Simulation of MBI Perovskite Solar cell on Silvaco TCAD

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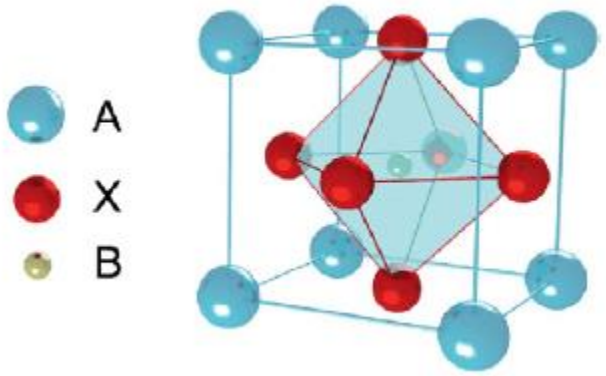
1. Introduction:

In recent years, perovskite solar cells have garnered increasing attention due to their significant efficiency improvement. Their power conversion efficiency (PCE) has risen from 3.8% to 23.3% since 2009. These cells are appealing because of multiple reasons. Firstly, they have a low production cost due to the relatively uncomplicated chemical and physical processes required to manufacture the cells. Secondly, perovskites can be deposited at low temperatures and do not require the high-temperature processing steps that are typical for manufacturing silicon cells. Additionally, unlike traditional silicon solar cells that primarily absorb visible light, perovskite solar cells have a broader absorption spectrum, capturing both visible and near-infrared light. All these factors make Perovskite Solar cells (PCS) a more efficient alternative to silicon solar cells. Our simulation study aims to explore the performance characteristic of a PSC using Silvaco TCAD Software, extracting relevant metrics such as its structure, IV, Generation, Recombination profiles, band diagram, and performance metrics of the cell.

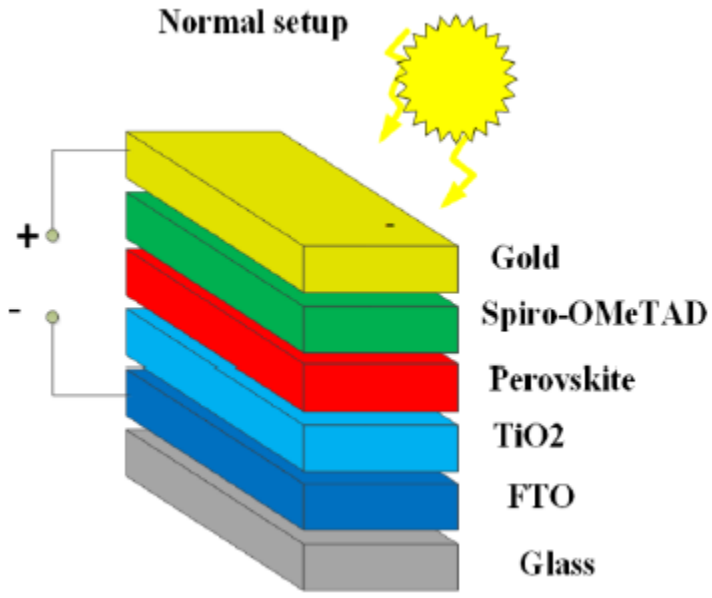
2. Structure of the Perovskite Solar Cell:

Perovskites have a crystal structure represented by the formula ABX_3 represents where A is a large organic or organic cation, B is the small inorganic cation and X_3 is an ion from the halogen group. This structure creates a flexible framework that can accommodate a variety of different ions. Hence, Perovskites are characterized by tunable electronic properties such as the bandgap. Besides, Perovskites have a high absorption coefficient and a direct bandgap that makes them function well as the absorber layer. Their bandgap is between 1.3 to 2.2 eV which as discussed in the subsection before, allows them to harvest both near-infrared and ultraviolet light.



