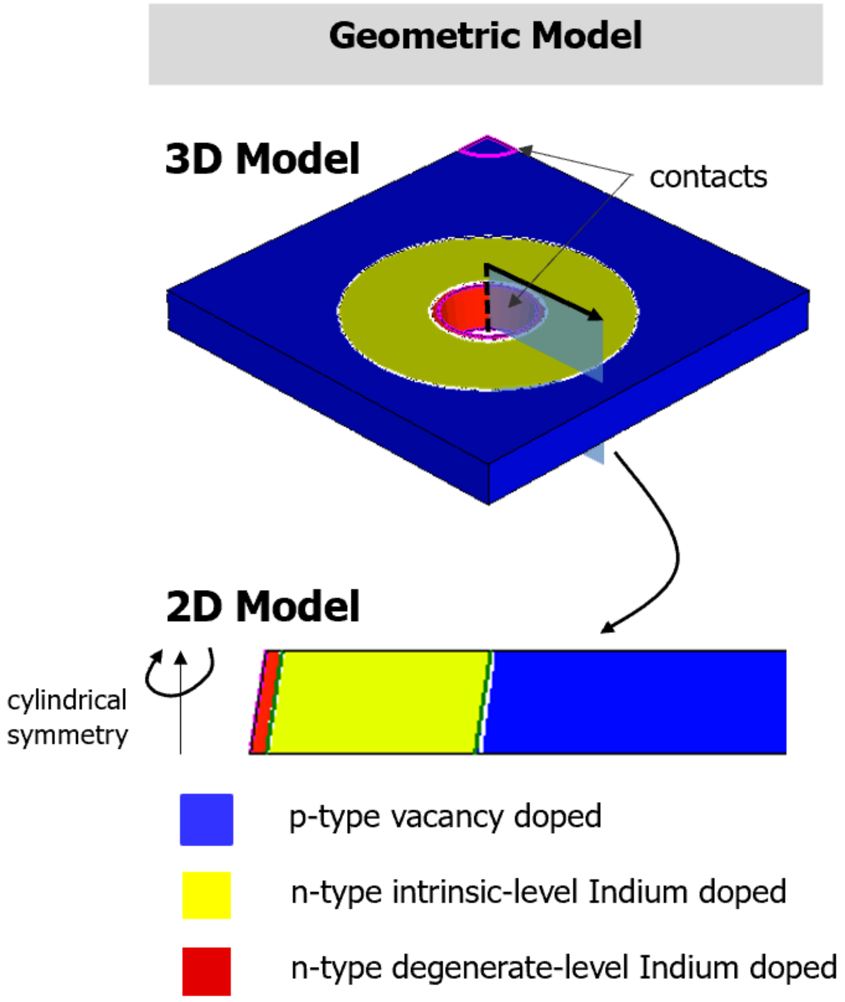
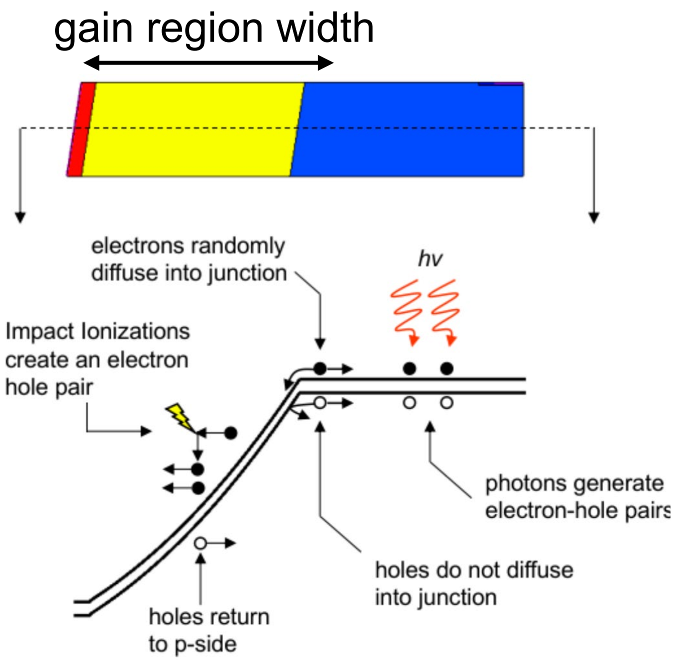
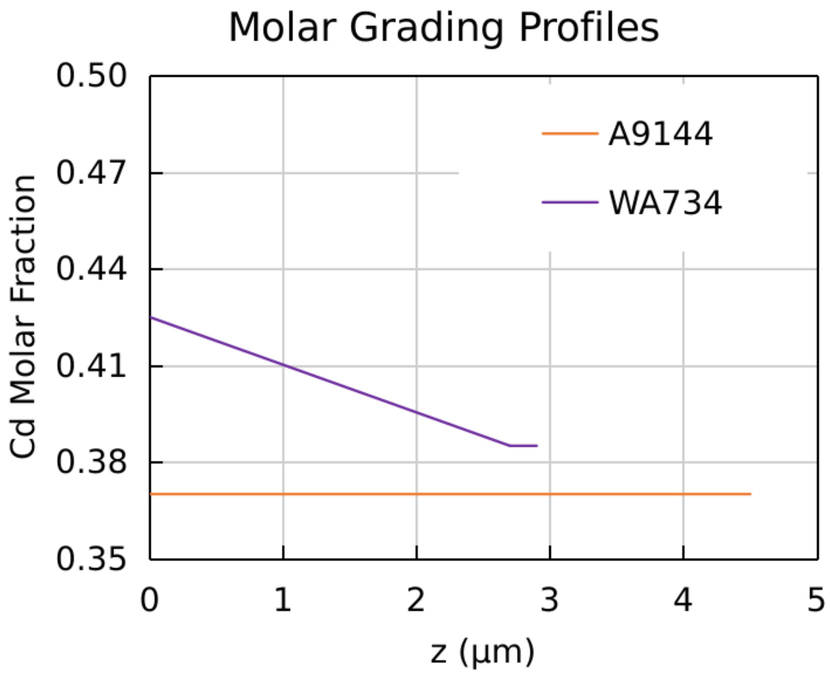
I. Prigozhin *et al.*, *IEEE TED*, 69(7), pp. 3791-3797 (2022)

Example: High-Density Vertically Integrated Photodiode (HDVIP)

Geometric Model and Device Operation







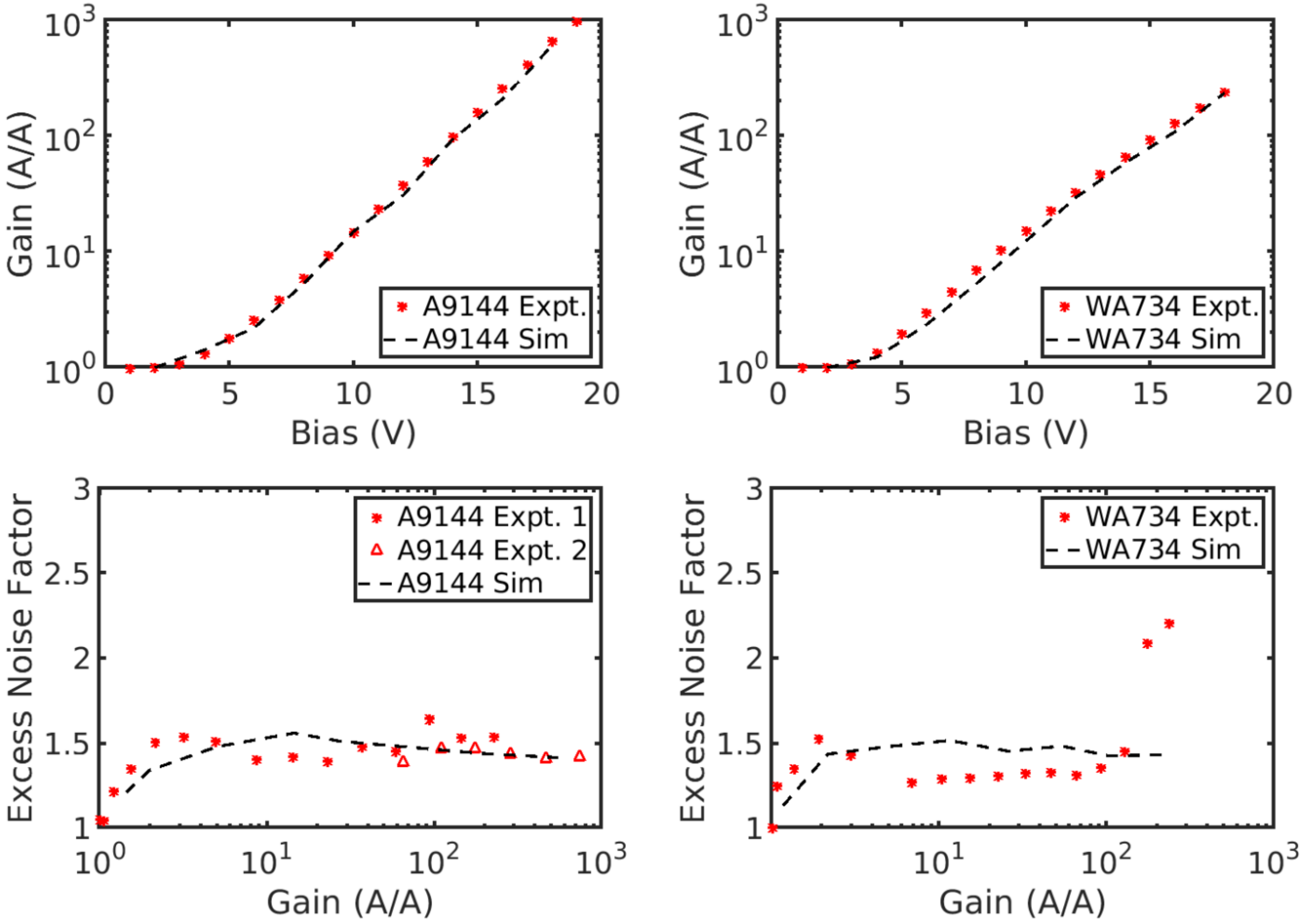
	Low	High
gain region width	5.5 μm	6.5 μm
Cd composition	37%	42.5%

- Experimental devices provided by Leonardo DRS
- Two best behaved HDVIP APDs are chosen
- One graded, one homogeneous

M. Zhu *et al.*, *IEEE TED*, Vol. 69(9), pp. 4962-4969 (2022)
M. Zhu *et al.*, *Proc. SPIE,* Vol. 12687, Paper 126870D (2023)

Example: High-Density Vertically Integrated Photodiode (HDVIP)

Gain & Excess Noise Factor Compared to Experimental Data

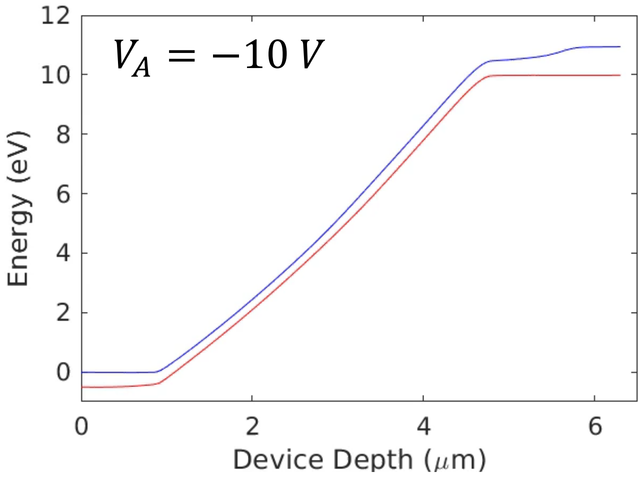


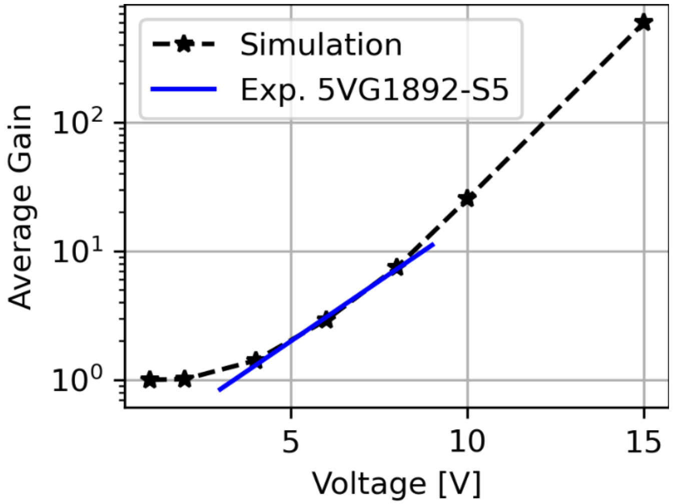
- Simulated gain and excess noise are plotted against experimental measurements
- Simulations also include bandgap grading
- Models are calibrated to the experimental gain values
- Resulting simulated excess noise values are similar to the experimental values

M. Zhu *et al.*, *IEEE TED*, Vol. 69(9), pp. 4962-4969 (2022)
M. Zhu *et al.*, *Proc. SPIE*, Vol. 12687, Paper 126870D (2023)

