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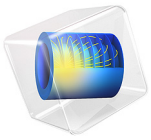

A Solar Cell with InAs Quantum Dots Embedded in AlGaAs/GaAs Quantum Wells

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This example shows an approximate approach to model a dot-in-well solar cell as described by Asahi et al. in the reference paper. The quantum wells and the layers of quantum dots are each treated as lumped energy levels in the bandgap. The authors specify transitions between the dot/well levels and the energy bands. The continuum part of the current density is otherwise unimpeded by the wells and dots. This description is equivalent to the trapping feature in the Semiconductor interface, so it is used to model the wells and dots in this example. The computed trend of the photocurrent and occupancy of the quantum dot states agrees well with the result shown in the paper.

Introduction

In Ref. 1, Asahi et al. studied the photocurrent generation process in a dot-in-well solar cell by shining two lasers at different wavelengths to look at the two-step photon absorption in the device. The solar cell is composed of an $Al_{0.3}Ga_{0.7}As$ p-i-n structure. The intrinsic region contains in addition 10 repeating units, with each unit consisting of a GaAs quantum well (QW) and a layer of InAs quantum dots (QD) embedded in the QW. The authors observed a saturation behavior of the photocurrent with respect to the laser intensities, and used a simple model to explain this behavior. Here we show how this kind of model can be built using the Semiconductor Module.

Model Definition

The authors' modeling approach is to treat the QW and QD as lumped energy levels. The transitions between these levels and the conduction/valence bands are described with simple lifetimes or rates in an unidirectional fashion (no detailed balancing). Other than these transitions, the current flow in the energy bands is not affected by the QW and QD. There is also a transition from the QW to the QD specified by the authors. See Fig. 6 in Ref. 1 for a summary of their model.

This description of the system is essentially the same as considering, in the Semiconductor interface, a bulk $Al_{0.3}Ga_{0.7}As$ p-i-n structure with some layers of traps in the intrinsic region, where the trap energy levels represent the layers of QW and QD. The unidirectional transitions can be implemented by setting the **Carrier Capture** probabilities to zeros and using the **Additional Carrier Capture Rate** option to specify the unidirectional rates. The transition from the QW to the QD can be implemented using the **Transition Between Discrete Levels** feature. To minimize the reverse transition from the QD to the QW, a large energy difference between the two trap levels are used.

For simplicity, only two repeating units are implemented in this example. Additional substrate buffer layers are also neglected. The default mesh is modified to use coarser

spacing in regions with very small gradients, in order to minimize round-off error. In Study 1, the double dogleg nonlinear method is used to help convergence.

See the comments in the section Modeling Instructions for more detailed discussions on the model construction, solution processes, and result visualization.

Results and Discussion

Figure 1 shows the photocurrent as a function of the 780 nm light while keeping the 1300 nm light at a few fixed values, to be compared with Fig. 7(a) in Ref. 1. The qualitative trend of saturation occurring at higher intensity of 780 nm light for higher level of 1300 nm light is well reproduced.

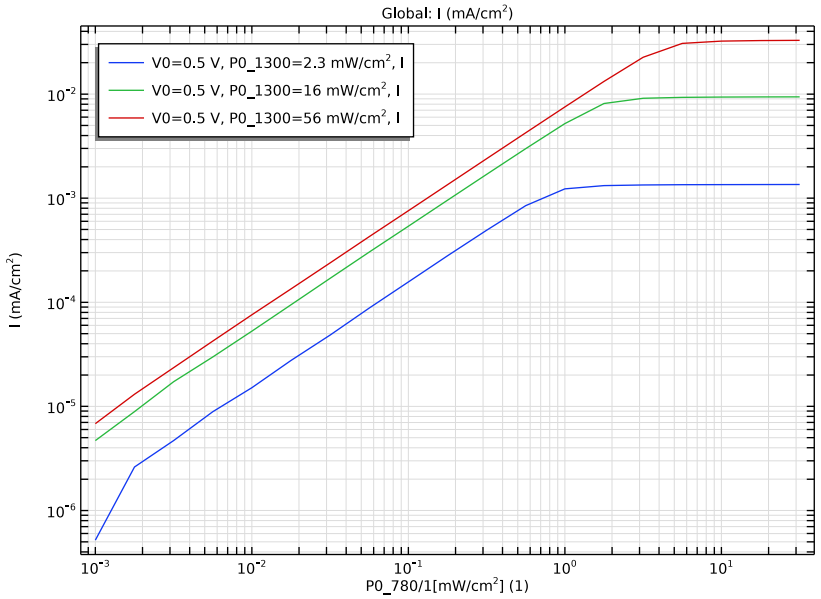


Figure 1: Photocurrent as a function of the 780 nm light while keeping the 1300 nm light at a few fixed values.

Figure 2 plots the occupancy of the QD states corresponding to the conditions shown in Figure 1, to be compared with Fig. 7(b) in Ref. 1. The qualitative trend is also well reproduced.