In our simulation, the choice of our perovskite was Methylammonium Bismuth Iodide ($CH_3NH_3BiI_3$) which is the material of interest in our experimental lab. Methylammonium Bismuth Iodide has an indirect bandgap of approximately 1.99 eV and can be cheaply and abundantly synthesized in the lab environment. It is known to possess excellent electrical and optical properties, low-temperature solution processability and long lifetime.

3. Perovskite Solar Cell:



The perovskite Solar cell consists of the following layers:

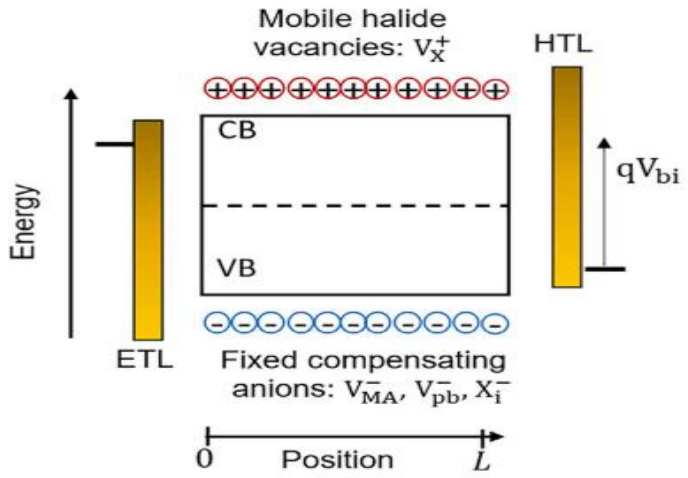
1. **<u>Front Electrode (Cathode)</u>**: This is made up of Fluorine-Doped Tin Oxide (FTO) which is a transparent, conducting metal oxide. Since FTO is transparent in the visible spectrum, it allows photons to reach the perovskite layer where they can be absorbed and converted

into electricity without impeding their path. Their conductivity ensures they carry out the role of electrodes which is to transport electrons to the external circuit. Our choice of FTO over Indium Tin oxide is motivated by several factors. FTO is generally less expensive than ITO and is chemically stable under the environmental conditions typical for solar cell fabrication.

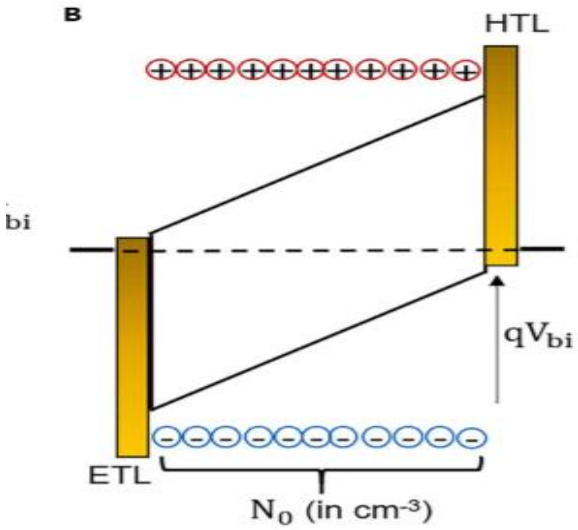
2. **Electron Transport Layer (ETL)**: The TiO_2 layer serves as the electron transport layer (ETL). It selectively transports electrons from the perovskite layer to the FTO layer while blocking the holes. This prevents recombination of charge carriers within the cell. TiO_2 is used because its conduction band aligns well with that of the perovskite material. This minimizes energy barriers at the interface.
3. **MBI Perovskite Layer**: Methylammonium bismuth iodide (MBI) is the active layer where light absorption and photo-generated charge carrier (electron-hole pairs) generation occur. Methylammonium bismuth iodide, in particular, stands out for its unique crystal structure and electronic properties. Its perovskite structure comprises organic cations like methylammonium (MA) and inorganic ions like bismuth and iodide. This combination results in desirable characteristics such as tunable bandgap, high carrier mobility, and good stability under light exposure.
4. **Hole Transport Layer (HTL)**: HAT-6 acts as the hole transport layer (HTL). It facilitates the movement of holes from the perovskite layer to the back electrode while blocking electrons. One of the key requirements for an effective HTL is that its highest occupied molecular orbital (HOMO) level should align well with the valence band of the perovskite material. HAT6 exhibits a favorable HOMO level, which facilitates efficient hole extraction from the perovskite layer to the HTL. This alignment ensures that there is minimal energy loss during hole transfer.
5. **Back Electrode (Anode)**: This is made up Gold which is used because of its excellent conductivity and inert properties, ensuring that it does not react with the materials in the cell.