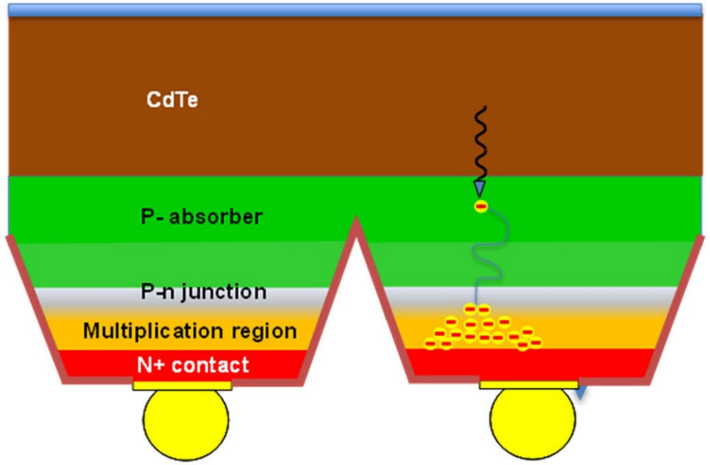
FBMC3D Field-Aided eAPD (FAeAPD) Simulations – Temporal Dependence

Band diagram (with particles)





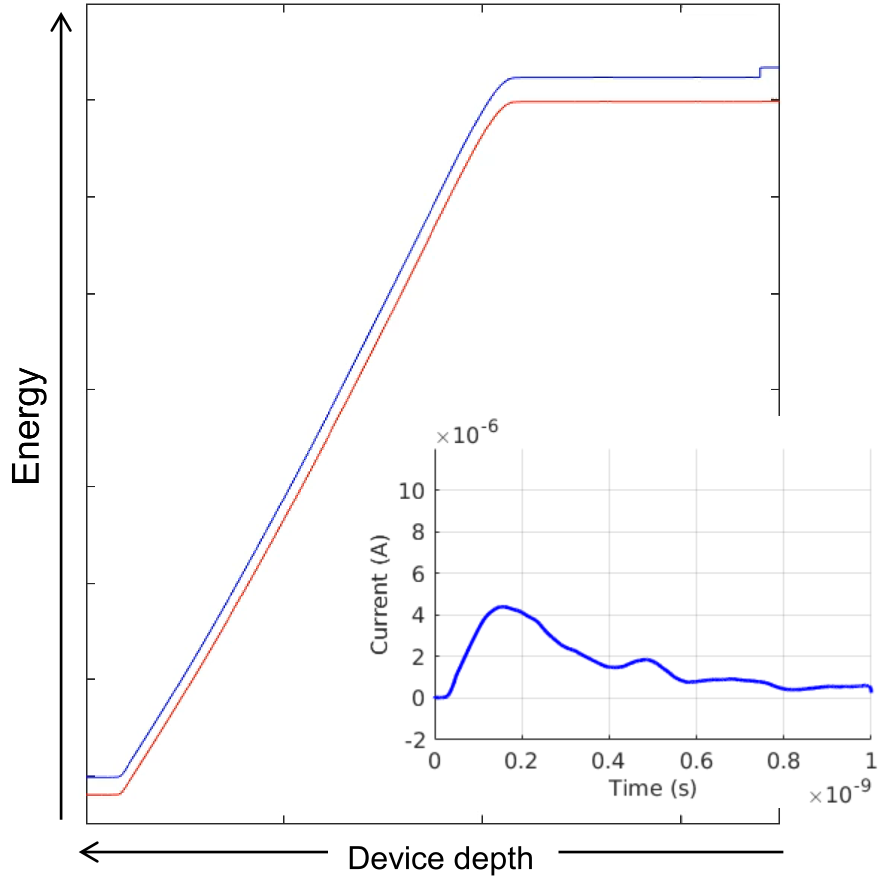
- ➢ Models applied to FAeAPD design
- ➢ Frozen field simulation (does not re-solve Poisson's equation)
  - Electric field profile obtained from previous self-consistent simulation
  - Faster way to evaluate gain, avoids classical confinement in 1D
- ➢ 100 particles injected (from the right) at beginning of the simulation



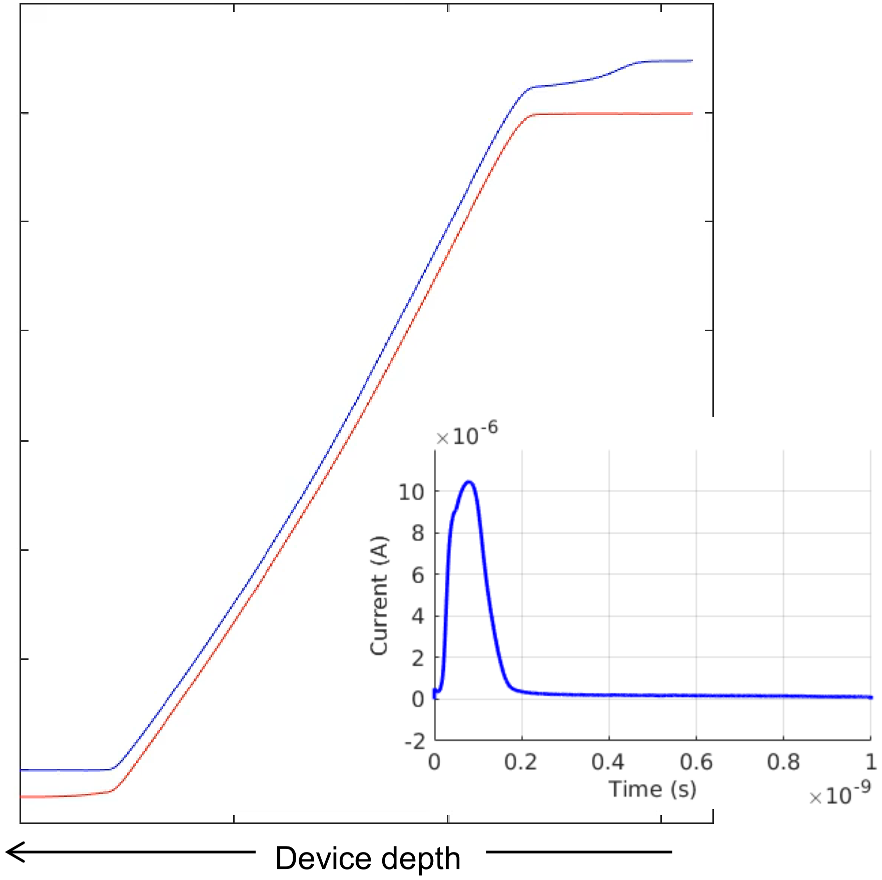
J. Rothman, *J. Electron. Mater.*, 47(10), pp. 5657–5665 (2018)

High Bandwidth FAeAPD – Impulse Response Comparison

SAPHIRA APD



Field-aided APD



Modeling Used to Confirm & Explain High Speed Operation

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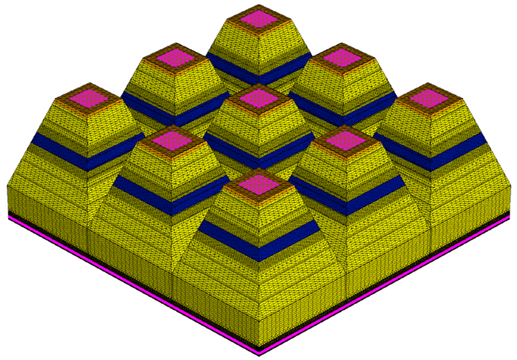
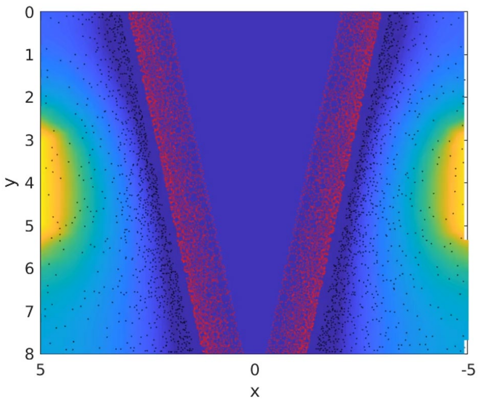
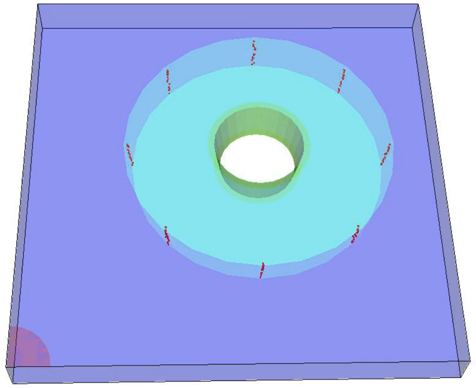
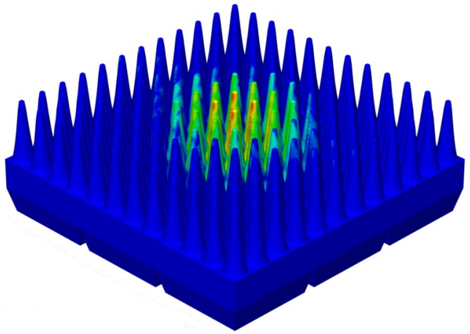
Outline

- Why Perform Modeling?
- Modeling Overview and Capabilities
  - What Numerical Modeling Buys You!
- Modeling Device Metrics – Single Devices & Arrays
  - Alloy Semiconductors (*e.g.*, HgCdTe, InGaAs, Alloy nBn, *etc.*)
  - Type II Superlattices (T2SL)
    - Nonequilibrium Green's Function (NEGF)
    - Quantum Corrected Drift Diffusion (QCDD)
  - Avalanche Photodiodes (APDs)
    - Full Band Monte Carlo (FBMC)
- Modeling Imaging Metrics – Modulation Transfer Function (MTF)
- Summary & Takeaways









Modulation Transfer Function (MTF) – Image Quality: Contrast and Resolution

- Modulation transfer function (MTF) describes how well an optical system reproduces an objects contrast in the image at different spatial frequencies

$$MTF = |OTF(\xi)| = \mathcal{F}\{h(x)\}$$

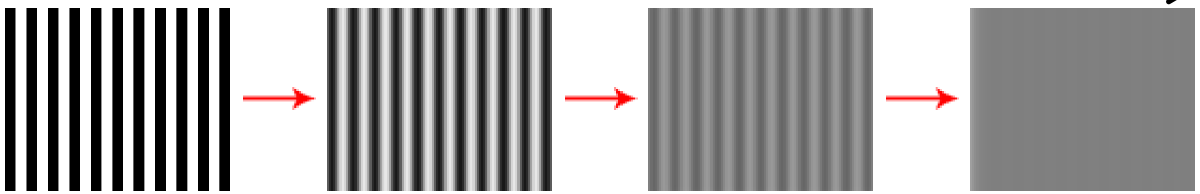
$$h(x) = \text{imaging system impulse response}$$

Target

Images

Reducing modulation depth (lower MTF)

Bar Target

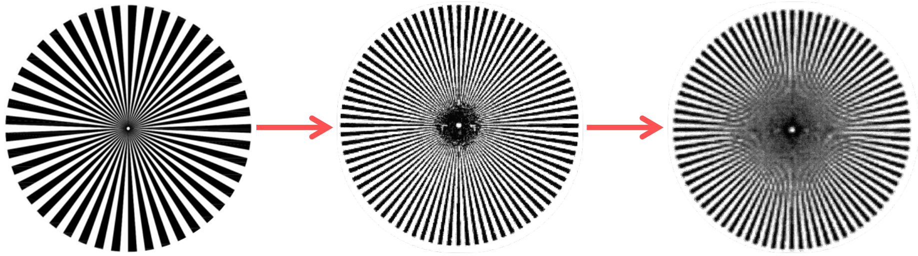


Applied Imaging, Inc; www.aig-imaging.com

Reduced $MTF(\xi)$ blurs higher spatial frequencies

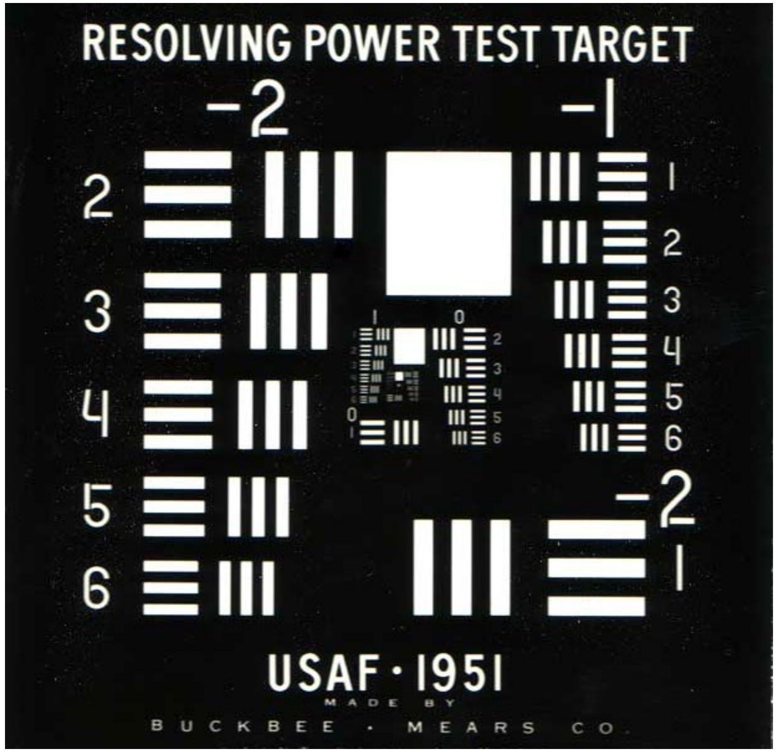
Spoke Target

$\left(\begin{array}{c}\text{spatial frequency}\\ \text{larger in center}\end{array}\right)$



