SRI VENKATESWARA INTERNSHIP PROGRAM
FOR RESEARCH IN ACADEMICS
(SRI-VIPRA)
Student Internship

SRI-VIPRA

Project Report of 2025: SVP-2521

"Polymer Composites for Photo-Voltaic Application"

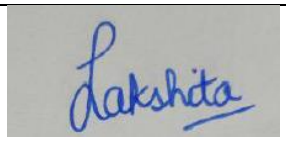
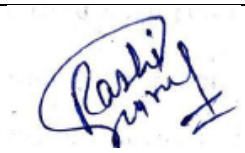
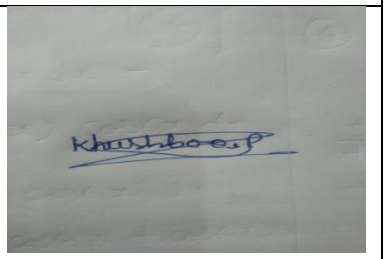
IQAC
Sri Venkateswara College
University of Delhi
Benito Juarez Road, Dhaula Kuan, New Delhi
New Delhi -110021

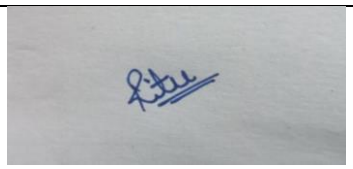
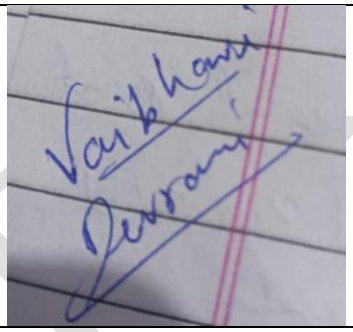
SRIVIPRA PROJECT 2025

Title : Polymer Composites for Photo-Voltaic Application

Name of Mentor: Dr. Vinita Kapoor **Name of Department: Chemistry** **Designation: Assistant Professor**	
Name of Mentor: Dr. Rakhi Narang **Name of Department: Electronics** **Designation: Assistant Professor**	

List of students under the SRIVIPRA Project

S.No	Photo	Name of the student	Roll number	Course	Signature
1		Lakshita	1623049	BSc (H) Electronics	
2		Rashi Sharma	1623055	BSc (H) Electronics	
3		Khushboo Pal	1623036	BSc (H) Electronics	

4		Ritu Rawat	1623024	BSc (H) Electronics	
5		Vaibhavi Devrani	1623054	BSc (H) Electronics	

Signature of Mentor

Certificate of Originality

This is to certify that the aforementioned students from Sri Venkateswara College have participated in the summer project SVP-2521 titled "Polymer Composites for Photo-Voltaic Application**"**.The participants have carried out the research project work under my guidance and supervision from 1st July, 2025 to 30th September 2025. The work carried out is original and carried out in an online/offline/hybrid mode.

Signature of Mentor

TABLE OF CONTENTS

S.No	Topic	Page No.
	Introduction	5
	Photovoltaic (PV) Cells	5
	Types of Photovoltaic Cells	5
	Organic Solar Cells	5
	Polyaniline (PANI)	5
	Advantages and Challenges	6
	Semiconductor Device Simulation using Silvaco TCAD (NanoHub)	7
	Conclusion	24

Introduction:

As the world is shifting towards renewable resources, and solar energy is one of the finest sources. Renewable resources are essential for obtaining sustainable development for growth of society. Solar energy is affordable and abundant renewable resource. It uses sun's power to generate electricity through photovoltaic cells or solar thermal systems.

Photovoltaic (PV) Cells:

Photovoltaic cells are the building blocks of solar panels. It is a device that converts solar energy into electrical energy through the photovoltaic effect. When electrons hit the cell, it excites electrons, exciting electric currents. This device is made up of semiconductor materials that can be organic and inorganic.

Types of Photovoltaic Cells:

- Monocrystalline Silicon Cells
- Polycrystalline Silicon Cells
- Thin-Film Solar Cells
- Perovskite Solar Cells
- Organic Photovoltaic (OPV) Cells

Organic Solar Cells:

Organic Solar Cells or Organic Photovoltaic cells (OPVs) are a type of solar cells that uses organic materials for converting solar energy to electric energy. Organic materials include carbon compounds, polymers etc.

Polyaniline (PANI):

Sustainable energy sources are becoming more and more popular worldwide, which has raised interest in renewable technologies like solar energy conversion. A lightweight, flexible, and possibly affordable substitute for conventional silicon-based solar cells is organic photovoltaic, or OPPs. Of the different materials Polyaniline stands out among the examined compounds because of its special blend of stability, electrical conductivity, and manufacturing simplicity. It is an organic polymer that conducts electricity and has numerous uses.

Advantages and Challenges

Advantages of OPVs (like PANI-based ones):

- Lightweight and flexible
- Low cost production
- Less energy used in manufacturing

Challenges:

- Lower efficiency as compared to silicon based OPV
- Not stable
- Mass production is difficult
- High purity of organic material is challenging

Semiconductor Device Simulation using Silvaco TCAD (NanoHub)

Objective

The main goal of this project is to design, simulate, and analyze semiconductor devices using the Silvaco TCAD toolset on the NanoHub platform. The work focuses on two devices:
1. Diode
2. Two-Junction PN Structure (PNPN device)

The simulations were executed in DeckBuild using the 'go victory device' command, and the results were observed in Visual through plots of current–voltage (I–V) characteristics.

Tools and Platform

- Platform: NanoHub.org
- Software Used: Silvaco TCAD
- Modules:
  - DeckBuild – for creating and running .in files
  - Victory Device – for physical device simulation
  - Visual – for viewing structures and electrical characteristics
- Command Used:
  go victory device
- File Type: .in (input deck files)

Device 1 – Diode

Theoretical Background

A diode is a two-terminal semiconductor device formed by joining P-type and N-type regions. When forward biased, charge carriers diffuse across the junction, resulting in current flow. In reverse bias, the depletion region widens, preventing current flow except for a small leakage current. The ideal diode equation is:

$I = I_0 (\exp(qV/kT) - 1)$

where I_0 is saturation current, q is electron charge, V is applied voltage, k is Boltzmann constant, and T is absolute temperature.