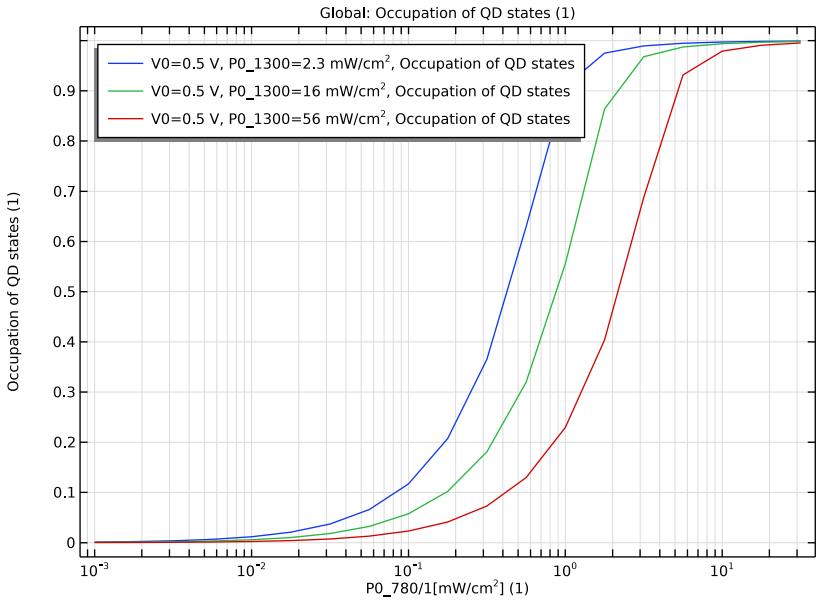


Figure 2: Occupancy of the QD states corresponding to the conditions shown in Figure 1.

Figure 3 shows the photocurrent as a function of the 1300 nm light while keeping the 780 nm light at a few fixed values, to be compared with Fig. 7(c) in Ref. 1. The qualitative trend is also well reproduced.

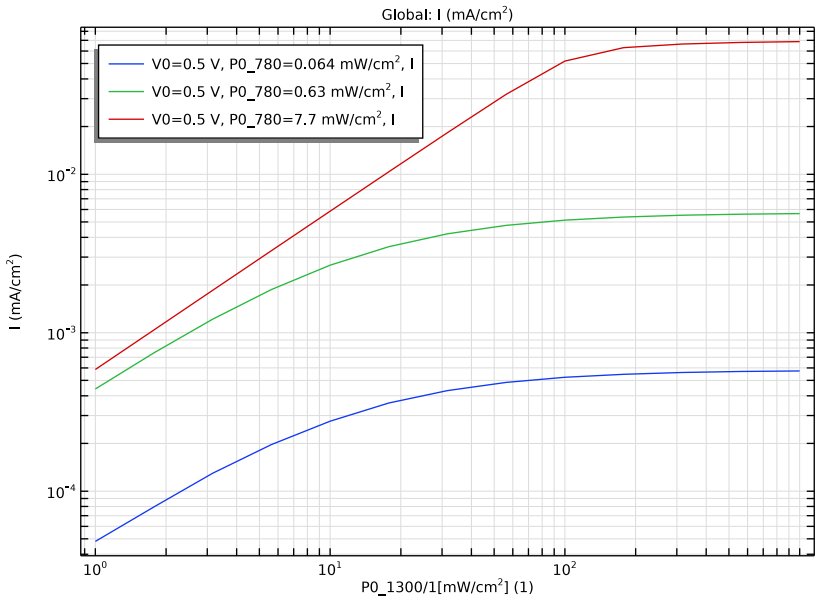


Figure 3: Photocurrent as a function of the 1300 nm light while keeping the 780 nm light at a few fixed values.

Figure 4 plots the occupancy of the QD states corresponding to the conditions shown in Figure 3, to be compared with Fig. 7(d) in Ref. 1. The qualitative trend is also well reproduced.

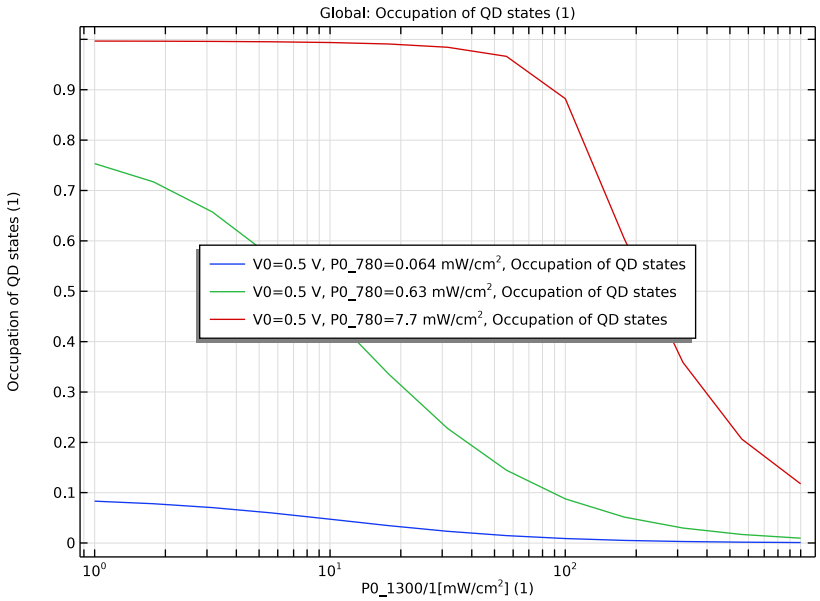


Figure 4: Occupancy of the QD states corresponding to the conditions shown in Figure 3.

References

1. S. Asahi, H. Teranishi, N. Kasamatsu, T. Kada, T. Kaizu and T. Kita, "Saturable Two-Step Photocurrent Generation in Intermediate-Band Solar Cells Including InAs Quantum Dots Embedded in Al$_{0.3}$Ga$_{0.7}$ As/GaAs Quantum Wells," in IEEE Journal of Photovoltaics, vol. 6, no. 2, pp. 465-472, March 2016, doi: 10.1109/JPHOTOV.2015.2504796.

Application Library path: `Semiconductor_Module/Photonic_Devices_and_Sensors/dot_in_well_solar_cell`

From the **File** menu, choose **New**.

NEW

In the **New** window, click **Model Wizard**.

MODEL WIZARD

1. In the **Model Wizard** window, Use 1D geometry to model the dot-in-well solar cell.
2. click **1D**.
3. In the **Select Physics** tree, select **Semiconductor>Semiconductor (semi)**.
4. Click **Add**.
5. Click **Study**.