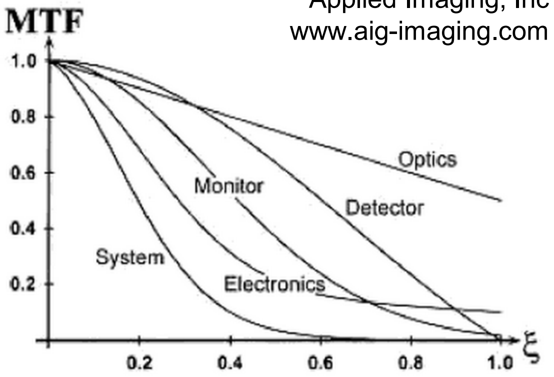
www.aig-imaging.com, G. Boreman, SPIE Press (2001)

Measurement Test Target



Applied Imaging, Inc
www.aig-imaging.com

Cascade Property of MTF



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Selected Performance Metrics: QE, Crosstalk and MTF @ Nyquist

External Quantum Efficiency

- Ratio of collected electron/hole pairs to photons incident on FPA
- Ideally 1.0

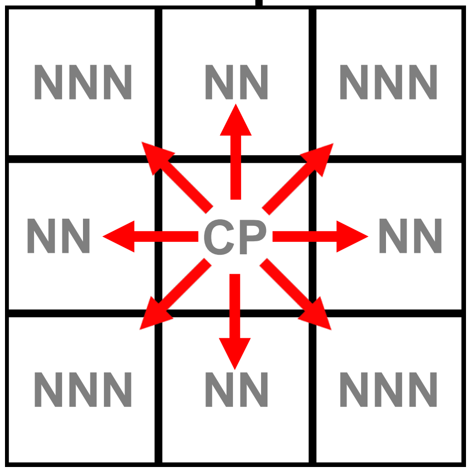
$$QE \stackrel{\text{def}}{=} \frac{I_{photo,center}}{q \times incident\ flux \times Area}$$

Inter Pixel Crosstalk

- Due to carrier diffusion from center to neighboring pixels
- Ideally 0.0

$$Crosstalk \equiv \frac{I_{Photo,\,non-center}}{I_{Photo,\,center}}$$

Pixel Map: 3 × 3



- CP = Center Pixel
- NN = Nearest Neighbor
- NNN = Next Nearest Neighbor

Detector MTF at Nyquist frequency – $MTF_{Detector}(\xi_{Ny})$

- Frequency at which the detector samples the target at a rate of two-samples per- cycle*
- Often used as system specification
- Maximum value is $\mathrm{MTF_{FP}}(\xi_{Ny}) = 0.64$

$$\xi_{Ny} = \frac{1}{2 \times \text{pixel pitch}}$$

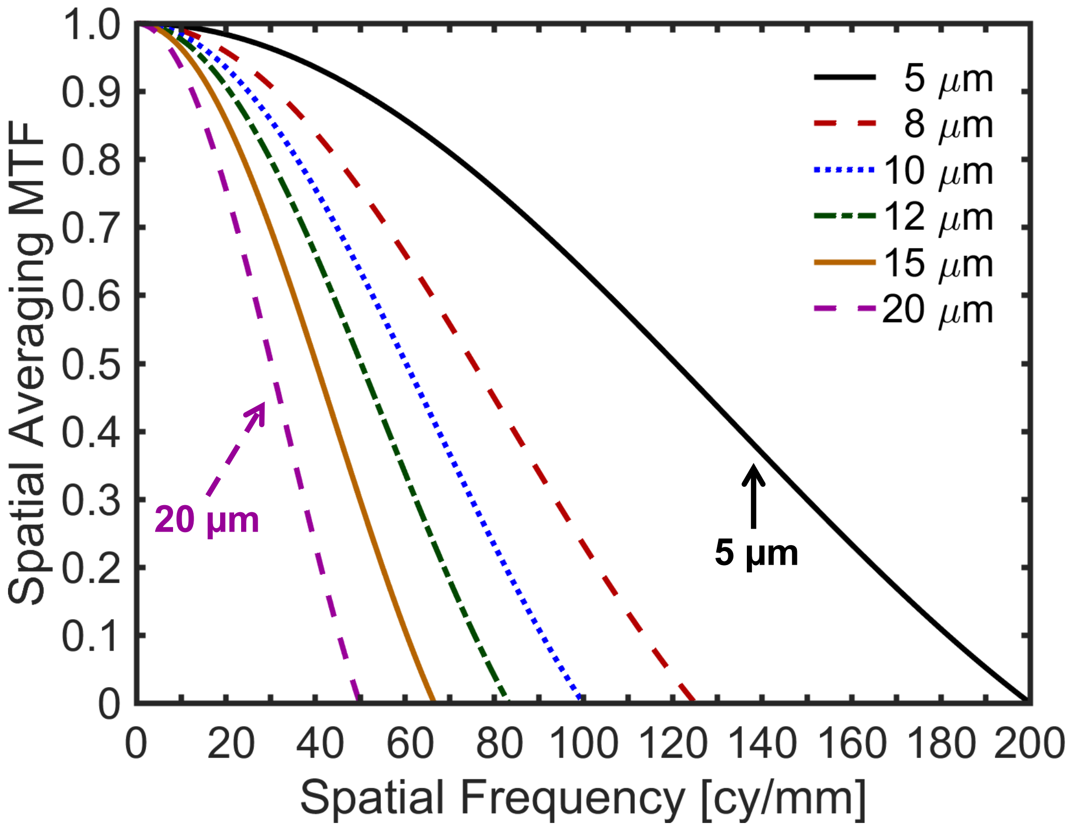
*G. D. Boreman, "Modulation Transfer Function in Optical and Electrooptical Systems," Bellingham, WA, USA: SPIE, 2001.

Metrics usually vary based on voltage, wavelength & temperature

Conflicting Tradeoffs Associated with Optimizing Each of These Metrics!

MTF Challenges: Drive to Smaller Pixels

- Detector MTF directly related to the size of the pixels (footprint)
- Reducing pixel pitch increases MTF (ideally), thereby improving the image contrast.
- Drive to smaller pixels in the IR industry
- Ultimate pixel pitch goal being†
  - 5 um for LWIR imaging
  - 3 um for MWIR imaging
- Reducing the pixel pitch poses numerous technological challenges
  - Obvious fabrication challenges
  - Drastically higher crosstalk due to inter-pixel diffusion of photocarriers
  - Crosstalk directly reduces overall detector MTF
  - MTF optimizing techniques often degrade QE



$$MTF_{\mathrm{FP}} = \mathrm{sinc}(\xi p) \quad \xi = \text{spatial frequency}$$
$$p = \text{pixel pitch}$$

†Driggers et al., “Infrared detector size: how low should you go?," Optical Engineering 51(6), 063202 (2012)

Modeling Required to Realize Benefits of Reducing the Pixel Pitch?

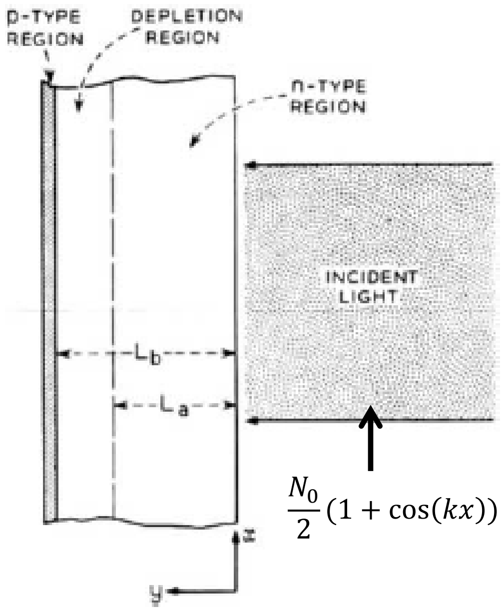
MTF Analytical Model – Applicable to Planar Arrays

The Silicon Diode Array Camera Tube

By MERTON H. CROWELL and EDWARD F. LABUDA

(Manuscript received November 26, 1968)

THE BELL SYSTEM TECHNICAL JOURNAL, MAY–JUNE 1969



Limitations

- Planar only (no etched structures)
- Ignores junctions in neighboring pixels
- MTF diffusion term is still pitch independent
- Assumes all photo-carriers within a diffusion length of central junction are collected (ignores spatial crosstalk)

$$\eta_k = \frac{\alpha L(1-R)}{\alpha^2 L^2 - 1}\left[\frac{2(\alpha L + SL/D) - (\beta_+ - \beta_-)\exp(-\alpha L_a)}{\beta_+ + \beta_-} - \frac{\exp(-\alpha L_a)}{\alpha L}\right] - (1-R)\exp(-\alpha L_b)$$

where L_a = thickness of undepleted region
L_b = thickness of undepleted region + depletion region
L_0 = diffusion length
$\beta_\pm = (1 \pm SL/D)\exp(\pm L_a/L)$, S = surface rec. velocity
$1/L^2(k) = 1/L_0^2 + k^2$
$k = 2\pi f$, f = spatial frequency

$$MTF_{Diff} = \frac{\eta_k}{\eta_0}, \qquad \eta_0 = \eta_k\Big|_{k=0}$$

$$MTF_{Footprint} = \frac{\sin(kd_p)}{kd_p}, \qquad d_p = \frac{1}{2}pitch$$

$$MTF_{Total} = \frac{\eta_k}{\eta_0}\left[\frac{\sin(kd_p)}{kd_p}\right]$$

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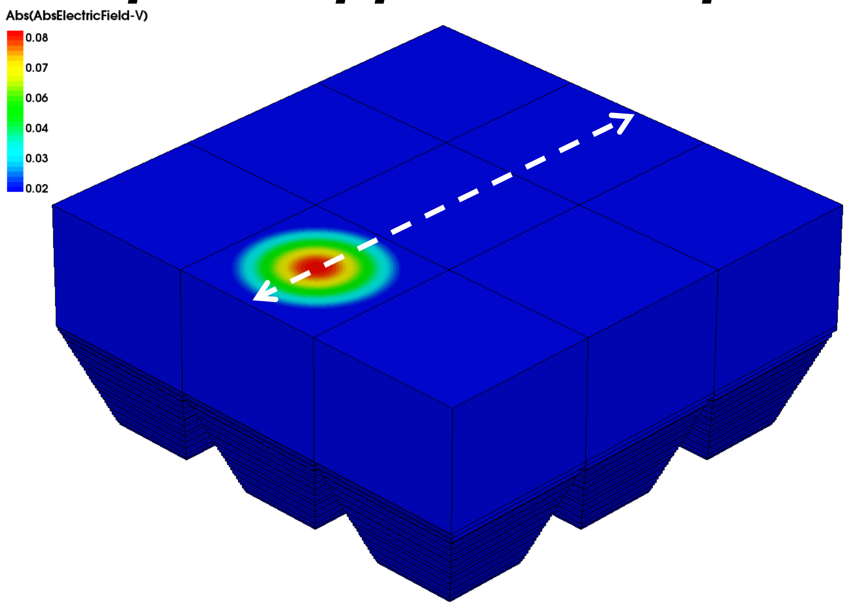
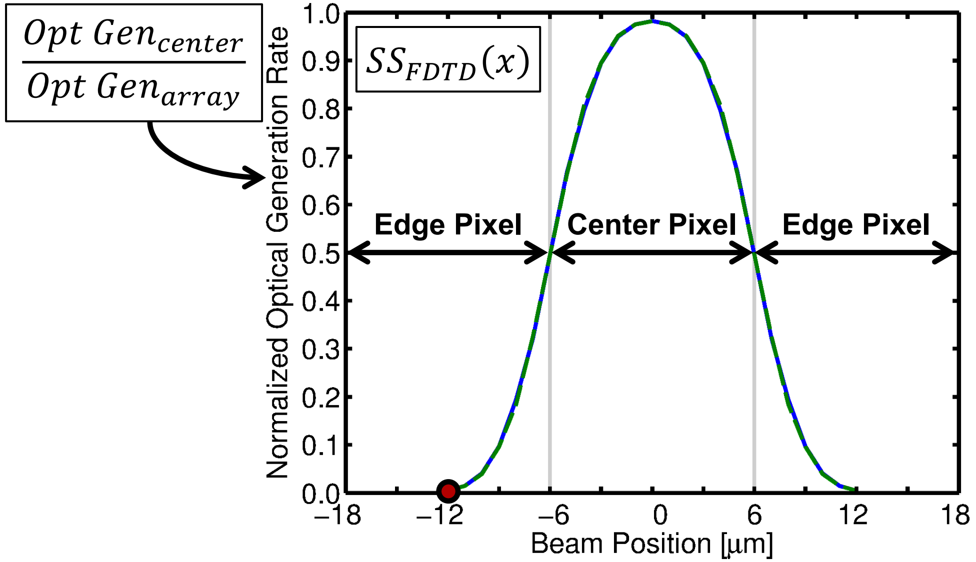
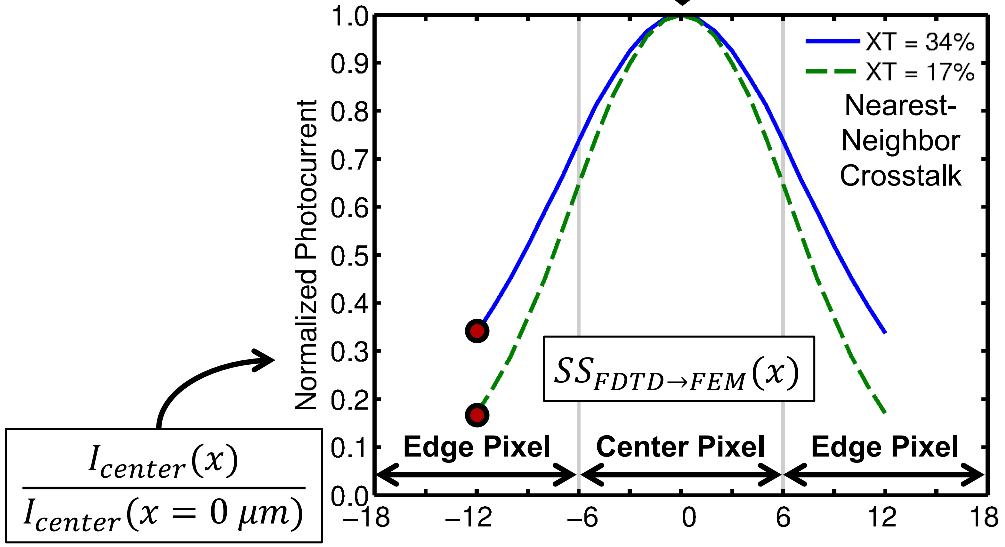
Subsequent Work Has Extended Model to Mesa Structures