Simulation Steps

1. Open DeckBuild in NanoHub and write the input code.
2. Begin with: go victory device
3. Define material as silicon.
4. Create regions for P and N doping.
5. Set doping concentrations and mesh grid.
6. Define electrical contacts.
7. Perform bias sweep analysis to extract I–V characteristics.
8. Visualize the results using Visual.

Silvaco Tcad Simulations:

1) Photodiode

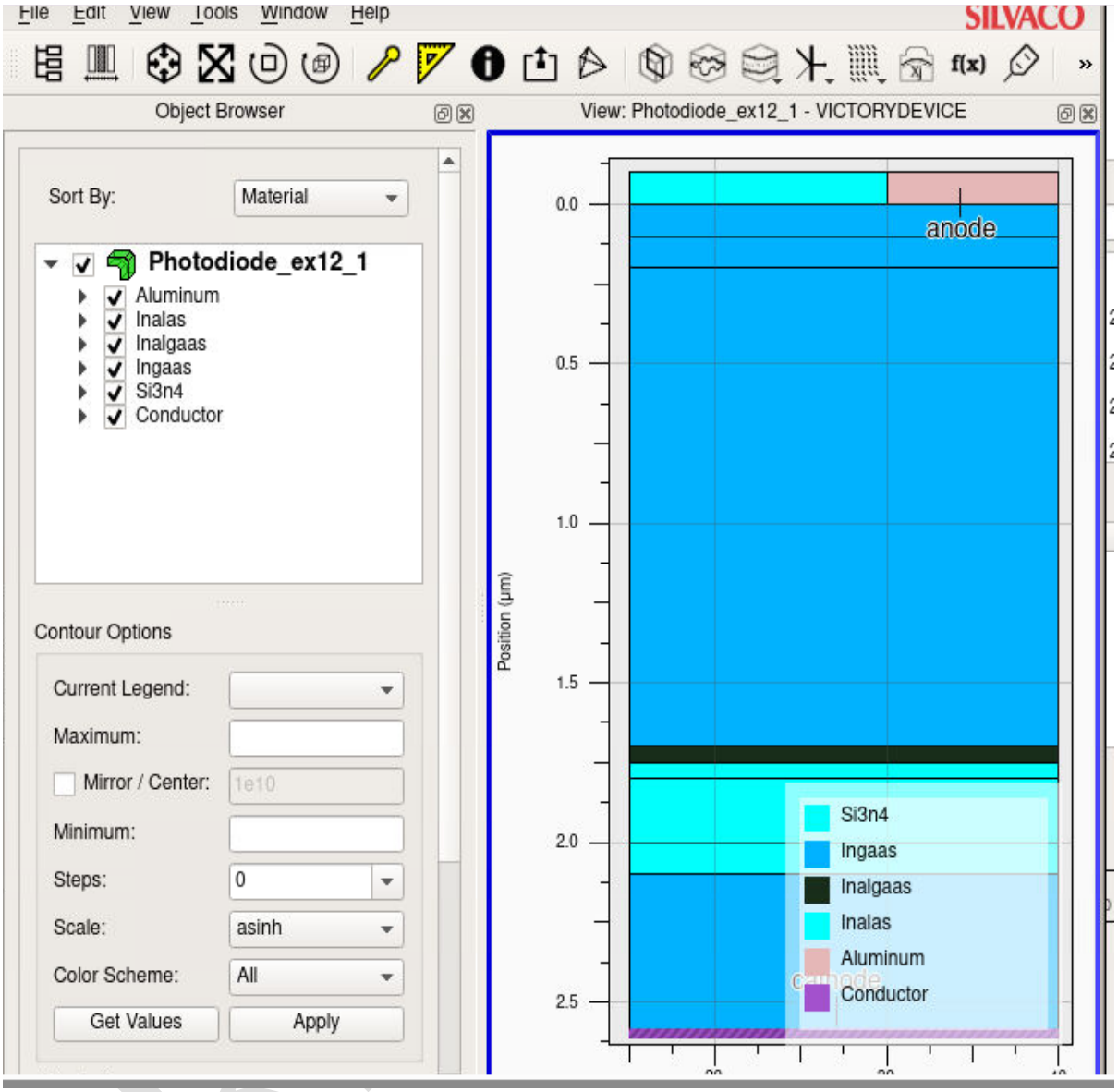
```
####### DEVICE SIMULATION #######
GO victorydevice simflags="-P 4"

#### STRUCTURE SPECIFICATION ####
MESH cylindr ^diag.flip

#x-mesh
X.MESH location=15 spacing=5
X.MESH location=30 spacing=5
X.MESH location=40 spacing=5

#y-mesh
Y.MESH location=-0.1 spacing=0.05
Y.MESH location=0 spacing=0.025
Y.MESH location=0.05 spacing=0.02
Y.MESH location=0.1 spacing=0.005
Y.MESH location=0.15 spacing=0.01
Y.MESH location=0.2 spacing=0.005
Y.MESH location=0.95 spacing=0.2
Y.MESH location=1.7 spacing=0.002
Y.MESH location=1.725 spacing=0.01
Y.MESH location=1.75 spacing=0.002
Y.MESH location=1.775 spacing=0.01
Y.MESH location=1.8 spacing=0.002
Y.MESH location=1.9 spacing=0.03
Y.MESH location=2 spacing=0.005
Y.MESH location=1.95 spacing=0.04
Y.MESH location=2.1 spacing=0.005
Y.MESH location=2.6 spacing=0.1
```