   It is usually a good practice to start the first study with a **Semiconductor Equilibrium** study step, which is easier to converge and provides a good initial condition for subsequent study steps.
6. In the **Select Study** tree, select **Preset Studies for Selected Physics Interfaces> Semiconductor Equilibrium**.
7. Click **Done**.

GEOMETRY 1

Set the length unit to a convenient one, in this model, nanometer.

1. In the **Model Builder** window, under **Component 1 (comp1)** click **Geometry 1**.
2. In the **Settings** window for **Geometry**, locate the **Units** section.
3. From the **Length unit** list, choose **nm**.

GLOBAL DEFINITIONS

Parameters 1 - Geometry & QW, QD

Enter model parameters in a few Parameters node, first, for the geometry and the quantum well (QW) and quantum dot (QD). Hide these parameters from the Auxiliary sweep parameter drop-down menu.

1. In the **Model Builder** window, under **Global Definitions** click **Parameters 1**.
2. In the **Settings** window for **Parameters**, type `Parameters 1 - Geometry & QW, QD` in the **Label** text field.

3 Click to expand the **Visibility** section. Clear the **Show in parameter selections** check box.

In this example, the QW and QD are modeled as trap levels, to match the simulation approach taken by the authors of the reference paper. Following that approach, where the QW and QD are considered "lumped" energy levels, the trap levels of the QW and QD will have the same spatial extent in this model, given by the parameter `t_well`. The parameter `t_dot` will only be used for optical absorption calculations. The transition from QW to QD is considered unidirectional (no excitation from QD to QW) in the paper. To achieve this effect, an arbitrary large energy gap of 600 meV is used to separate the corresponding trap levels in this model, in the definition of the parameter `DeltaE_dot` Some parameters are not specified in the paper and guess values are used and indicated in the descriptions.

4 Locate the **Parameters** section. In the table, enter the following settings:

Name	Expression	Value	Description
area	1[cm^2]	1E-4 m²	Cross-section area
t_well	16[nm]	1.6E-8 m	Thickness of QW
t_dot	4[nm]	4E-9 m	Effective thickness of QD
t_unit	t_well+50[nm]	6.6E-8 m	Thickness of repeating unit
tau_welltodot	0.3[ns]	3E-10 s	Lifetime of transition from QW to QD
alpha_well	7000[cm^-1]	7E5 1/m	Absorption coefficient of QW
alpha_dot	1000[cm^-1]	1E5 1/m	Absorption coefficient of QD
N_dot	2e10[cm^-2]/ t_well	1.25E22 1/m³	Effective density of QD states
N_well	N_dot*10	1.25E23 1/m³	Guessed density of QW states
tau_thermal	50[ms]	0.05 s	Lifetime of thermal excitation from QW to conduction band
tau_dot	1[ms]	0.001 s	Lifetime of transition from QD to valence band

Name	Expression	Value	Description
tau_well	10[ns]	1E-8 s	Guessed lifetime of transition from QW to valence band
T0	300[K]	300 K	Temperature
Vth	k_B_const*T0/e_const	0.025852 V	Thermal voltage
gD	1	1	Degeneracy factor
DeltaE_well	220[mV]	0.22 V	Effective QW level from conduction band edge
DeltaE_dot	600[mV]+DeltaE_well	0.82 V	Effective QD level from conduction band edge
gamma	1/tau_thermal*gD*exp(DeltaE_well/Vth)	99281 1/s	Guessed transition rate from conduction band to QW

Parameters 2 - Swept

1 In the **Home** toolbar, click Pi **Parameters** and choose **Add>Parameters**.

Enter the parameters that will be used in the Auxiliary sweep.

2 In the **Settings** window for **Parameters**, type `Parameters 2 - Swept` in the **Label** text field.

3 Locate the **Parameters** section. In the table, enter the following settings:

Name	Expression	Value	Description
V0	0[V]	0 V	Bias voltage
P0_780	0[mW/cm^2]	0 W/m²	Input power of 780 nm light
P0_1300	0[mW/cm^2]	0 W/m²	Input power of 1300 nm light

Parameters 3 - Optical

1 In the **Home** toolbar, click Pi **Parameters** and choose **Add>Parameters**.

Enter the parameters for optical transitions and also hide them from the Auxiliary sweep parameter drop-down menu.

2 In the **Settings** window for **Parameters**, type `Parameters 3 - Optical` in the **Label** text field.

3 Locate the **Visibility** section. Clear the **Show in parameter selections** check box.

4 Locate the **Parameters** section. In the table, enter the following settings:

Name	Expression	Value	Description
alpha_780	exp(-alpha_well*t_well)	0.98886	Fraction of 780 nm light remaining after absorption by one QW
hv_780	h_const*c_const/780[nm]	2.5467E-19 J	Energy of a 780 nm photon
P1_780	P0_780/hv_780*(1-0.33)	0 1/(m²·s)	780nm photon flux entering the first QW after 33% of surface reflection
P2_780	P1_780*alpha_780	0 1/(m²·s)	780nm photon flux entering the 2nd QW after absorption by the 1st QW
G1_780	P1_780*(1-alpha_780)/t_well	0 1/(m³·s)	Generation rate in the 1st QW due to 780 nm light
G2_780	P2_780*(1-alpha_780)/t_well	0 1/(m³·s)	Generation rate in the 2nd QW due to 780 nm light
hv_1300	h_const*c_const/1300[nm]	1.528E-19 J	Energy of a 1300 nm photon
P1_1300	P0_1300/hv_1300*(1-0.298)	0 1/(m²·s)	1300 nm photon flux entering the first QD layer after 29.8% of surface reflection

Build the geometry with 2 repeating units of the dot-in-well structure. There are 10 repeating units in the paper. In this model we illustrate the procedure with 2 units. Some of the substrate layers are also neglected for simplicity.