MTF Numerical Simulation Procedure – Approach 1)

Real Space Approach – Spot Scan (SS) → MTF







$$MTF_{optical}(\xi) = |\mathcal{F}\{SS_{FDTD}(x)\}|$$

$$MTF_{total}(\xi) = |\mathcal{F}\{SS_{FDTD \rightarrow FEM}(x)\}|$$

Decompose

- Footprint
- Gaussian Beam
- Optical Crosstalk
- Diffusion Crosstalk
- Detector

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B. Pinkie *et al.*, Opt. Lett., Vol. 38(14), pp. 2546-2549 (2013)
J. Schuster, Proc. SPIE, Vol. 10526, Paper 105261I (2018)

MTF Example: MWIR HgCdTe Planar P-on-n Detector

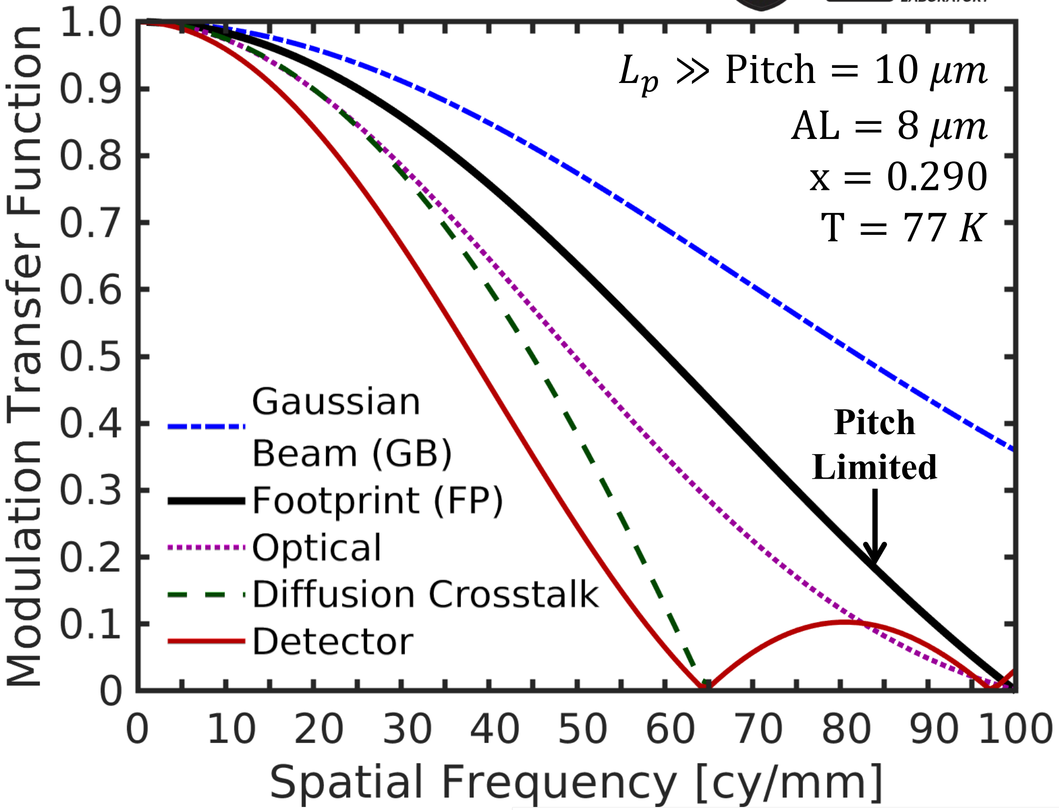
$$MTF_{Total} \approx \underbrace{MTF_{FP} \times MTF_{GB}}_{\text{Optical (FDTD)}} \times \underbrace{MTF_{Diff}}_{\text{Diffusion (FEM)}}$$

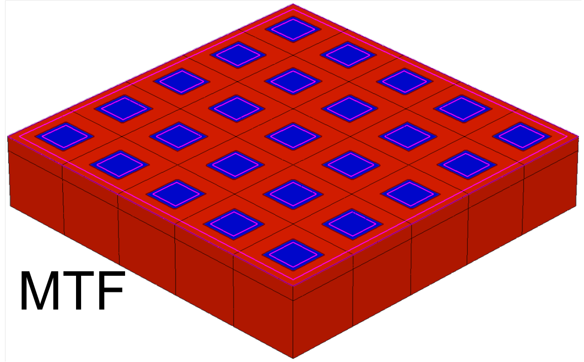
$$MTF_{Diff} = \frac{\mathcal{F}\{SS_{FDTD \rightarrow FEM}(x)\}}{\mathcal{F}\{SS_{FDTD}(x)\}}$$

$$MTF_{Detector} = MTF_{Total}/MTF_{GB}$$

$$MTF_{FP} = \text{sinc}(\xi p)$$

$$MTF_{GB} = \mathcal{F}\{[\exp(-x^2/\omega^2)]^2\}$$

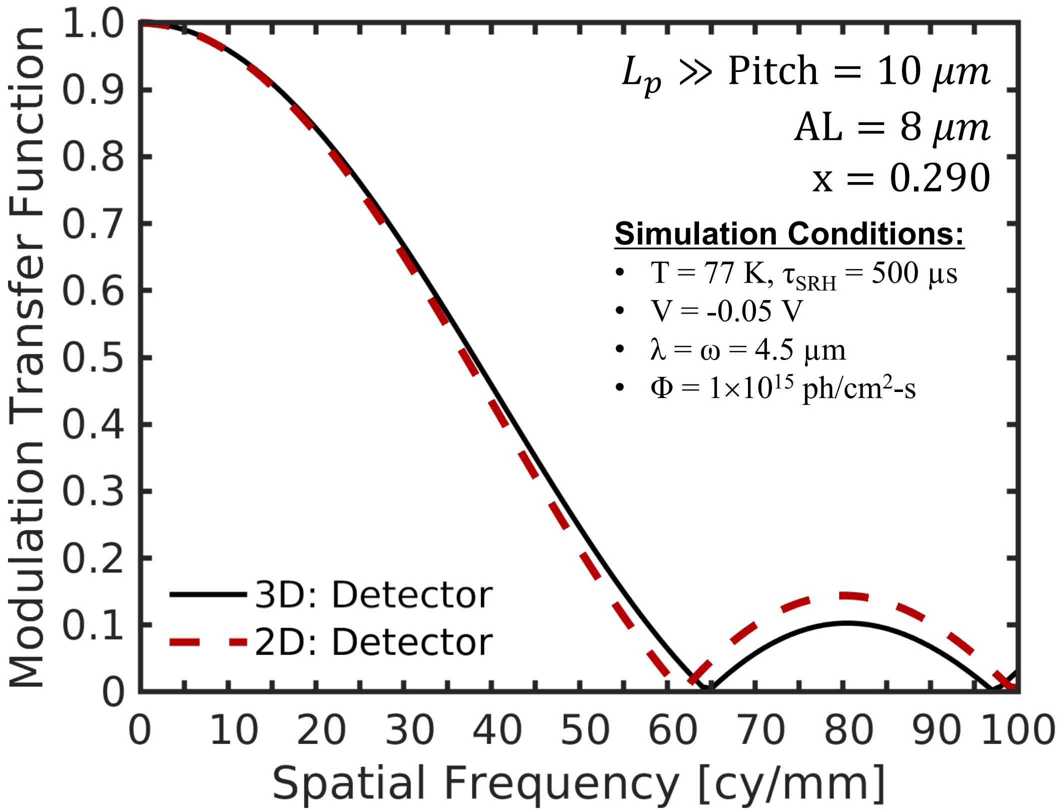




- Analytical formulas not used in simulation
- MTF_{Total} simulated using numerical methods
  - Finite Difference-Time Domain (FDTD) for optical generation rates
  - Finite Element Method (FEM) for drift-diffusion analysis
- Constituent contributions then decoupled
- In this example, diffusion of photo-carriers (spatial crosstalk) limiting total MTF

J. Schuster, Proc. SPIE., Vol. 10526, Paper 1052653 (2018)

Computational Complexity and Reducing Dimensionality



$$\mathrm{MTF}_{\mathrm{FP}}(\xi_{Ny}) = 0.64$$

Dimensionality	NN Crosstalk	$MTF_{Detector}(\xi_{Ny})$
3D	35.1	0.25
2D	37.4	0.21

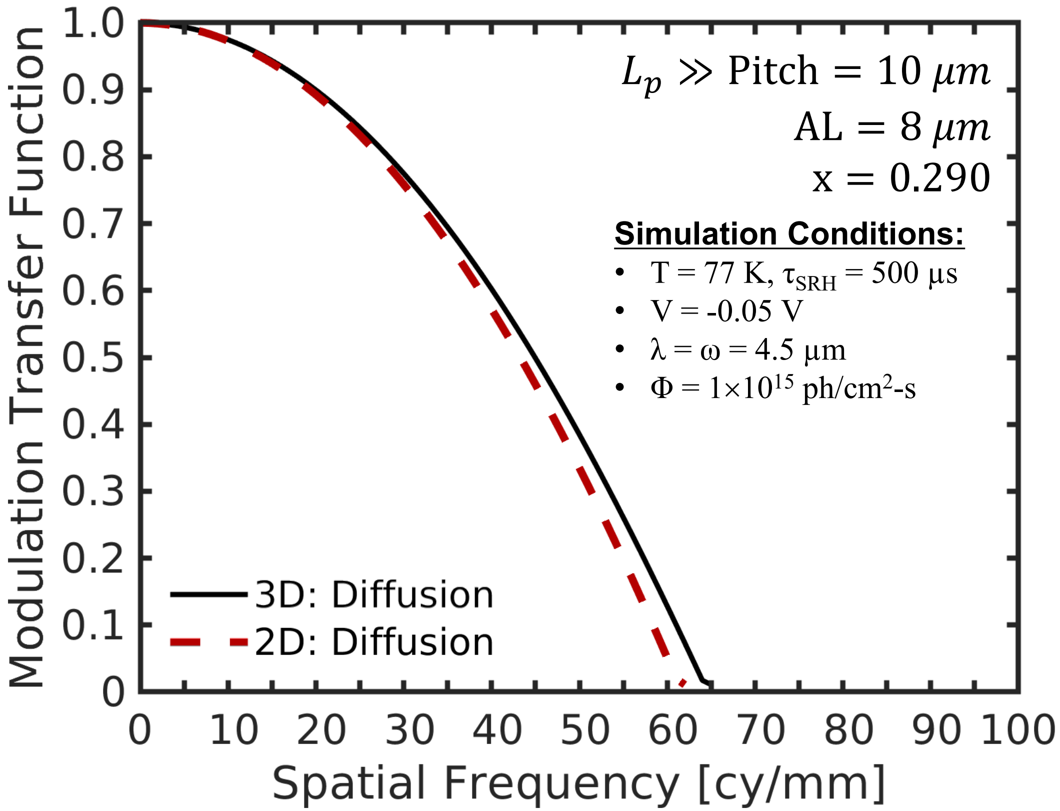
Tradeoff in reducing dimensionality from 3D to 2D