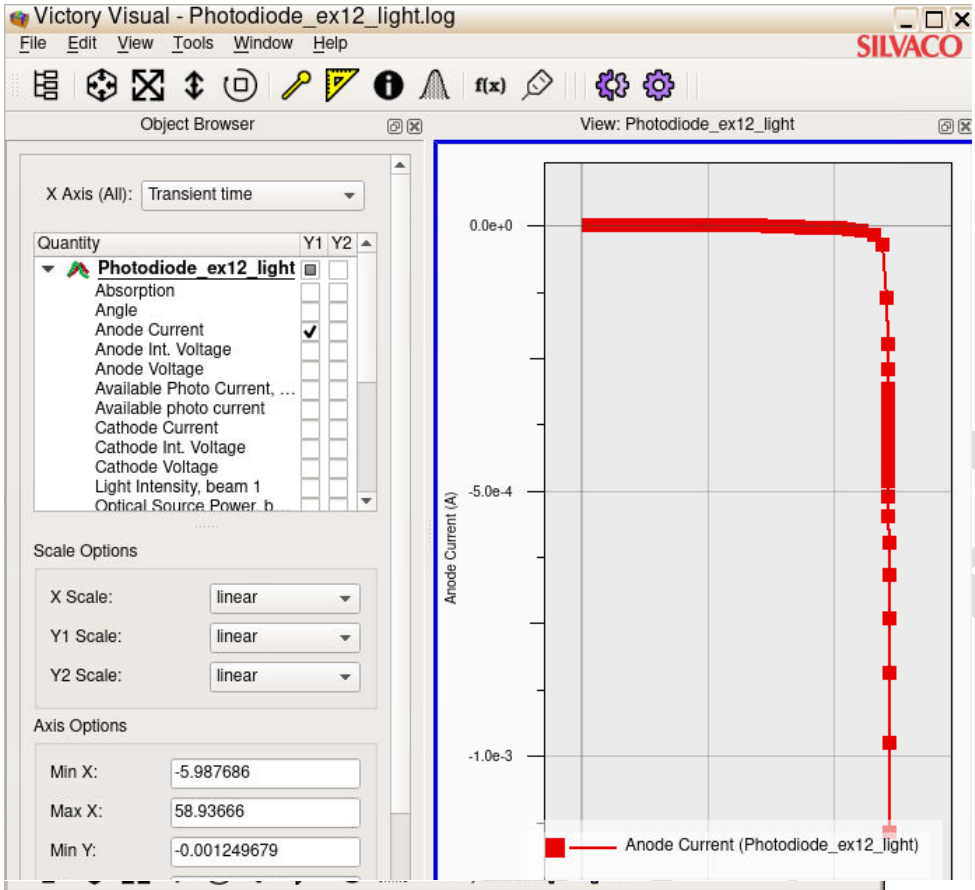
```
REGION num=1 material=nitride

#In(1-x)Ga(x)As In0.53Ga0.47As
REGION num=2 material=InGaAs x.comp=0.47 x.min=0 \
 x.max=40 y.min=0 y.max=0.1 name=pcontact

REGION num=3 material=InGaAs x.comp=0.47 x.min=0 \
 x.max=40 y.min=0.1 y.max=0.2 name=pclad

REGION num=4 material=InGaAs x.comp=0.47 x.min=0 \
 x.max=40 y.min=0.2 y.max=1.7 name=absorb

#Al0.22Ga0.25In0.52As -> In(1-x-y)Al(x)Ga(y)As
REGION num=5 material=InAlGaAs x.comp=0.22 y.comp=0.25 x.min=0 x.max=40 \
        y.min=1.7 y.max=1.75 name=grad

#Al0.48In0.52As -> In(1-x)Al(x)As
REGION num=6 material=InAlAs x.comp=0.48 name=charge x.min=0 x.max=40 \
        y.min=1.75 y.max=1.8

REGION num=7 material=InAlAs x.comp=0.48 name=mult x.min=0 x.max=40 \
        y.min=1.8 y.max=2

REGION num=8 material=InAlAs x.comp=0.48 x.min=0 x.max=40 y.min=2 \
        y.max=2.1 name=nclad

REGION num=9 material=InGaAs x.comp=0.47 y.min=2.1 \
        y.max=2.6 name=ncontact
ELECTRODE num=1 name=anode x.min=30 x.max=40 y.min=-0.1 y.max=0 material=Aluminum
ELECTRODE num=2 name=cathode bottom

DOPING region=2 uniform p.type conc=2e19

DOPING region=3 uniform p.type conc=5e18

# absorb i-1.5um
DOPING region=4 uniform p.type conc=5e14

DOPING region=5 uniform p.type conc=1e17*3.03

#crfitical DOPING layer: charge fixed
DOPING region=6 uniform p.type conc=6.2e17

#Mult layer
DOPING region=7 uniform n.type conc=3e16

DOPING region=8 uniform n.type conc=1e19

DOPING region=9 uniform n.type conc=2e19

#### MATERIAL/PHYSICAL MODELS ####
INTERFACE s.s thermionic

MODELS material=InAlGaAs cubic35

MATERIAL material=InGaAs taun0=100e-9 taup0=100e-9 mun0=11000 mup0=110 \
        m.vthn=0.042 m.vthp=0.46 affinity=4.5 permit=13.9 eg300=0.85
```