4. Physical Processes inside the Perovskite Solar Cell

Let us now consider the physical framework inside the Perovskite Solar Cell. For an intrinsic Perovskite in the dark without any contact, the conduction band and valence band of both ETL and HTL layer are aligned (see the figure below. Note the dotted lines represent the Fermi Level).



After contacting the film with an ETL on the left (x = 0) and an HTL on the right (x = L), a built-in voltage V_{bi} results due to the difference in contact work functions. This voltage drops linearly between the HTL and ETL.



The ETL (usually made of materials like TiO_2or ZnO) collects the excited electrons. Electrons move from the MBI layer to the ETL due to their energy difference. The HTL (often made of materials like spiro-OMeTAD or HAT-5 and HAT-6) collects the positive holes. Holes move from the MBI layer to the HTL. The separated electrons and holes flow through their respective transport layers. This movement of charge carriers creates an electrical current. The current is collected by electrodes (usually transparent conductive oxide layers) and sent to an external circuit. The external circuit connected to the solar cell receives the generated current. This current can power electronic devices or charge batteries. Researchers optimize the thickness and quality of the MBI layer to minimize defects (such as pinholes) that could reduce performance. Improving the morphology of the MBI layer enhances the overall efficiency of MBI perovskite solar cells.

When considering the nature of the energy-band diagram, it must be mentioned that perovskite solar cell is a p-i-n or n-i-p solar cell where "p" stands for the p-type (positive) layer, "i" stands for the intrinsic layer, and "n" stands for the n-type (negative) layer. For our simulation, the p layer is HAT6, the n layer is TiO2 and i layer is MBI perovskite.

Unlike traditional solar cells where light absorption in the doped regions contributes to photogeneration, light absorption in p-i-n or n-i-p junctions at doped regions does not contribute to photogeneration. Photogeneration occurs only for light that is collected in the “i" intrinsic region. As a result, p and n are usually 10 nm thick to ensure that maximum amount of light reaches the ‘i’ region. On the other hand, i region is around 100 nm thick in traditional p-i-n cells to ensure that maximum photogeneration in the i region can occur. Our simulation follows this structure, with TiO2 (n-type) and HAT-6 (p-type) being of length 80 nm and 70 nm respectively and the MBI perovskite i region is around 320 nm thick in n-i-p cell to ensure that maximum photogeneration in the i region can occur. The anode contact is gold with the thickness of 25 nm while the cathode is FTO layer with the thickness of 55nm.

5-Challenges and Ongoing Research

1. Stability Issues: Despite improvements, MBI perovskite solar cells still face challenges related to long-term stability, particularly in humid and high-temperature environments. Efforts are ongoing to develop robust encapsulation techniques and explore alternative perovskite formulations.
2. Lead-Free Alternatives: Environmental concerns associated with lead in perovskite materials have led to the exploration of lead-free alternatives. However, achieving comparable performance without compromising stability remains a major research focus.
3. Commercialization Hurdles: Transitioning from lab-scale prototypes to mass-produced, market-ready solar modules require addressing cost, scalability, and reliability concerns. Collaborations between academia and industry are crucial for overcoming these hurdles.

6- Future Prospects

1. Efficiency Boost: Further optimization of MBI perovskite compositions, interface engineering, and tandem cell integration could push efficiencies closer to the theoretical limits, surpassing conventional solar technologies.