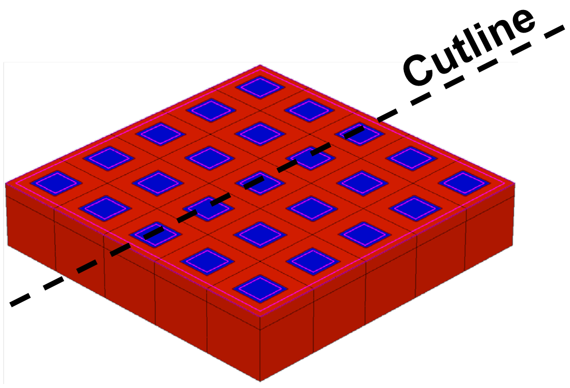
- 2D slightly overestimates crosstalk
- 2D predicts MTF at Nyquist that is 16% smaller than 3D
- 3D simulations only required when highly accurate MTF values needed! (*e.g.*, final design)
- Run time of 2D simulations can be ~200 – 800 times faster than 3D
  - Simulations finish in hours, not days (for complicated devices with poor convergence)

Architecture	3D (hours)	2D (hours)	Speed Up
Planar HgCdTe	23.94	0.03	798.0
Two-Color HgCdTe	13.58	0.03	452.7
Two-Color T2SL	463.06	2.21	209.5

J. Schuster, Proc. SPIE., Vol. 10526, Paper 1052653 (2018)

MWIR HgCdTe Planar P-on-n Detector MTF: 2D vs 3D





$$Crosstalk \equiv \frac{I_{Photo,\,non-center}}{I_{Photo,\,center}}$$

3D Crosstalk Map: 5 × 5

1.7	4.0	5.9	4.0	1.7
4.0	16.9	35.2	16.9	4.0
6.0	35.2	100	34.9	6.0
4.0	16.9	35.2	16.9	4.0
1.7	4.0	6.0	4.0	1.7

→

2D Crosstalk Map: 5 × 1

6.4	37.4	100	37.4	6.4

- Diffusion MTF slightly lower in 2D than 3D
  - Apparent from crosstalk values

2D MTF Simulations May be Acceptable Depending on Required Precision

J. Schuster, Proc. SPIE., Vol. 10526, Paper 1052653 (2018)

MTF Numerical Simulation Procedure – Approach 2)
Frequency Space Approach

- Spot scan approach replicates experimental procedures
  - Extremely computational expensive
- Alternatively, MTF can be computed in Fourier space using generation profile of only pertinent frequency

In-phase cosine excitation: $GP_1 = \frac{1}{2}[1 + \cos(2\pi f x)]$

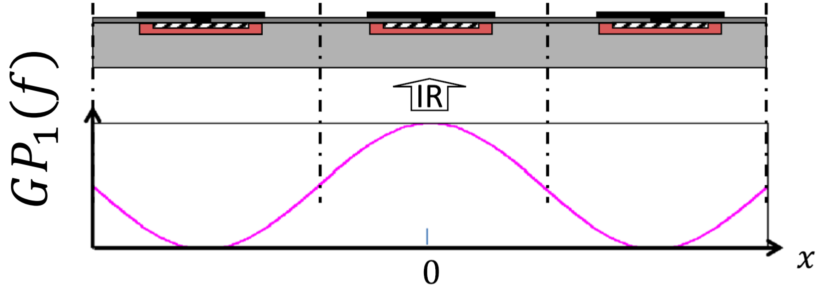
Antiphase excitation: $GP_2(x, f) = 1 - GP_1(x, f)$

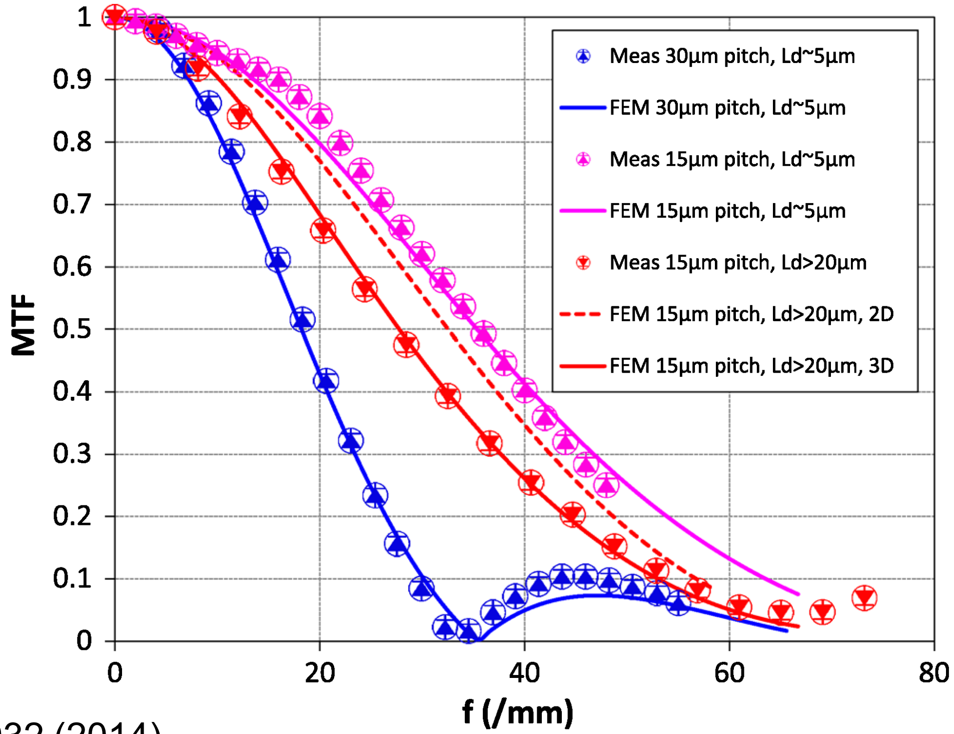
Current response: $I_i(f) = \int h(\vec{x}) \times GP_i(x, f) d\,\vec{x}$

$$MTF(\mathrm{f}) = \frac{I_1(f) - I_2(f)}{I_1(f) + I_2(f)} = \frac{2I_1(f) - I(0)}{I(0)} = 2\frac{I_1(f)}{I(0)} - 1$$

- MTF estimated using only one computation per excitation frequency!

Direct frequency space measurement





O. Gravrand *et al.*, *J. Electron. Mater.*, Vol. 43(8), pp. 3025–3032 (2014)
J. Berthoz *et al.*, *J. Electron. Mater.*, Vol. 44, pp. 3157–3162 (2015)

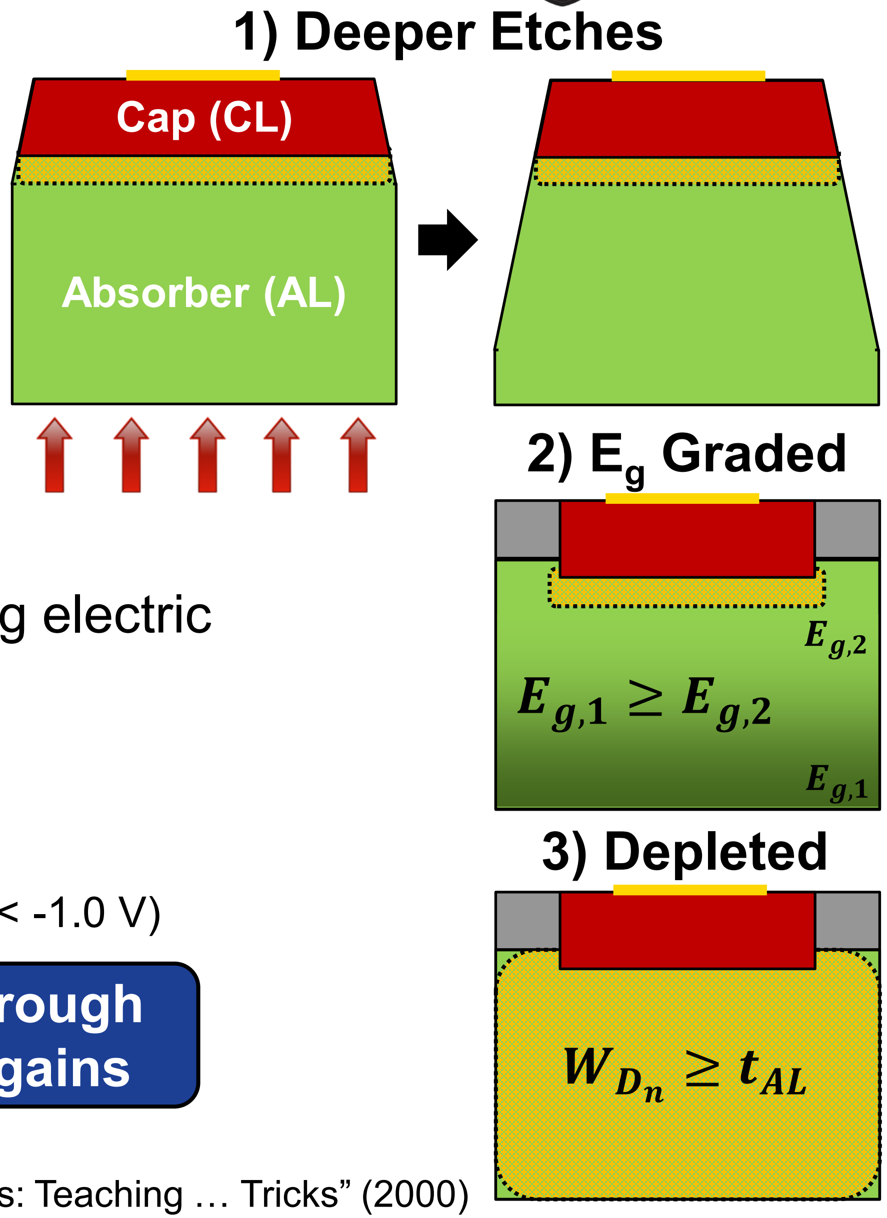
Crosstalk Mitigation → Improving (Maximizing) the MTF

$MTF_{Detector}$ limited by $MTF_{Diffusion}$ (<<1) → require crosstalk mitigation

Three primary crosstalk mitigation approaches:

- <u>Physically</u> isolate photocarriers – delineate pixels
  1) Etch Mesas
     - Requires switching from planar to mesa architecture (not necessarily possible)
     - Is full delineation required?
     - Tradeoff: Significantly degrades QE if etch angle is shallow
- <u>Electrically</u> isolate photocarriers – confine photocarriers using electric fields
  2) Incorporate bandgap grading* → forms "quasi"-electric field*
     - Practical in HgCdTe, III-V SL, not InGaAs
  3) Deplete absorber layer → forms electric field
     - Trick is achieving "full" depletion at reasonable small reverse biases (< -1.0 V)

All approaches benefit from numerical simulations through improved understanding & quantifying performance gains



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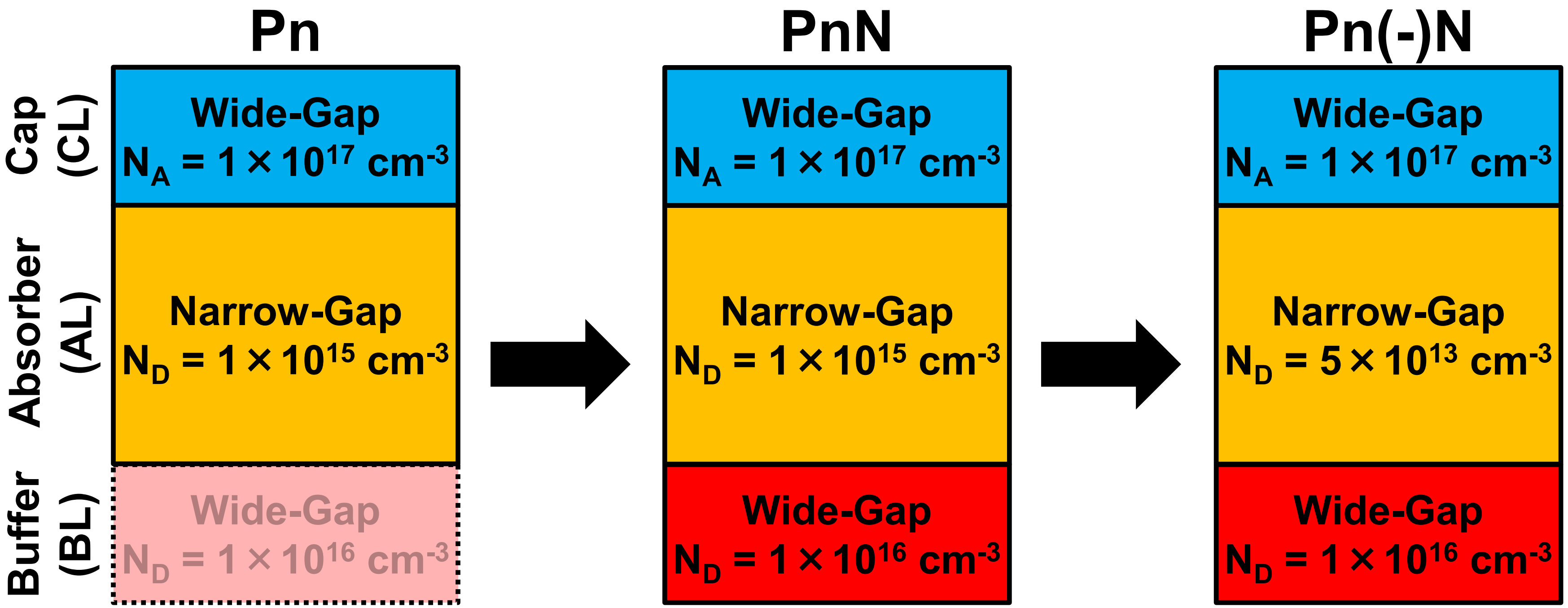
J. Schuster, Proc. SPIE., Vol. 10526, Paper 1052653 (2018)