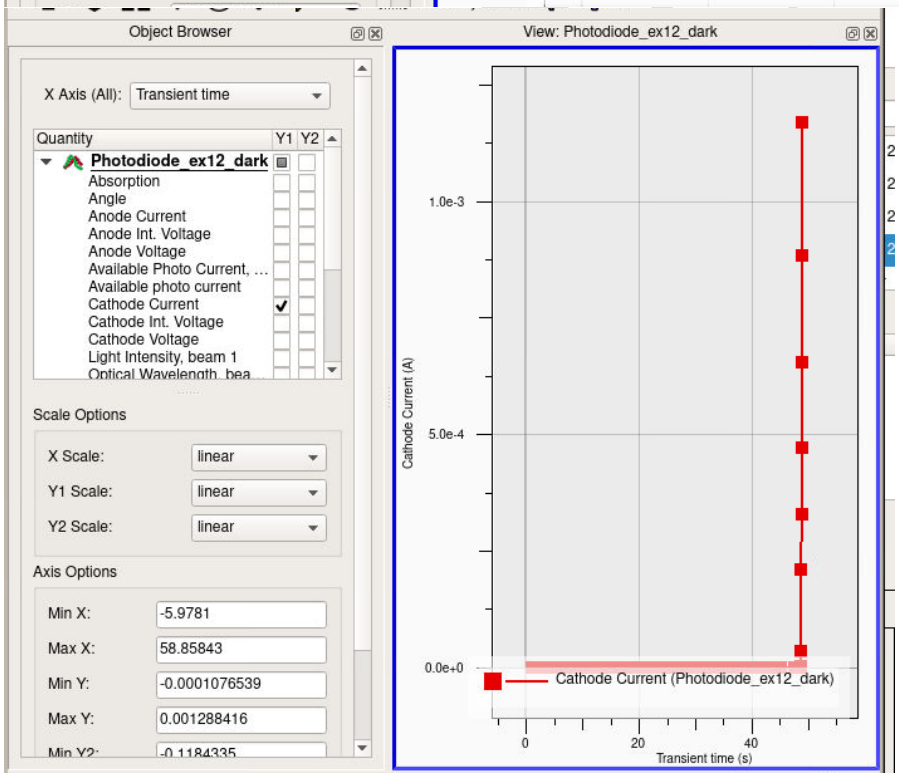
```
MATERIAL material=InAlAs taun0=1e-11 taup0=1e-11 mun0=4500 mup0=45 \
         m.vthn=0.085 m.vthp=0.6 affinity=4.25 permit=12.2 eg300=1.2 \

MATERIAL material=InAlGaAs mun0=2300 mup0=23 taun0=1e-11 taup0=1e-11 \
        m.vthn=0.06 m.vthp=0.61 affinity=4.38 permit=12.5 eg300=1.2

MATERIAL name=clad vsatn=1.5e7 vsatp=1.5e7
MATERIAL name=charge vsatn=2.5e6 vsatp=2.5e6
MATERIAL name=mult vsatn=1e7 vsatp=1e7
MATERIAL name=absorb vsatn=1.5e7 vsatp=1.5e7
MATERIAL name=pcontact vsatn=1.5e7 vsatp=1.5e7
MATERIAL name=ncontact vsatn=1.5e7 vsatp=1.5e7

MATERIAL material=InGaAs augn=1e-31 augp=1e-31 copt=2e-9
MATERIAL material=InAlGaAs augn=1e-29 augp=1e-29 copt=2e-7
MATERIAL material=InAlAs augn=1e-28 augp=1e-28 copt=2e-6

MATERIAL material=InGaAs indx.imag=In0.53GaAs_k.dat

MODELS srh fermi fldmob print auger optr

MODELS material=InAlGaAs cubic35

IMPACT selb an1=8.6e6 ap1=2.3e7 bn1=3.5e6*1 bp1=4.5e6*1 betan=1 betap=1 \
        an2=8.6e6 ap2=2.3e7 bn2=3.5e6*1 bp2=4.5e6*1 egran=1e4

OUTPUT con.band val.band band.param

BEAM num=1 x.orig=15 y.orig=-2 angle=90 orient.xz.y wavelength=1.55 \
```

```
IMPACT selb an1=8.6e6 ap1=2.3e7 bn1=3.5e6*1 bp1=4.5e6*1 betan=1 betap=1 \
        an2=8.6e6 ap2=2.3e7 bn2=3.5e6*1 bp2=4.5e6*1 egran=1e4

OUTPUT con.band val.band band.param

BEAM num=1 x.orig=15 y.orig=-2 angle=90 orient.xz.y wavelength=1.55 \
        reflect=4 rays=20 raytrace=$'name'_1.str \
         back.refl front.refl xmin=0 xmax=15

PROBE name=field x=25 y=0.01 field

#### NUMERICAL METHODS ####
METHOD pas climit=1e-4 dt.max=10 itlimit=40 tstep.incr=1.25

#### SOLUTION SOLVING ####
# dark IV
SOLVE init

SAVE outf=$'name'_Init_dark.str

SOLVE vanode=0 ramptime=1e-9 tstop=1 dt=1e-11

LOG outfile=$'name'_dark.log
SOLVE vanode=-50 ramptime=1e2 tstop=1e3 dt=1e-1 compl=-1e-3 cname=anode
LOG off

# light IV
SOLVE init
```

```
set r=15e-4
set area=3.141592*$r*$r
SOLVE b1=1e-9
SOLVE b1=1e-6
SOLVE b1=1e-6/($area)*0.5

SAVE outf=$'name'_Init_light.str

SOLVE vanode=0 ramptime=1e-9 tstop=1 dt=1e-11

LOG outfile=$'name'_light.log
SOLVE vanode=-50 ramptime=1e2 tstop=1e2 dt=1e-1 compl=-1e-3 cname=anode
LOG off

GO victoryextract
LOAD in="$'name'_dark.log"
CURVE name=curve x="Anode Voltage" y="abs(Anode Current)"
EXTRACT.CSV csvfile="$'name'_dark"
LOAD in="$'name'_light.log"
CURVE name=curve x="Anode Voltage" y="abs(Anode Current)"
EXTRACT.CSV csvfile="$'name'_light"

victoryvisual -V 1.8.3.C \
$'name'_dark.csv:$'name'_csv.set+\
dark_exp.csv:$'name'_csv.set+\
$'name'_light.csv:$'name'_csv.set+\
light_exp.csv:$'name'_csv.set

QUIT
```


File Edit View Tools Window Help
SILVACO
Object Browser
View: Photodiode_ex12_1 - VICTORYDEVICE
Sort By:
Material
Photodiode_ex12_1
Aluminum
Inalas
Inalgaas
Ingaas
Si3n4
Conductor
Contour Options
Current Legend:
Maximum:
Mirror / Center:
1e10
Minimum:
Steps:
0
Scale:
asinh
Color Scheme:
All
Get Values
Apply
anode
cathode
Position (μm)
0.0
0.5
1.0
1.5
2.0
2.5
Si3n4
Ingaas
Inalgaas
Inalas
Aluminum
Conductor