GEOMETRY 1

Interval 1 - Top

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Geometry 1** and choose **Interval**.

2 In the **Settings** window for **Interval**, type `Interval 1 - Top` in the **Label** text field.

3 Locate the **Interval** section. From the **Specify** list, choose **Interval lengths**.

4 In the **Left endpoint** text field, type `-150-540`.

5 In the table, enter the following settings:

Lengths (nm)
150
540

Interval 2 - 1st unit

1 In the **Model Builder** window, right-click **Geometry 1** and choose **Interval**.

2 In the **Settings** window for **Interval**, type `Interval 2 - 1st unit` in the **Label** text field.

3 Locate the **Interval** section. In the table, enter the following settings:

Coordinates (nm)
0
t_well
t_unit

4 Locate the **Selections of Resulting Entities** section. Find the **Cumulative selection** subsection. Click **New**.

5 In the **New Cumulative Selection** dialog box, type `1st unit` in the **Name** text field.

6 Click **OK**.

Array 1 - all units

1 Right-click **Geometry 1** and choose **Transforms>Array**.

2 In the **Settings** window for **Array**, type `Array 1 - all units` in the **Label** text field.

3 Locate the **Input** section. From the **Input objects** list, choose **1st unit**.

4 Locate the **Size** section. In the **Size** text field, type `2`.

5 Locate the **Displacement** section. In the **x** text field, type `t_unit`.

Interval 3 - Bottom

1 Right-click **Geometry 1** and choose **Interval**.

2 In the **Settings** window for **Interval**, type `Interval 3 - Bottom` in the **Label** text field.

3 Locate the **Interval** section. From the **Specify** list, choose **Interval lengths**.

4 In the **Left endpoint** text field, type `2*t_unit`.

5 In the table, enter the following settings:

Lengths (nm)
200
700

6 Click **Build All Objects**.

7 Click the **Zoom Extents** button in the **Graphics** toolbar.

Add AlGaAs material from the built-in library and set the Al mole fraction to 0.3.

ADD MATERIAL

1 In the **Home** toolbar, click **Add Material** to open the **Add Material** window.

2 Go to the **Add Material** window.

3 In the tree, select **Semiconductors>Al(x)Ga(1-x)As - Aluminium Gallium Arsenide**.

4 Click **Add to Component** in the window toolbar.

5 In the **Home** toolbar, click **Add Material** to close the **Add Material** window.

MATERIALS

Al(x)Ga(1-x)As - Aluminium Gallium Arsenide (mat1)

1 In the **Settings** window for **Material**, locate the **Material Contents** section.

2 Find the **Local properties** subsection. In the table, enter the following settings:

Name	Expression	Unit	Description	Property group
x	0.3			Basic

Define domain selections for the QW and QD to be used later.

DEFINITIONS

1st well/dot

1 In the **Definitions** toolbar, click **Explicit**.

2 In the **Settings** window for **Explicit**, type `1st well/dot` in the **Label** text field.

3 Select Domain 3 only.

2nd well/dot

1 In the **Definitions** toolbar, click **Explicit**.

2 In the **Settings** window for **Explicit**, type `2nd well/dot` in the **Label** text field.

3 Select Domain 5 only.

all wells/dots

1 In the **Definitions** toolbar, click **Union**.

2 In the **Settings** window for **Union**, type `all wells/dots` in the **Label** text field.

3 Locate the **Input Entities** section. Under **Selections to add**, click **Add**.

4 In the **Add** dialog box, select **1st well/dot** in the **Selections to add** list.

5 Click **OK**.

6 In the **Settings** window for **Union**, locate the **Input Entities** section.

7 Under **Selections to add**, click **Add**.

8 In the **Add** dialog box, select **2nd well/dot** in the **Selections to add** list.

9 Click **OK**.

Set up doping, metal contacts, and discrete trap energy levels representing the QW and QD. Use the **Transition Between Discrete Levels** feature for the transition from the QW to the QD. Use the "Additional carrier capture rate" option for other transitions. This option is more convenient for arbitrary unidirectional transitions as those adopted in the paper.

SEMICONDUCTOR (SEMI)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Semiconductor (semi)**.

2 In the **Settings** window for **Semiconductor**, locate the **Cross-Section Area** section.

3 In the A text field, type `area`.

Analytic Doping Model 1

1 In the **Physics** toolbar, click **Domains** and choose **Analytic Doping Model**.

2 Select Domain 1 only.

3 In the **Settings** window for **Analytic Doping Model**, locate the **Impurity** section.

4 In the N_{A0} text field, type `2e18[1/cm^3]`.

Analytic Doping Model 2

1 In the **Physics** toolbar, click **Domains** and choose **Analytic Doping Model**.

2 Select Domain 8 only.

3 In the **Settings** window for **Analytic Doping Model**, locate the **Impurity** section.

4 From the **Impurity type** list, choose **Donor doping (n-type)**.

5 In the N_{D0} text field, type `5e16[1/cm^3]`.

Metal Contact 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Metal Contact**.

2 Select Boundary 9 only.

Metal Contact 2

1 In the **Physics** toolbar, click **Boundaries** and choose **Metal Contact**.

2 Select Boundary 1 only.

3 In the **Settings** window for **Metal Contact**, locate the **Terminal** section.

4 In the V_0 text field, type `V0`.

Trap-Assisted Recombination 1

1 In the **Physics** toolbar, click **Domains** and choose **Trap-Assisted Recombination**.

2 In the **Settings** window for **Trap-Assisted Recombination**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **all wells/dots**.

4 Locate the **Trap-Assisted Recombination** section. From the **Trapping model** list, choose **Explicit trap distribution**.