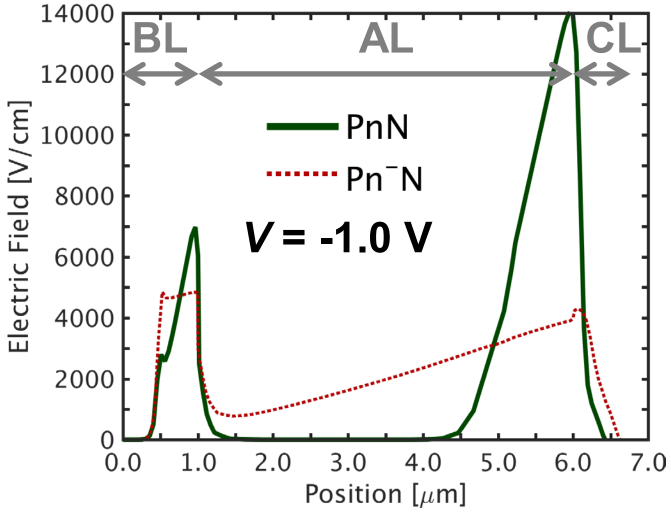
*H. Kroemer, "Nobel Lecture: "Quasi-Electric Fields and Band Offsets: Teaching … Tricks" (2000)

Depleted Architecture: Crosstalk Mitigation Approach #3)



Goal: Reduce crosstalk (diffusion) by depleting absorber layer

- ➢ Collection now through drift not diffusion
- ➢ Approach
  1) Switch from Pn to PnN architecture
  2) Reduce AL doping† by 15× → enable "full depletion" at less than -1 V for 5 μm absorber



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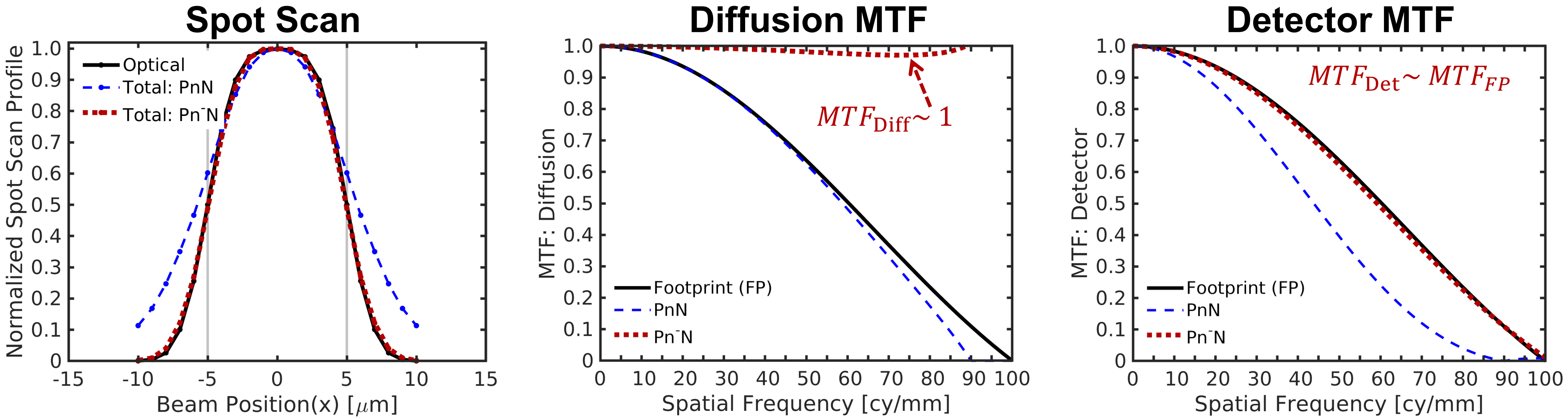
†D. Lee, *et al.*, *J. Electron. Mater.*, Vol. 45, No. 9, pp. 4587-4595 (2016)
J. Schuster, Proc. SPIE., Vol. 10526, Paper 1052653 (2018)

Depleted Architecture: Crosstalk Mitigation Approach #3)



Switching to depleted architecture

- Diffusion of photocarriers eliminated
- Spot scan: Total nearly identical to optical (no deviation)
- MTF diffusion ~ 1
- MTF detector ~ MTF footprint (ideal performance)

$$Crosstalk \equiv \frac{I_{Photo,\,non-center}}{I_{Photo,\,center}} \qquad MTF_{Detector} = \frac{MTF_{Total}}{MTF_{GB}}$$

Simulation Conditions:

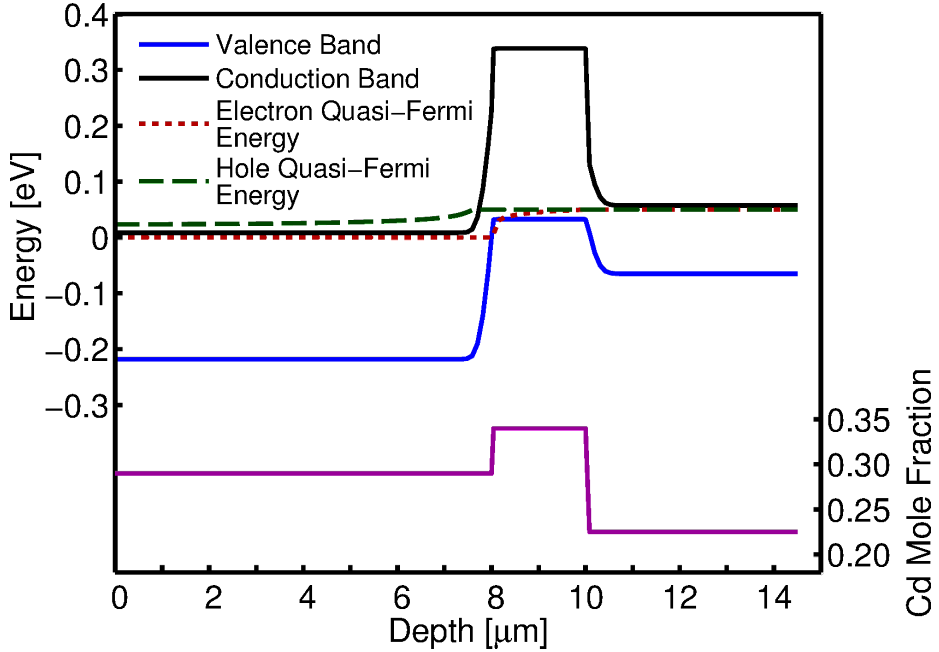
- T = 150 K • λ = ω = 3.0 μm
- **V = -1.0 V** • $\Phi = 1\times10^{15}$ ph/cm²-s

$$\mathrm{MTF_{FP}}(\xi_{Ny}) = 0.64$$

Detector	Crosstalk		$\mathrm{MTF_{Detector}}(\xi_{Ny})$	
	-0.1 V	-1.0 V	-0.1 V	-1.0 V
PnN	17.7%	12.1%	0.34	0.40
Pn-N	6.5%	0.3%	0.47	0.62

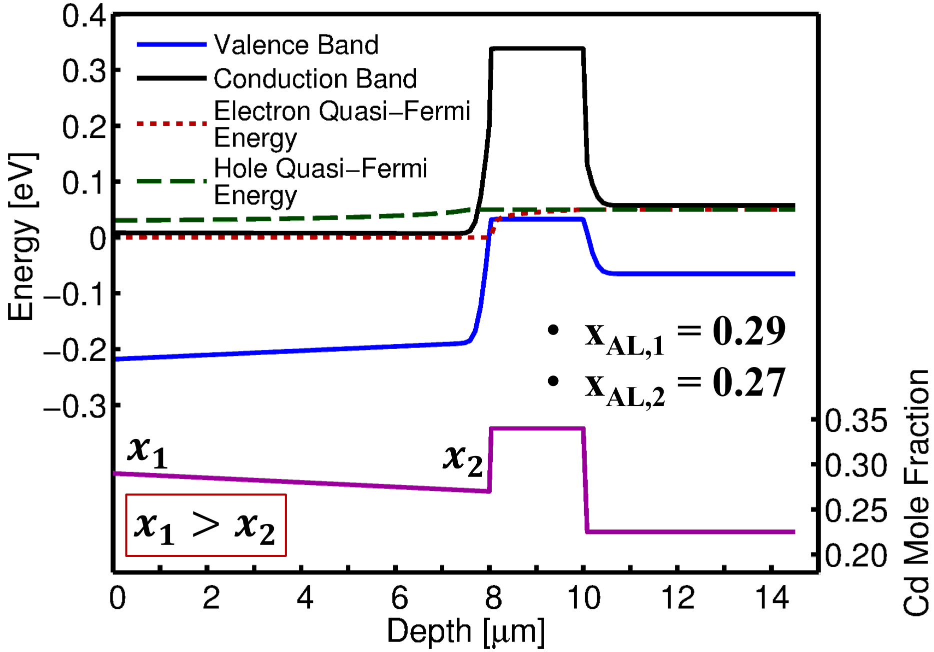
J. Schuster, Proc. SPIE., Vol. 10526, Paper 1052653 (2018)

Grading MW Bandgap: Crosstalk Mitigation Approach #2)



Grading

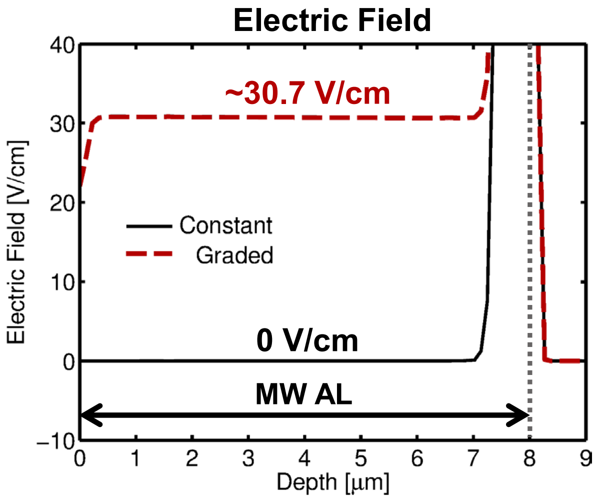
- $\Delta x = 0.02$
- $\Delta E_g = 31.9$ meV



- Grading the AL mole fraction results in a quasi-electric field forming in the MW AL
- Quasi-electric field
  - Aids collection of photocarriers via drift
  - Reduces number of photocarriers diffusing to adjacent pixels:
    - ✓ Reduces spatial crosstalk
    - ✓ Increases MTF

Simulation Conditions:

- T = 77 K
- $\tau_{SRH} = 500$ μs
- **V = -0.05 V**



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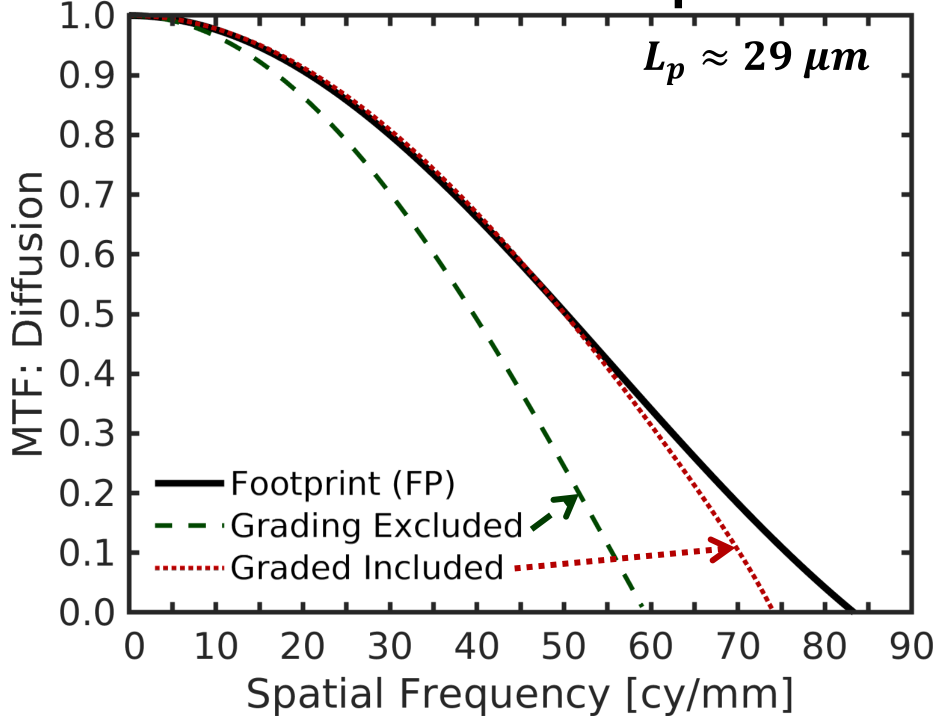
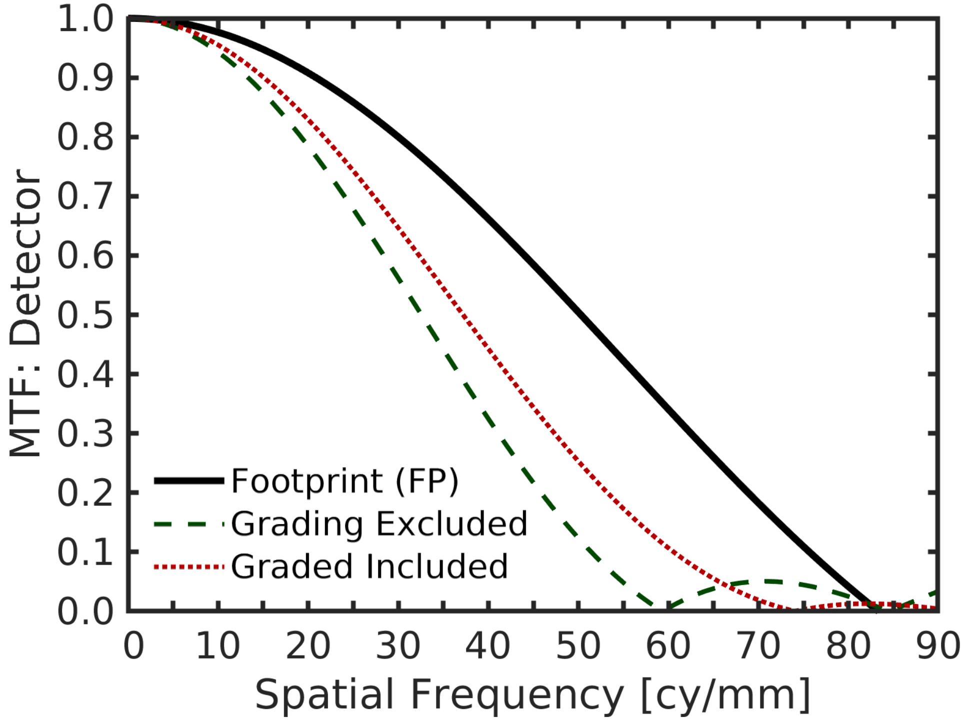
Grading MW Bandgap: Crosstalk Mitigation Approach #2)