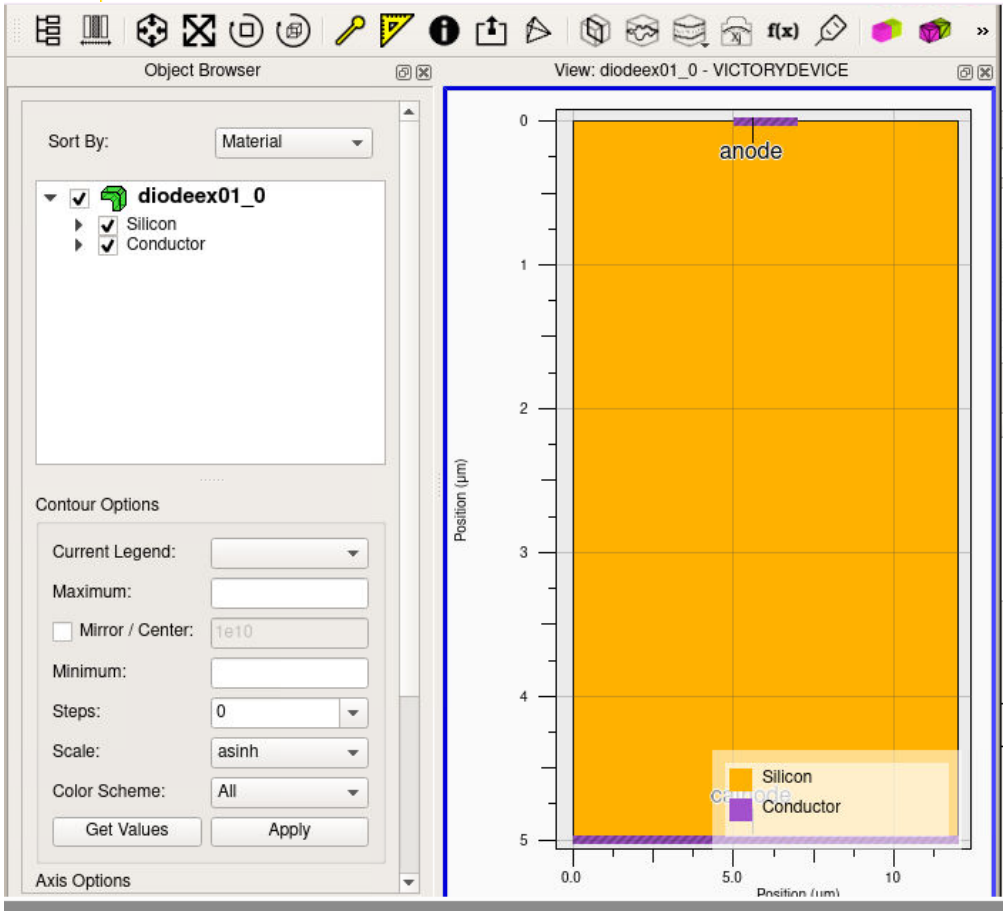

Victory Visual - Photodiode_ex12_light.log
File Edit View Tools Window Help
SILVACO
Object Browser
View: Photodiode_ex12_light
X Axis (All): Transient time
Quantity Y1 Y2
Photodiode_ex12_light
Absorption
Angle
Anode Current
Anode Int. Voltage
Anode Voltage
Available Photo Current, ...
Available photo current
Cathode Current
Cathode Int. Voltage
Cathode Voltage
Light Intensity, beam 1
Optical Source Power, b...
Scale Options
X Scale: linear
Y1 Scale: linear
Y2 Scale: linear
Axis Options
Min X: -5.987686
Max X: 58.93666
Min Y: -0.001249679
0.0e+0
-5.0e-4
-1.0e-3
Anode Current (A)
Anode Current (Photodiode_ex12_light)

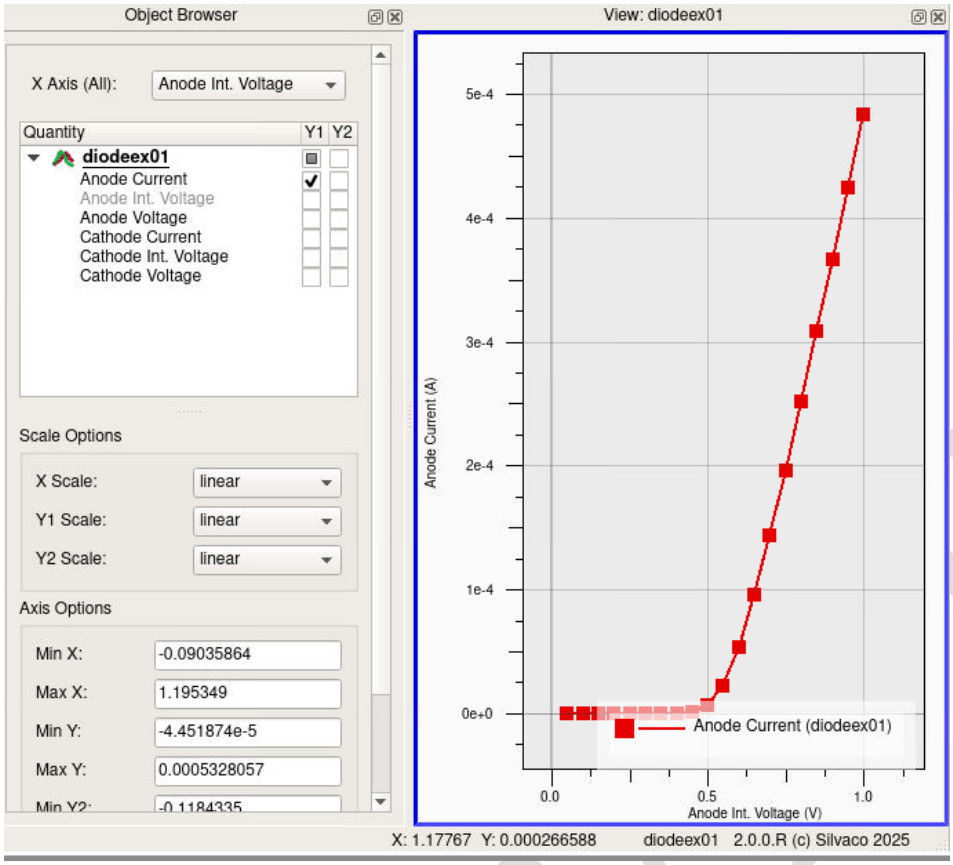

Object Browser
View: Photodiode_ex12_dark
X Axis (All): Transient time
Quantity Y1 Y2
Photodiode_ex12_dark
Absorption
Angle
Anode Current
Anode Int. Voltage
Anode Voltage
Available Photo Current, ...
Available photo current
Cathode Current
Cathode Int. Voltage
Cathode Voltage
Light Intensity, beam 1
Optical Wavelength, bea...
Scale Options
X Scale: linear
Y1 Scale: linear
Y2 Scale: linear
Axis Options
Min X: -5.9781
Max X: 58.85843
Min Y: -0.0001076539
Max Y: 0.001288416
Min Y2: -0.1184335
1.0e-3
5.0e-4
0.0e+0
Cathode Current (A)
0
20
40
Transient time (s)
Cathode Current (Photodiode_ex12_dark)