5 Locate the **Trapping** section. Select the **Specify trap species** check box.

Discrete Energy Level - wells

1 In the **Physics** toolbar, click **Attributes** and choose **Discrete Energy Level**.

2 In the **Settings** window for **Discrete Energy Level**, type `Discrete Energy Level - wells` in the **Label** text field.

3 Locate the **Trap Type** section. From the **Trap type** list, choose **Neutral electron traps**.

4 Locate the **Traps** section. In the $N_{t,ne}$ text field, type `N_well`.

5 From the **Impurity energy level** list, choose **From conduction band edge**.

6 In the $E_{t,0}$ text field, type `DeltaE_well`.

7 In the g_D text field, type `gD`.

8 Locate the **Carrier Capture** section. From the **Probability of electron capture** list, choose **User defined**. In the C_n text field, type `0`.

9 From the **Probability of hole capture** list, choose **User defined**. In the C_p text field, type `0`.

Discrete Energy Level - dots

1 Right-click **Discrete Energy Level - wells** and choose **Duplicate**.

2 In the **Settings** window for **Discrete Energy Level**, type `Discrete Energy Level - dots` in the **Label** text field.

3 Locate the **Traps** section. In the $N_{t,ne}$ text field, type `N_dot`.

4 In the $E_{t,0}$ text field, type `DeltaE_dot`.

Before continuing the physics setup, define variables for the QW and QD populations and transition rates. First define two integration operators over the domain of the two QW/QD. Then define 3 sets of variables.

DEFINITIONS

Integration - 1st well/dot

1 In the **Definitions** toolbar, click **Nonlocal Couplings** and choose **Integration**.

2 In the **Settings** window for **Integration**, type `Integration - 1st well/dot` in the **Label** text field.

3 Locate the **Source Selection** section. From the **Selection** list, choose **1st well/dot**.

Integration - 2nd well/dot

1 In the **Definitions** toolbar, click **Nonlocal Couplings** and choose **Integration**.

2 In the **Settings** window for **Integration**, type `Integration - 2nd well/dot` in the **Label** text field.

3 Locate the **Source Selection** section. From the **Selection** list, choose **2nd well/dot**.

Variables - all wells/dots

1 In the **Model Builder** window, right-click **Definitions** and choose **Variables**.

2 In the **Settings** window for **Variables**, type `Variables - all wells/dots` in the **Label** text field.

3 Locate the **Geometric Entity Selection** section. From the **Geometric entity level** list, choose **Domain**.

4 From the **Selection** list, choose **all wells/dots**.

5 Locate the **Variables** section. In the table, enter the following settings:

Name	Expression	Unit	Description
`ft_well`	`semi.tar1.dtd1.ft`		`Occupation of QW`
`ft_dot`	`semi.tar1.dtd2.ft`		`Occupation of QD`
`n_well`	`ft_well*N_well`	1/m³	`Density of occupied QW`
`n_dot`	`ft_dot*N_dot`	1/m³	`Density of occupied QD`

Name	Expression	Unit	Description
alpha1	exp(-alpha_dot* intop1(n_dot)/N_dot* t_dot/t_well)		Fraction of 1300 nm light remaining after absorption by 1st QD
alpha2	exp(-alpha_dot* intop2(n_dot)/N_dot* t_dot/t_well)		Fraction of 1300 nm light remaining after absorption by 2nd QD
P2_1300	P1_1300*alpha1	1/(m²·s)	1300 nm photon flux entering the 2nd QD

Variables - 1st well/dot

1 Right-click **Definitions** and choose **Variables**.

2 In the **Settings** window for **Variables**, type `Variables - 1st well/dot` in the **Label** text field.

3 Locate the **Geometric Entity Selection** section. From the **Geometric entity level** list, choose **Domain**.

4 From the **Selection** list, choose **1st well/dot**.

5 Locate the **Variables** section. In the table, enter the following settings:

Name	Expression	Unit	Description
G_780	G1_780	1/(m³·s)	Generation rate in the 1st QW due to the 780 nm light
G_1300	P1_1300*(1-alpha1)/ t_well	1/(m³·s)	Generation rate in the 1st QD due to the 1300 nm light

Variables - 2nd well/dot

1 Right-click **Definitions** and choose **Variables**.

2 In the **Settings** window for **Variables**, type `Variables - 2nd well/dot` in the **Label** text field.

3 Locate the **Geometric Entity Selection** section. From the **Geometric entity level** list, choose **Domain**.

4 From the **Selection** list, choose **2nd well/dot**.

5 Locate the **Variables** section. In the table, enter the following settings:

Name	Expression	Unit	Description
G_780	G2_780	1/(m³·s)	Generation rate in the 2nd QW due to the 780 nm light
G_1300	P2_1300*(1-alpha2)/t_well	1/(m³·s)	Generation rate in the 2nd QD due to the 1300 nm light

Finish setting up the physics. Be careful about the signs of the additional carrier capture rates: the additional electron capture rate is positive for a transition of an electron from the conduction band to the trap level, and the additional hole capture rate is positive for a transition of an electron from the trap level to the valence band.

SEMICONDUCTOR (SEMI)

Discrete Energy Level - wells

1 In the **Model Builder** window, under **Component 1 (comp1)>Semiconductor (semi)>Trap-Assisted Recombination 1** click **Discrete Energy Level - wells**.

2 In the **Settings** window for **Discrete Energy Level**, click to expand the **Additional Carrier Capture Rate** section.