Diffusion MTF Component



Detector MTF



- Bandgap graded by ~31 meV over 8 µm AL
- Via drift quasi-electric field in the AL (~30.7 V/cm) reduces number of photocarriers diffusing to neighboring pixels → significantly reducing the diffusion MTF component

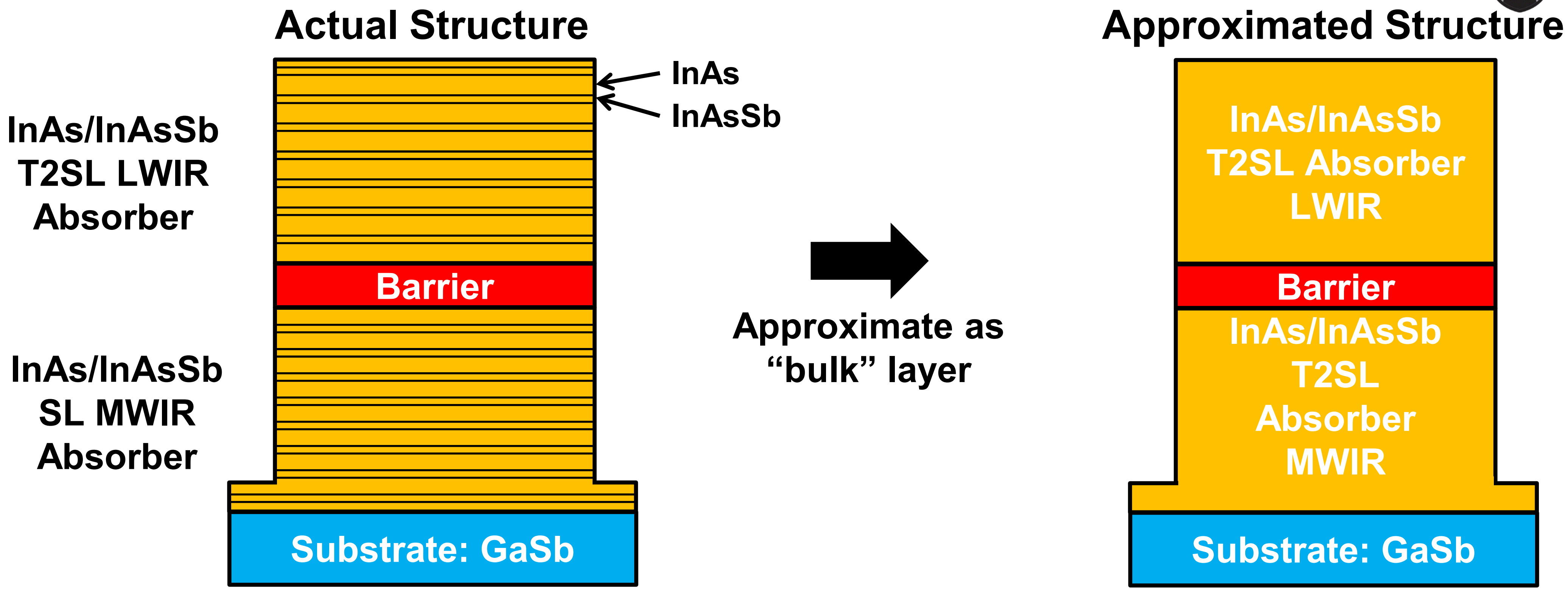
Simulation Conditions:

- T = 77 K
- τ_{SRH} = 500 µs
- V = -0.05 V
- λ = ω = 4.0 µm
- Φ = 1×10[15] ph/cm[2]-s

$$\mathrm{MTF_{FP}}(\xi_{Ny}) = 0.64$$

MW Grading	Crosstalk		$\mathrm{MTF_{Detector}}(\xi_{Ny})$
	NN	NNN	
Excluded	24.1%	9.2%	0.29
Included	10.9%	1.7%	0.41

T2SL nBn Device Modeling Challenges



- Drift-diffusion is a semi-classical model, well suited to alloy semiconductors, not quantized structures
- Approach: T2SL using drift-diffusion
  1) Approximate T2SL layers as “bulk”-like layers with “global” material properties
  2) Obtain parameters externally ($k \cdot P$ or measurement) ← lacking material database
  3) Perform drift-diffusion simulations on “approximated” device

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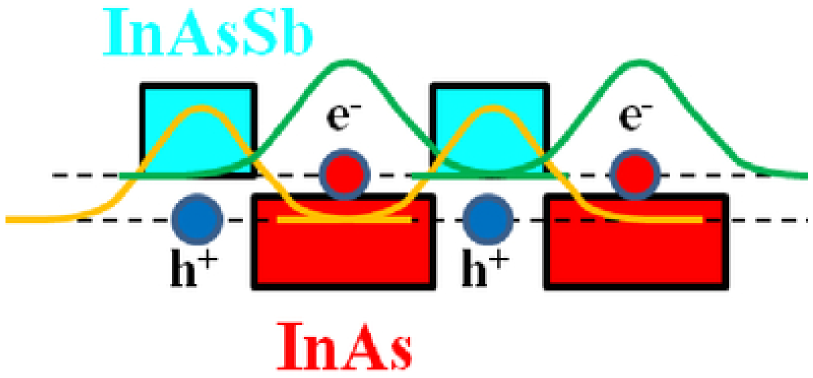
J. Schuster, IEEE Trans. Electron Devices, Vol. 66, No. 3, pp. 1338-1344 (2019)

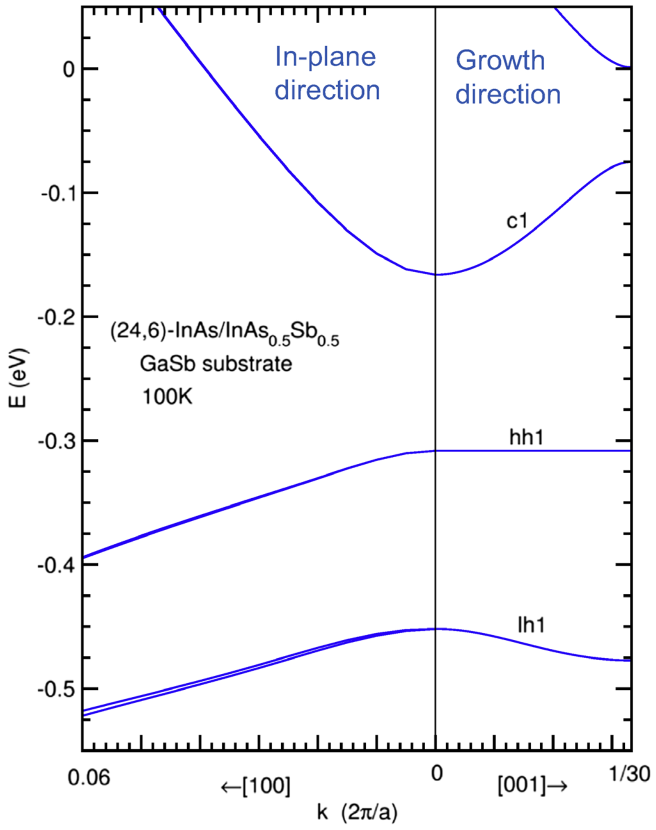
Superlattice Anisotropic Mobilities



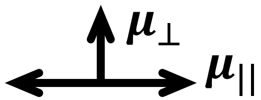
Effective Conduction Band

Effective Valence Band

M. Razeghi *et al.*, “InAs/InAs$_{1-x}$Sb$_x$ type-II superlattices for high performance long wavelength infrared detection," Proc. SPIE 9819, 981909 (2016)

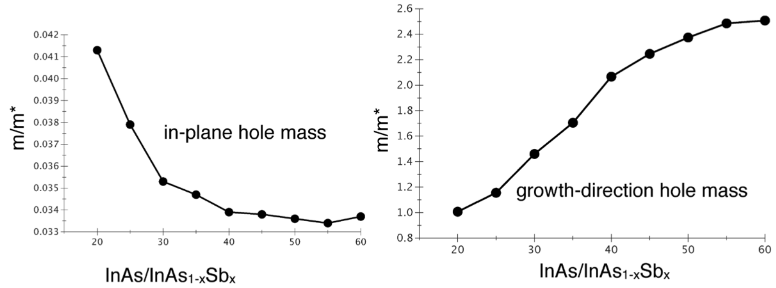


D. Ting *et al.*, Infrared Phys. Tech., 84, pp. 102–106 (2017)



- Confinement in vertical direction, but not lateral direction → anisotropic effective masses → anisotropic mobilities ($\mu_{||} \gg \mu_{\perp}$)
  - $\mu_{||} = 1200$ cm²/V-s → $L_{||} = 43.7\ \mu$m
  - $\mu_{\perp} = 60$ cm²/V-s → $L_{||} = 9.8\ \mu$m
- Ideal situation (for MTF) would be $\mu_{\perp} \gg \mu_{||}$

Objective: Use 2D/3D modeling capability to quantify effect of anisotropic mobilities on MTF