2) Normal Diode:

```
# (c) Silvaco Inc., 2019
GO victorydevice simflags="-P 4"

mesh  space.mult=1.0
#
x.mesh loc=0.00 spac=0.5
x.mesh loc=3.00 spac=0.2
x.mesh loc=5.00 spac=0.25
x.mesh loc=7.00 spac=0.25
x.mesh loc=9.00 spac=0.2
x.mesh loc=12.00 spac=0.5
#
y.mesh loc=0.00 spac=0.1
y.mesh loc=1.00 spac=0.1
y.mesh loc=2.00 spac=0.2
y.mesh loc=5.00 spac=0.4


region  num=1  silicon

electr  name=anode  x.min=5  length=2
electr  name=cathode  bot

#....   N-epi doping
doping  n.type conc=5.e16 uniform

#....   Guardring doping
doping   p.type conc=1e19 x.min=0  x.max=3  junc=1 rat=0.6 gauss
doping   p.type conc=1e19 x.min=9 x.max=12 junc=1 rat=0.6 gauss
```

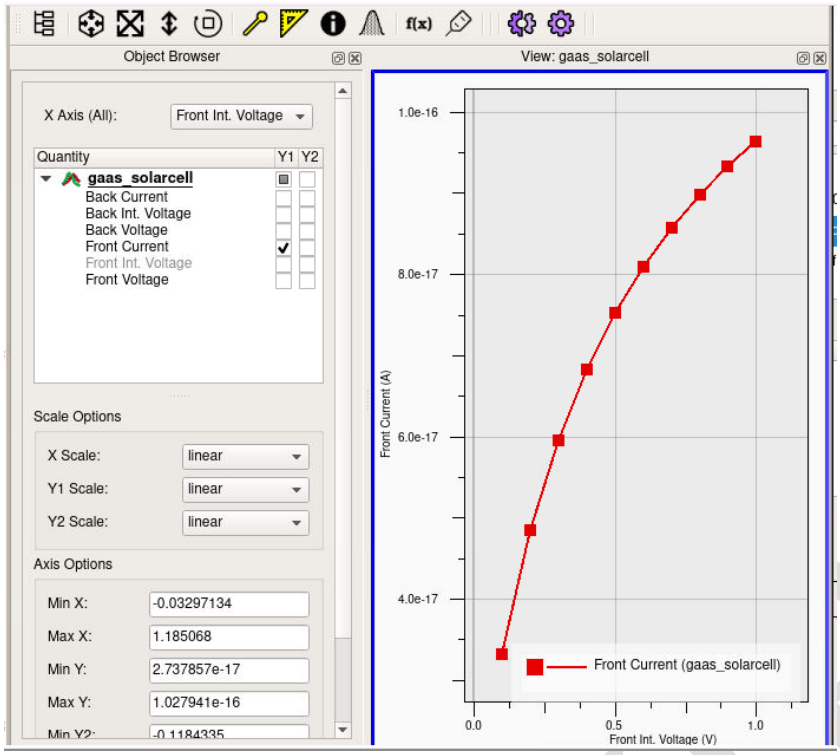
```
#....   N+ doping
doping  n.type conc=1e20 x.min=0 x.max=12 y.top=2 y.bottom=5 uniform

save outf=diodeex01_0.str



model    conmob  fldmob  srh  auger  bgn
contact    name=anode workf=4.97

solve      init

method newton

log   outfile=diodeex01.log
solve      vanode=0.05  vstep=0.05  vfinal=1  name=anode

quit
```