3 In the $R_{\mathrm{n,extra}}$ text field, type `-n_well/tau_thermal+gamma*semi.N`.

4 In the $R_{\mathrm{p,extra}}$ text field, type `-G_780+n_well/tau_well`.

Discrete Energy Level - dots

1 In the **Model Builder** window, click **Discrete Energy Level - dots**.

2 In the **Settings** window for **Discrete Energy Level**, locate the **Additional Carrier Capture Rate** section.

3 In the $R_{\mathrm{n,extra}}$ text field, type `-G_1300`.

4 In the $R_{\mathrm{p,extra}}$ text field, type `n_dot/tau_dot`.

Trap-Assisted Recombination 1

In the **Model Builder** window, click **Trap-Assisted Recombination 1**.

Transition Between Discrete Levels 1

1 In the **Physics** toolbar, click **Attributes** and choose **Transition Between Discrete Levels**.

2 In the **Settings** window for **Transition Between Discrete Levels**, locate the **Transition Between Discrete Levels** section.

3 From the **Upper level (2)** list, choose **Discrete Energy Level - wells**.

4 From the **Lower level (1)** list, choose **Discrete Energy Level - dots**.

5 In the τ_{21} text field, type `tau_welltodot`.

Modify the default mesh to use coarser spacing in regions with very small gradients, in order to minimize round-off error.

MESH 1

Size

In the **Model Builder** window, under **Component 1 (comp1)** right-click **Mesh 1** and choose **Edit Physics-Induced Sequence**.

Size 1

Select Boundaries 2–8 only.

Size 2

1 Right-click **Component 1 (comp1)>Mesh 1>Size 1** and choose **Duplicate**.

2 Right-click **Size 2** and choose **Move Up**.

3 In the **Settings** window for **Size**, locate the **Geometric Entity Selection** section.

4 From the **Geometric entity level** list, choose **Domain**.

5 Select Domain 8 only.

6 Locate the **Element Size** section. From the **Predefined** list, choose **Extra coarse**.

7 Click **Build All**.

In study 1, ramp up the bias voltage `V0` from 0 to 0.5 V, while keeping the lights off. Sometimes the double dogleg nonlinear method works better than the Newton method.

STUDY 1 - RAMP V0 FROM 0 TO 0.5 V, NO LIGHT

1 In the **Model Builder** window, click **Study 1**.

2 In the **Settings** window for **Study**, type `Study 1 - ramp V0 from 0 to 0.5 V, no light` in the **Label** text field.

Stationary

1 In the **Study** toolbar, click **Study Steps** and choose **Stationary>Stationary**.

2 In the **Settings** window for **Stationary**, click to expand the **Study Extensions** section.

3 Select the **Auxiliary sweep** check box.

4 Click **Add**.

5 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
V0 (Bias voltage)	0 0.1 0.5	V

Solution 1 (sol1)

1 In the **Study** toolbar, click **Show Default Solver**.

2 In the **Model Builder** window, expand the **Solution 1 (sol1)** node.

3 In the **Model Builder** window, expand the **Study 1 - ramp V0 from 0 to 0.5 V, no light> Solver Configurations>Solution 1 (sol1)>Stationary Solver 1** node, then click **Fully Coupled 1**.

4 In the **Settings** window for **Fully Coupled**, click to expand the **Method and Termination** section.

5 From the **Nonlinear method** list, choose **Double dogleg**.

6 Click **Compute**.

Group the plots by study.

RESULTS

Carrier Concentrations (semi), Electric Potential (semi), Energy Levels (semi)

1 In the **Model Builder** window, under **Results**, Ctrl-click to select **Energy Levels (semi)**, **Carrier Concentrations (semi)**, and **Electric Potential (semi)**.

2 Right-click and choose **Group**.

Study 1

In the **Settings** window for **Group**, type `Study 1` in the **Label** text field.

Create a new study to ramp the 780 nm light while keeping the 1300 nm light at a few fixed values. Set the bias voltage at the operating point of 0.5 V, and use the corresponding solution from Study 1 as the initial condition.

ADD STUDY

1 In the **Study** toolbar, click **Add Study** to open the **Add Study** window.

2 Go to the **Add Study** window.

3 Find the **Studies** subsection. In the **Select Study** tree, select **General Studies>Stationary**.

4 Click **Add Study** in the window toolbar.

5 In the **Study** toolbar, click **Add Study** to close the **Add Study** window.

STUDY 2

Step 1: Stationary

1 In the **Settings** window for **Stationary**, locate the **Study Extensions** section.

2 Select the **Auxiliary sweep** check box.

3 From the **Sweep type** list, choose **All combinations**.

4 Click + **Add**.

5 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
V0 (Bias voltage)	`0.5`	V

6 Click + **Add**.

7 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
P0_1300 (Input power of 1300 nm light)	`0 2.3 16 56`	`mW/cm^2`

8 Click + **Add**.

9 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
P0_780 (Input power of 780 nm light)	`10^range(-3,0.25,1.5)`	`mW/cm^2`

10 Click to expand the **Values of Dependent Variables** section. Find the **Initial values of variables solved for** subsection. From the **Settings** list, choose **User controlled**.

11 From the **Method** list, choose **Solution**.

12 From the **Study** list, choose **Study 1 - ramp V0 from 0 to 0.5 V, no light, Stationary**.

13 From the **Parameter value (V0 (V))** list, choose **0.5 V**.

14 In the **Model Builder** window, click **Study 2**.

15 In the **Settings** window for **Study**, type `Study 2 - ramp P_780` in the **Label** text field.

16 In the **Study** toolbar, click = **Compute**.

Group the plots by study. Create plots to compare with Fig. 7 (a) and (b) in the reference paper. The qualitative trend of the photo current and the occupation of QD states is well

reproduced. (The current density with P_1300 off is visually much smaller than any of the values with P_1300 on. Therefore plotting those values "I" is sufficient, even though the paper plots the difference "Delta I".)