M. E. Flatté *et al.*, Proc. SPIE 9370, 93700K (2015)

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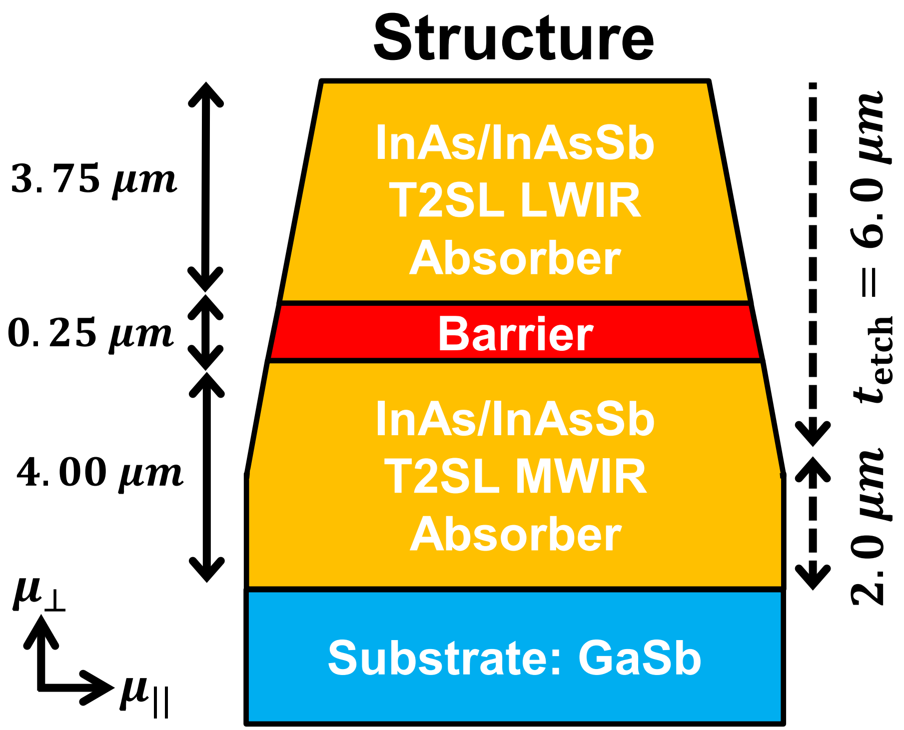
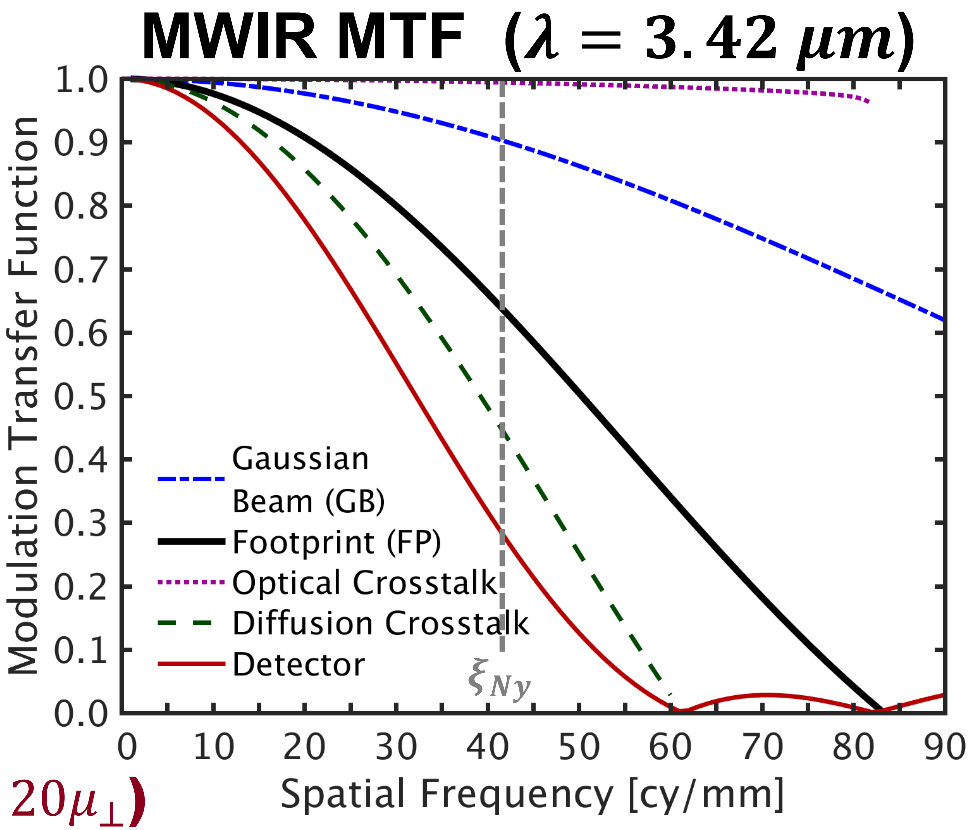
MW/LW Two Color T2SL nBn: Structure & MTF





T2SL MTF with anisotropic mobilities ($\mu_{||} \sim 20\mu_\perp$)

- Despite deep etch (only 2 µm un-etched AL remaining) detector MTF several reduced by crosstalk
  - Nearest-neighbor diffusion crosstalk = 29.4%
  - $\text{MTF}_{\text{Detector}}(\xi_{Ny}) = 0.28$ ($\xi_{Ny} = 41.7$ cy/mm, $\text{MTF}_{FP}(\xi_{Ny}) = 0.64$)

Simulation Conditions:

- $\tau_{\text{SRH(MW AL)}} = 2.4\ \mu s$
- $\tau_{\text{SRH(LW AL)}} = 1.0\ \mu s$
- $T = 77$ K
- $V = -0.1$ V
- $\lambda = \omega = 3.42\ \mu m$
- $\Phi = 1\times10^{15}$ ph/cm^2-s

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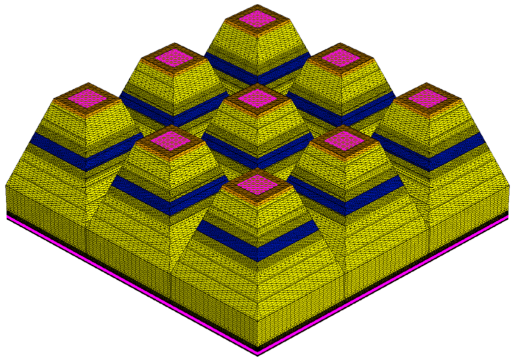
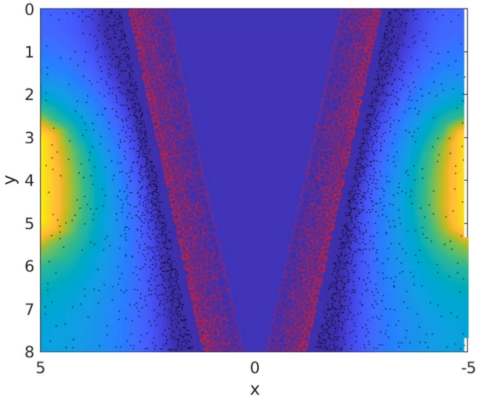
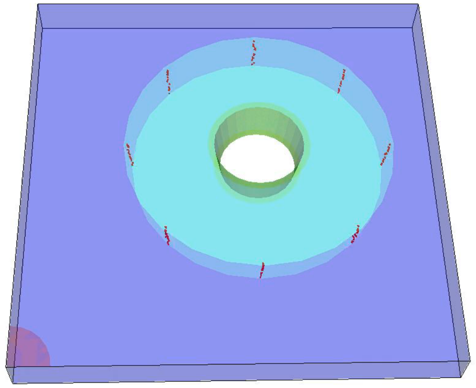
J. Schuster, IEEE Trans. Electron Devices, Vol. 66, No. 3, pp. 1338-1344 (2019)

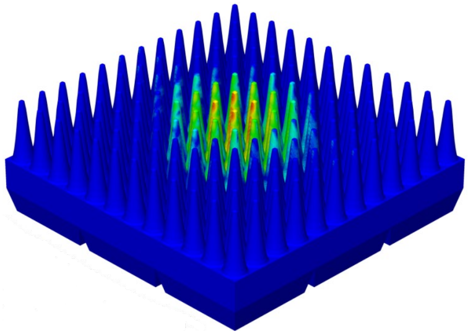
Outline

- ➢ Why Perform Modeling?
- ➢ Modeling Overview and Capabilities
  - What Numerical Modeling Buys You!
- ➢ Modeling Device Metrics – Single Devices & Arrays
  - Alloy Semiconductors (*e.g.*, HgCdTe, InGaAs, Alloy nBn, *etc.*)
  - Type II Superlattices (T2SL)
    - Nonequilibrium Green's Function (NEGF)
    - Quantum Corrected Drift Diffusion (QCDD)
  - Avalanche Photodiodes (APDs)
    - Full Band Monte Carlo (FBMC)
- ➢ Modeling Imaging Metrics – Modulation Transfer Function (MTF)
- ➢ Summary & Takeaways









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Modeling Software (Not Comprehensive)

Commercial Simulators are Prohibitively Expensive (except to Universities) → Hindering Widespread Use

Material Modeling

- $k \cdot P$
- Nonlocal pseudopotential method (NLPM)
- Density Functional Theory – Requires supercomputer
  - Vienna Ab initio Simulation Package (VASP, https://www.vasp.at)
  - Octopus (https://octopus-code.org)
  - Quantum ESPRESSO (https://www.quantum-espresso.org)
  - Synopsys QuantumATK (https://www.synopsys.com/manufacturing/quantumatk.html)

Transport & Device Modeling

- Analytical Codes
  - Minimal effort to develop → usually developed internally
- Commercial Drift-Diffusion (2D & 3D) – Extremely expensive
  - Synopsys TCAD Sentaurus (https://www.synopsys.com/manufacturing/tcad.html)
  - Silvaco Victory (https://silvaco.com/tcad/victory-device-3d)
  - COMSOL Semiconductor Module – not as tailored as Synopsys or Silvaco (https://www.comsol.com/semiconductor-module)
  - Ansys Lumerical CHARGE (https://www.ansys.com/products/photonics/charge)
- Quantum Corrected Drift-Diffusion
- 1D Non-equilibrium Green's Function
- 3D Monte Carlo

  - **Commercial solutions insufficient or non-existent**
  - **Extremely difficult to develop**

Notable References Summarized

- Drift-Diffusion
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  - J. Schuster *et al.*, "Numerical simulation of third-generation HgCdTe detector pixel arrays," IEEE J. Sel. Top. Quant. Electron., Vol. 19, 3800415 (2013)
  - J. Schuster and E. Bellotti, "Evaluation of quantum efficiency, crosstalk and surface recombination in HgCdTe photon trapping structures," J. Electron. Mater., Vol. 43, pp. 2808 (2014)
- T2SL (k·P, NEGF, SPDD)
  - kdotP
    - P. C Klipstein, "Operator ordering and interface-band mixing in the Kane-like Hamiltonian of lattice-matched semiconductor superlattices with abrupt interfaces," Phys. Rev. B, Vol. 81, Num. 23, Paper 235314 (http://dx.doi.org/10.1103/PhysRevB.81.235314)
  - NEGF:
    - F. Bertazzi *et. al.*, "Nonequilibrium Green's Function Modeling of type-II Superlattice Detectors and its Connection to Semiclassical Approaches," Phys. Rev. Appl. 14, 014083 (2020)
    - A. Tibaldi *et al*, "Analysis of Carrier Transport in Tunnel-Junction Vertical-Cavity Surface-Emitting Lasers by a Coupled Nonequilibrium Green's Function–Drift-Diffusion Approach," Phys. Rev. Appl. 14, 024037 (2020)
    - A. Tibaldi *et al.*, "Modeling Infrared Superlattice Photodetectors: From Nonequilibrium Green's Functions to Quantum-Corrected Drift Diffusion," Phys. Rev. Appl. 16, 044024 (2021)
    - E. Bellotti *et al.,* "Disorder-Induced Degradation of Vertical Carrier Transport in Strain-Balanced Antimony-Based Superlattices," Phys. Rev. Appl. 16, 054028 (2021)
  - SPDD
    - A. Tibaldi *et al.*, "Modeling Infrared Superlattice Photodetectors: From Nonequilibrium Green's Functions to Quantum-Corrected Drift Diffusion," Phys. Rev. Appl. 16, 044024 (2021)
- APD – Full Band Monte Carlo 3D (FBMC3D)
    - I. Prigozhin *et al.*, "FBMC3D—A Large-Scale 3-D Monte Carlo Simulation Tool for Modern Electronic Devices," *IEEE TED*, Vol. 68, No. 1, pp. 279-287 (2021)
    - I. Prigozhin *et al.*, "Numerical Modeling of Graded Bandgap Long Wavelength Infrared HgCdTe Avalanche Photodiodes," *IEEE TED*, 69(7), pp. 3791-3797 (2022)
    - M. Zhu *et al.*, "Dark Current and Gain Modeling of Mid-Wave and Short-Wave Infrared Compositionally Graded HgCdTe Avalanche Photodiodes," *IEEE TED*, Vol. 69(9), pp. 4962-4969 (2022)
    - M. Zhu *et al.*, "Monte carlo modeling of HgCdTe avalanche photodiodes," Proc. SPIE, Volume 12687, paper 126870D (2023)
- MTF
  - Approach 1)
    - B. Pinkie *et al.*, "Physics-based simulation of the modulation transfer function in HgCdTe infrared detector arrays," Optics Letters, Vol. 38, Number 14, pp. 2546-2549, 2013 (http://dx.doi.org/10.1364/ol.38.002546)
    - J. Schuster, "Numerical simulation of the modulation transfer function (MTF) in infrared focal plane arrays: simulation methodology and MTF optimization," Proceedings of SPIE, Vol. 10526, Paper 105261I, 2018 (http://dx.doi.org/10.1117/12.2295018)
    - J. Schuster, "Assessment of the modulation transfer function in infrared detectors with anisotropic material properties: Type II superlattices," IEEE Transactions on Electron Devices, Vol. 66, Num. 3, pp. 1338–1344, 2019 (http://dx.doi.org/10.1109/TED.2019.2892589)
  - Approach 2)
    - O. Gravrand *et al.*, "MTF issues in small-pixel-pitch planar quantum IR detectors," J. Electron. Mater., Vol. 43(8), pp. 3025–3032 (2014)
    - J. Berthoz *et al.*, "Modeling and characterization of MTF and spectral response at small pitch on Mercury Cadmium Telluride," J. Electron. Mater., Vol. 44, pp. 3157–3162 (2015)

Take-aways

- Numerical device modeling enables
  1) Understanding current state-of-the-art devices
     - Separating fundamental *versus* technological limitations
     - Interpreting data
  2) Exploring parameter space – design/formulate experiments → achieve optimum performance
  3) Conceptualizing new IR device architectures that will provide improvements over current state-of-the-art
- Robust and independently verified material parameters required for both analytical and numerical simulations
- Understanding interfaces is key → where most important physics happens
- Essential to understand the limitations and realm of validity of each model and to employ the physically correct model for each problem
  - *e.g.*, don't use a semi-classical drift-diffusion model to understand temperature dependent carrier transport in T2SL's where hopping & localization dictate transport
- NEGF and FBMC3D simulators developed as open platform for DoD applications – available to DoD Agencies & CSM members

THANK YOU.

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