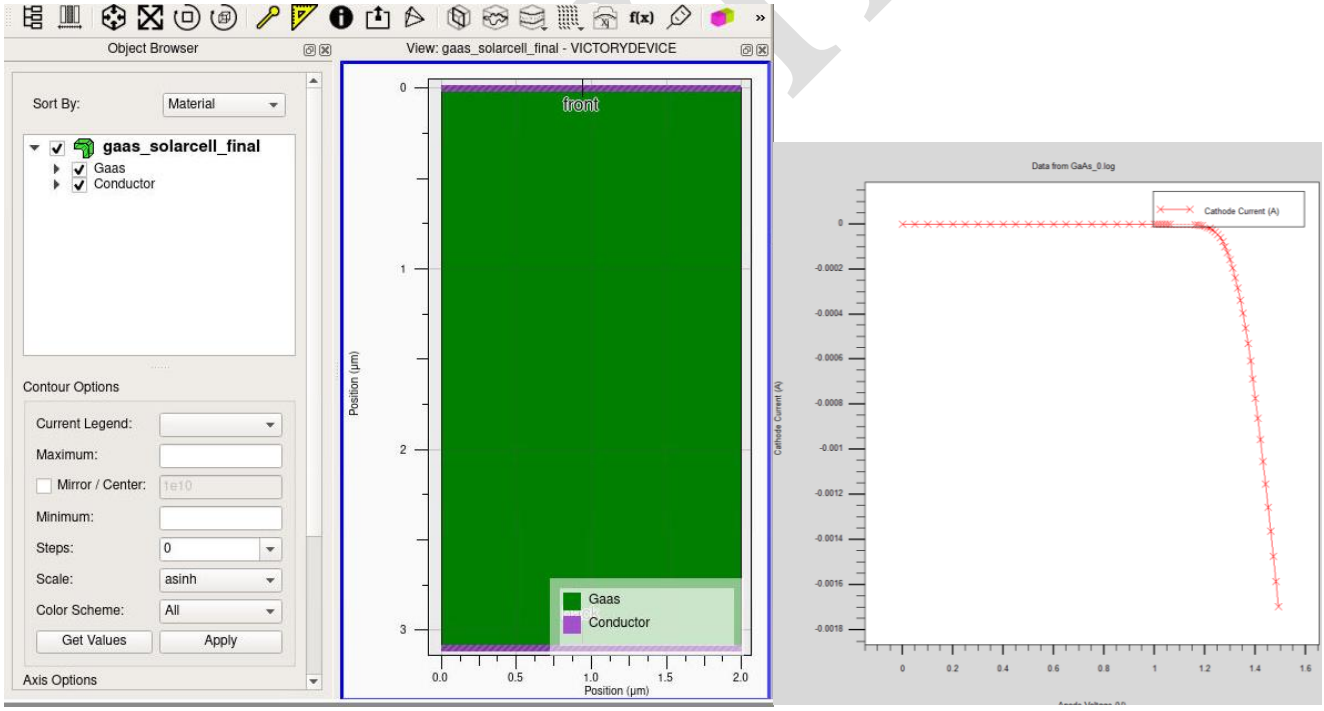




3) GaAs Cell

```
# (c) Silvaco Inc., 2019
GO victorydevice simflags="-P 4"

mesh  space.mult=1.0
#
x.mesh loc=0.00 spac=0.25
x.mesh loc=2.00 spac=0.25

#
y.mesh loc=0.00 spac=0.02
y.mesh loc=0.1 spac=0.02
y.mesh loc=3.1 spac=0.05

region  num=1  material=GaAs y.min=0.0 y.max=0.1
region num=2 material= GaAs y.min=0,1 y.max=3.1

electr  name=front top
electr  name=back  bottom


#....   N-epi doping
doping region=1 n.type conc=2e18 uniform
doping region=2 p.type conc=1e17 uniform

models srh auger conmob fldmob bgn

material region=1 taun0=1e-8 taup0=1e-8
material region=2 taun0=1e-8 taup0=1e-8

contact name=front work=4.5
contact name=back work=5.0

solve init

save outfile="gaas_solarcell_0.str"

log outfile="gaas_solarcell.log"
method newton

solve name=front vstep=0.1 vfinal=1.0

save outfile="gaas_solarcell_final.str"


quit
```





Improved GaAs cell

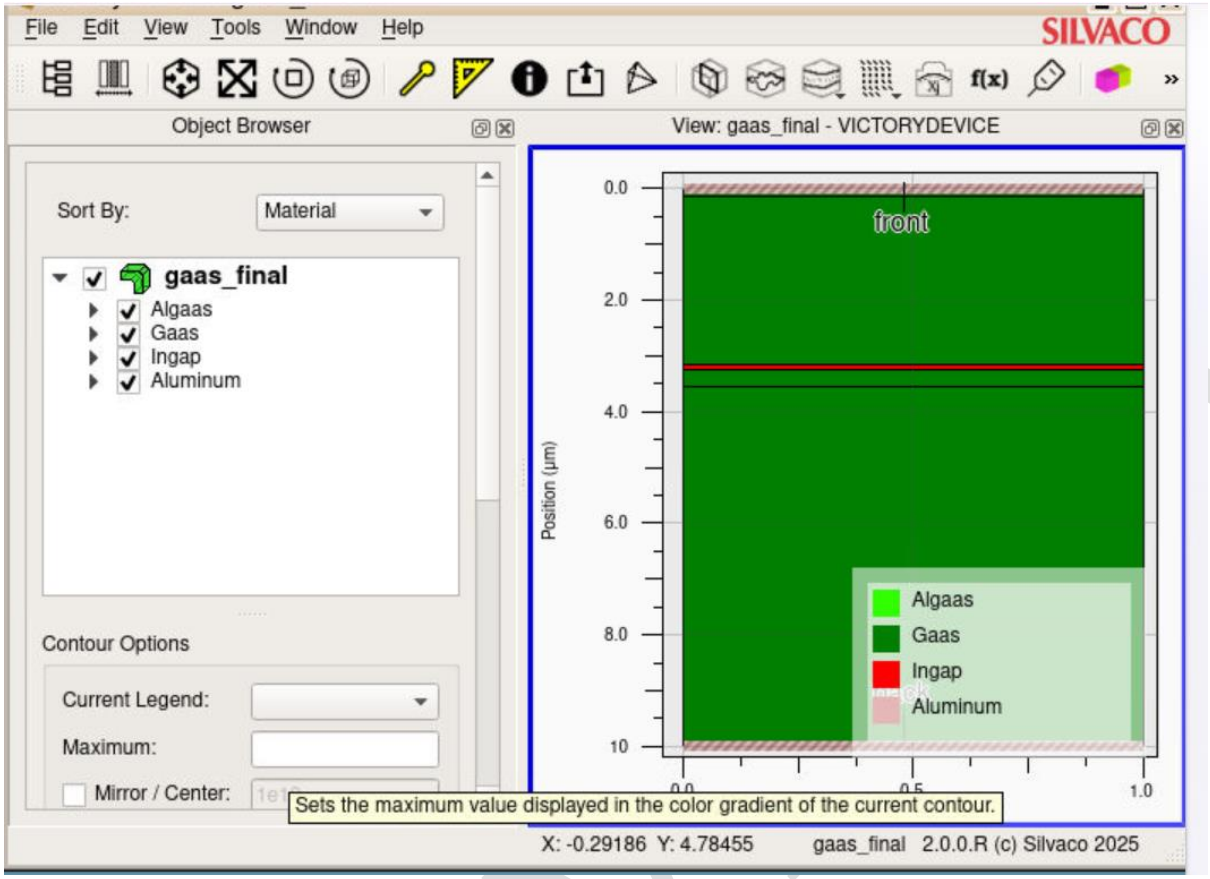
(c) Silvaco Inc., 2019
go atlas
#

```
mesh auto

#
x.m loc=0.0 s=0.25
x.m loc=1.0 s=0.25

#y.m loc=0.00 s=0.25
#y.m loc=3.1 s=0.25
#
#1 cap layer
region material=AlInP bot thick=0.05 ny=10 donors=1e19 x.comp=0.51
region material=GaAs bot thick=0.100 ny=20 donors=2e18
region material=GaAs bot thick=3.000 ny=100 acceptor=1e17
region material=InGaP bot thick=0.100 ny=20 acceptor=2e18 x.comp=0.495
region material=GaAs bot thick=0.300 ny=100 acceptor=7e18
region material=GaAs bot thick=300.000 ny=100 acceptor=1e19

# Electrodes on top and bottom
#
electrode name=anode   bottom
electrode name=cathode top
#
# The complex index data will mostly use the Sopra database.
# The index data for InGaP is supplied in a file.
#
material mat=GaAs      sopra=Gaas.nk
#material mat=InAlGaP    sopra=Againp7.nk
material mat=AlInP    sopra=againp10.nk
#material mat=AlGaAs     sopra=Algaas7.nk
material material=InGaP index.file=solarex03.nk
#
# Here we define the affinity for InGaP and AlGaAs to
# set up the band alignment
#
material material=GaAs EG300=1.42 PERMITTIVITY=13.1 AFFINITY=4.07
material material=GaAs MUN=8800 MUP=400
material material=GaAs NC300=4.7e17 NV300=7e18
material material=InGaP EG300=1.9 PERMITTIVITY=11.62 AFFINITY=4.16
material material=InGaP MUN=1945 MUP=141
material material=InGaP NC300=1.3e20 NV300=1.28e19
material material=InAsP EG300=2.4 PERMITTIVITY=11.7 AFFINITY=4.2
material material=InAsP MUN=2291 MUP=142
material material=InAsP NC300=1.08e20 NV300=1.28e19
#material material=AlGaAs  affinity=3.54
#
# Enable physical models
```