RESULTS

Carrier Concentrations (semi) 1, Electric Potential (semi) 1, Energy Levels (semi) 1

1. In the **Model Builder** window, under **Results**, Ctrl-click to select **Energy Levels (semi) 1**, **Carrier Concentrations (semi) 1**, and **Electric Potential (semi) 1**.
2. Right-click and choose **Group**.

Study 2

In the **Settings** window for **Group**, type `Study 2` in the **Label** text field.

I vs. P_780 (Fig. 7a)

1. In the **Home** toolbar, click  **Add Plot Group** and choose **1D Plot Group**.
2. In the **Settings** window for **1D Plot Group**, type `I vs. P_780 (Fig. 7a)` in the **Label** text field.
3. Locate the **Data** section. From the **Dataset** list, choose **Study 2 - ramp P_780/ Solution 3 (sol3)**.
4. From the **Parameter selection (P0_1300)** list, choose **Manual**.
5. In the **Parameter indices (1-4)** text field, type `2 3 4`.
6. Locate the **Axis** section. Select the **x-axis log scale** check box.
7. Select the **y-axis log scale** check box.
8. Locate the **Legend** section. From the **Position** list, choose **Upper left**.

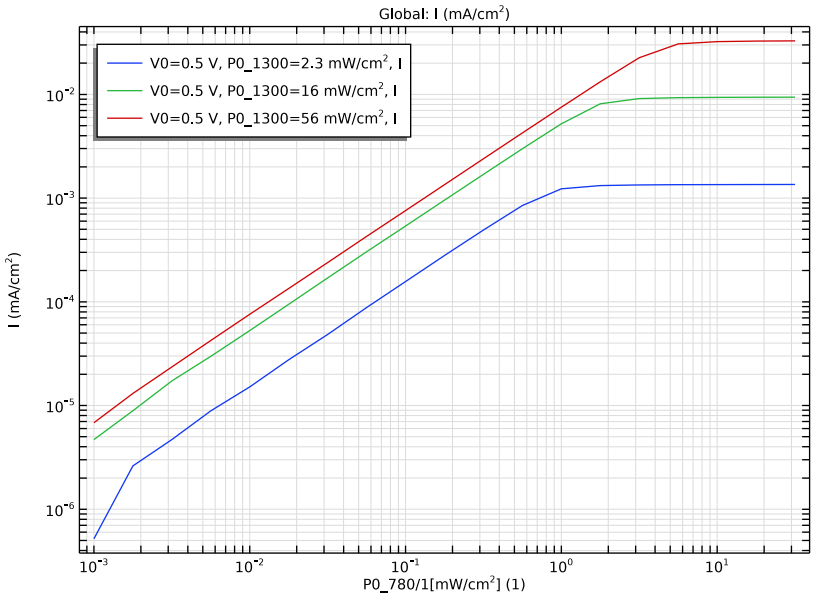
Global 1

1. In the **I vs. P_780 (Fig. 7a)** toolbar, click  **Global**.
2. In the **Settings** window for **Global**, locate the **y-Axis Data** section.
3. In the table, enter the following settings:

Expression	Unit	Description
`semi.IO_1/area`	`mA/cm^2`	`I`

4. Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.
5. In the **Expression** text field, type `P0_780/1[mW/cm^2]`.

6 In the **I vs. P_780 (Fig. 7a)** toolbar, click **Plot**.



ft_dot vs. P_780 (Fig. 7b)

1 In the **Model Builder** window, right-click **I vs. P_780 (Fig. 7a)** and choose **Duplicate**.

2 In the **Settings** window for **1D Plot Group**, type `ft_dot vs. P_780 (Fig. 7b)` in the **Label** text field.

3 Locate the **Axis** section. Clear the **y-axis log scale** check box.

Global I

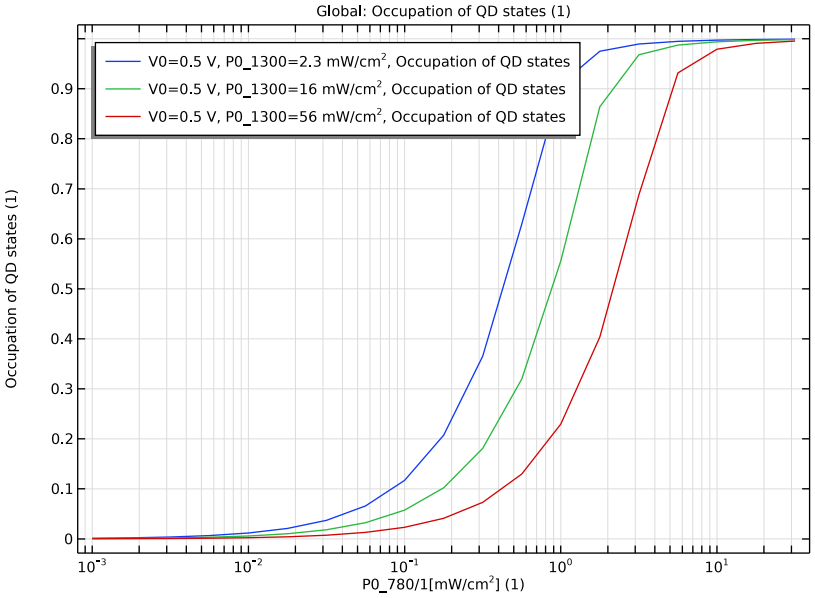
1 In the **Model Builder** window, expand the **ft_dot vs. P_780 (Fig. 7b)** node, then click **Global I**.

2 In the **Settings** window for **Global**, locate the **y-Axis Data** section.

3 In the table, enter the following settings:

Expression	Unit	Description
`intop1(ft_dot)/t_well`	1	`Occupation of QD states`

4 In the **ft_dot vs. P_780 (Fig. 7b)** toolbar, click **Plot**.



Create another new study to ramp the 1300 nm light while keeping the 780 nm light at a few fixed values. Set the bias voltage at the operating point of 0.5 V, and use the corresponding solution from Study 1 as the initial condition.