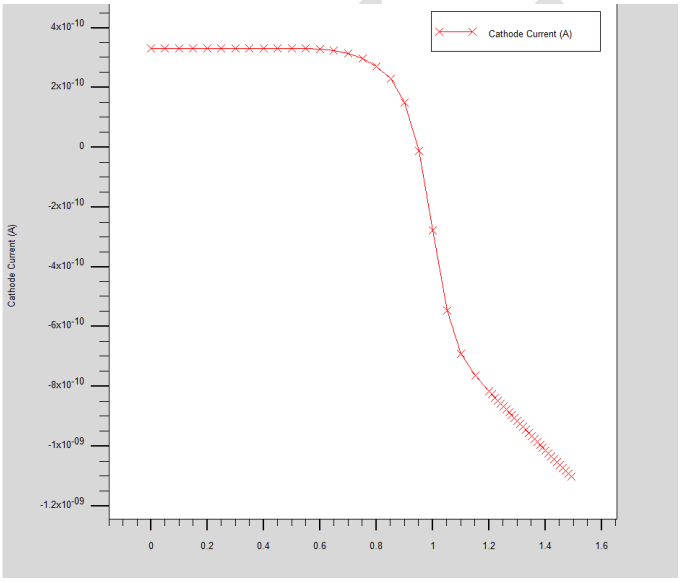
```
#
models srh fermi conmob optr auger bgn
#
method itlimit=40 maxtraps=10
#
#
beam num=1 x.o=0.5 y.o=-0.5 angle=90 \
    wavel.start=0.305 wavel.end=3.455 wavel.num=300 \
    power.file=solarex03_0.spec out.power=solarex03_0.log
#
# Plot input solar spectrum
#
#tonyplot solar_1TJ.log -set solar_1TJ_0.set
#
# Here is an alternate simplified am0 solar spectrum
#
#     power.file=solarex03_0.spec out.power=solarex03_0.log
#power.file=solarex03_15.spec out.power=solarex03_15.log
# Output optical intensity.
#
output band.temp opt.int
#
# save the initial structure
#
save outf=GaAs_improved_0_AM0_.str
#
#
log outf=GaAs_improved_AM0_dark.log

solve vanode=0.01
solve vanode=0.1
solve name=anode vstep=0.025 vfinal=0.8
solve name=anode vstep=0.01 vfinal=2.0

#
# Set NLBBT .
#
models srh fermi ni.fermi conmob optr auger bgn
# Here we ramp the beam.
#
solve b1=1e-02
solve b1=1e-01
solve b1=1
#
log outf=GaAs_improved_AM0_light.log
#
```

```
# Ramp the bias back.
#
solve name=anode vstep=-0.01   vfinal=1.2
solve name=anode vstep=-0.05    vfinal=0
#
# Extract important figures of merit.
#
extract init infile="GaAs_improved_AM0_light.log"
extract name="Jsc" max(curve(v."anode", i."cathode"))
extract name="JscmAcm2" $Jsc*1e08*1e03
extract name="Voc" x.val from curve(v."anode", i."cathode") where y.val=0.0
extract name="Pm" max(curve(v."anode", (v."anode" * i."cathode")))
extract name="Vm" x.val from curve(v."anode", (v."anode"*i."cathode") ) \
          where y.val=$"Pm"
extract name="Im" $"Pm"/$"Vm"
extract name="FF" ($"Pm"/($"Jsc"*$"Voc"))*100
extract name="Opt_int" max(beam."1")
extract name="Eff" (1e8*$Pm/$Opt_int)*100
#
# Plot the results
#
#tonyplot =GaAs_improved_0_AM0.log -set =GaAs_improved_0_AM0.set

quit
```

Structure:


File Edit View Tools Window Help
SILVACO
Object Browser
View: gaas_final - VICTORYDEVICE
Sort By:
Material
gaas_final
Algaas
Gaas
Ingap
Aluminum
Contour Options
Current Legend:
Maximum:
Mirror / Center:
front
Position (µm)
0.0
2.0
4.0
6.0
8.0
10
1.0
Algaas
Gaas
Ingap
Aluminum
Sets the maximum value displayed in the color gradient of the current contour.
X: -0.29186 Y: 4.78455
gaas_final 2.0.0.R (c) Silvaco 2025

Curve:


Cathode Current (A)
4x10^-10
2x10^-10
0
-2x10^-10
-4x10^-10
-6x10^-10
-8x10^-10
-1x10^-09
-1.2x10^-09
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6

Conclusion:

Photovoltaic cells have made significant strides in the renewable energy landscape. It has advances in material science, manufacturing techniques. However, challenges remain in developing sustainable, cost effective, reliable and high efficiency. So, continued research will be crucial in the innovation of Photovoltaic cells.