ADD STUDY

1 In the **Home** toolbar, click **Add Study** to open the **Add Study** window.

2 Go to the **Add Study** window.

3 Find the **Studies** subsection. In the **Select Study** tree, select **Empty Study**.

4 Click **Add Study** in the window toolbar.

5 In the **Home** toolbar, click **Add Study** to close the **Add Study** window.

STUDY 2 - RAMP P_780

Step 1: Stationary

In the **Model Builder** window, under **Study 2 - ramp P_780** right-click **Step 1: Stationary** and choose **Copy**.

STUDY 3 - RAMP P_1300

1 In the **Model Builder** window, click **Study 3**.

2 In the **Settings** window for **Study**, type `Study 3 - ramp P_1300` in the **Label** text field.

3 Right-click **Study 3 - ramp P_1300** and choose **Paste Stationary**.

Step 1: Stationary

1 In the **Settings** window for **Stationary**, locate the **Study Extensions** section.

2 In the table, click to select the cell at row number 3 and column number 2.

3 Click **Move Up**.

4 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
P0_780 (Input power of 780 nm light)	`0.064 0.63 7.7`	`mW/cm^2`
P0_1300 (Input power of 1300 nm light)	`10^range(0,0.25,3)`	`mW/cm^2`

5 In the **Home** toolbar, click **Compute**.

Group the plots by study. Create plots to compare with Fig. 7 (c) and (d) in the reference paper. The qualitative trend of the photo current and the occupation of QD states is well reproduced.

RESULTS

Carrier Concentrations (semi) 2, Electric Potential (semi) 2, Energy Levels (semi) 2

1 In the **Model Builder** window, under **Results**, Ctrl-click to select **Energy Levels (semi) 2**, **Carrier Concentrations (semi) 2**, and **Electric Potential (semi) 2**.

2 Right-click and choose **Group**.

Study 3

In the **Settings** window for **Group**, type `Study 3` in the **Label** text field.

I vs. P_780 (Fig. 7a)

In the **Model Builder** window, under **Results>Study 2** right-click **I vs. P_780 (Fig. 7a)** and choose **Copy**.

I vs. P_1300 (Fig. 7c)

1 In the **Model Builder** window, right-click **Study 3** and choose **Paste 1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, type `I vs. P_1300 (Fig. 7c)` in the **Label** text field.

3 Locate the **Data** section. From the **Parameter selection (P0_1300)** list, choose **All**.

4 From the **Dataset** list, choose **Study 3 - ramp P_1300/Solution 4 (sol4)**.

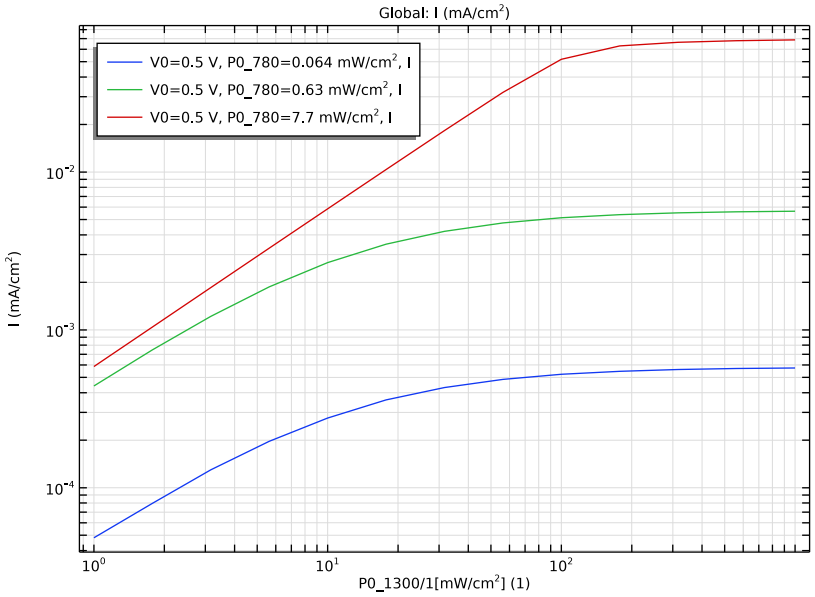
Global 1

1 In the **Model Builder** window, expand the **I vs. P_1300 (Fig. 7c)** node, then click **Global 1**.

2 In the **Settings** window for **Global**, locate the **x-Axis Data** section.

3 In the **Expression** text field, type `P0_1300/1[mW/cm^2]`.

4 In the **I vs. P_1300 (Fig. 7c)** toolbar, click **Plot**.



ft_dot vs. P_780 (Fig. 7b)

In the **Model Builder** window, under **Results>Study 2** right-click **ft_dot vs. P_780 (Fig. 7b)** and choose **Copy**.

ft_dot vs. P_1300 (Fig. 7d)

1 In the **Model Builder** window, right-click **Study 3** and choose **Paste 1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, type `ft_dot vs. P_1300 (Fig. 7d)` in the **Label** text field.

3 Locate the **Data** section. From the **Parameter selection (P0_1300)** list, choose **All**.

4 From the **Dataset** list, choose **Study 3 - ramp P_1300/Solution 4 (sol4)**.

5 Locate the **Legend** section. From the **Position** list, choose **Center**.

Global 1

1 In the **Model Builder** window, expand the **ft_dot vs. P_1300 (Fig. 7d)** node, then click **Global 1**.

2 In the **Settings** window for **Global**, locate the **x-Axis Data** section.

3 In the **Expression** text field, type `P0_1300/1[mW/cm^2]`.

4 In the **ft_dot vs. P_1300 (Fig. 7d)** toolbar, click **Plot**.