2. Environmental Sustainability: Development of lead-free MBI perovskites and eco-friendly manufacturing processes will align with sustainable energy initiatives and regulatory requirements.
3. Market Penetration: Successful commercialization and widespread adoption of MBI perovskite solar cells will depend on cost competitiveness, reliability, and addressing consumer confidence in long-term performance.

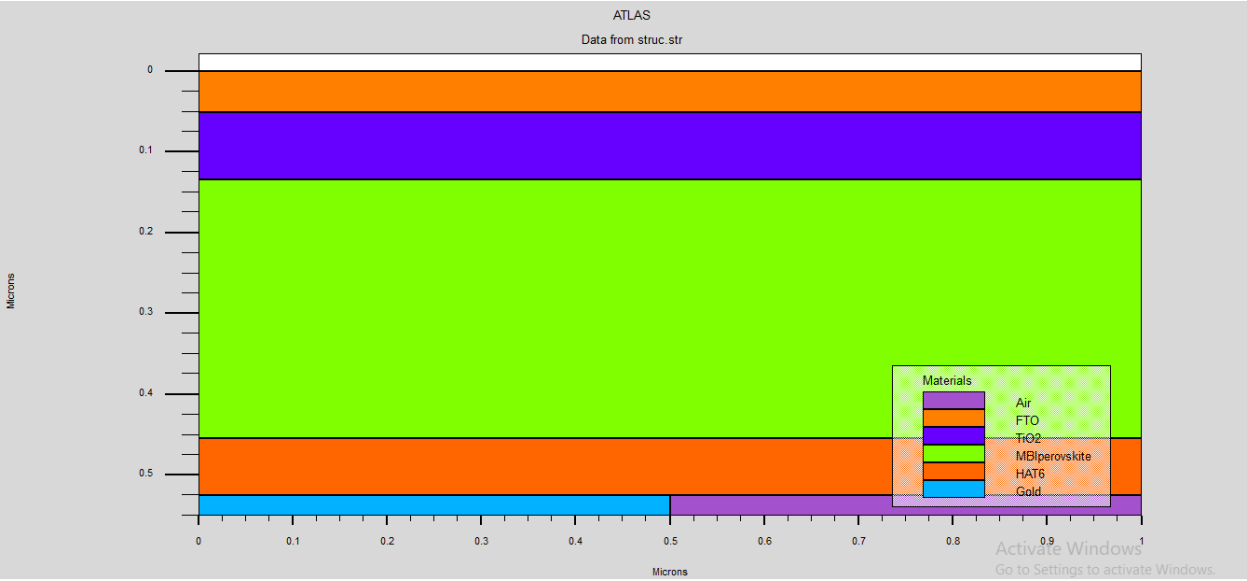
7-Simulation code:

```
go atlas

mesh space.mult=1

x.m l=0.0 s=.05
x.m l=1.0 s=.05

y.m l=0 s=0.01
y.m l=0.135 s=.01
y.m l=0.455 s=.02
y.m l=0.525 s=.01
y.m l=0.550 s=.1

#Defining regions
region num = 1 material = Air x.min = 0.00 y.min = 0
region num = 2 user.material = FTO x.min = 0.00 x.max = 1.0 y.min = 0 y.max = 0.055
region num = 3 material=TiO2 x.min = 0.00 x.max = 1.0 y.min = 0.055 y.max = 0.135
region num = 4 user.material= MBIperovskite x.min = 0.00 x.max = 1.0 y.min = 0.135 y.max
= 0.455
region num = 5 user.material=HAT6 x.min = 0.00 x.max = 1.0 y.min = 0.455 y.max = 0.525

#Defining Electrodes
electrode num=1 name=cathode x.min=0.00 x.max=1.65 y.min=0.0 y.max=0.055 mat=FTO
electrode num=2 name=anode x.min=0.00 x.max=0.5 y.min=0.525 y.max=0.550 mat=Gold

# Defining Doping
doping uniform n.type conc=2e16 reg=2
doping uniform n.type conc=5.6e16 reg=3
doping uniform n.type conc=1e15 reg=4
doping uniform p.type conc=1e16 reg=5

material material=air real.index=1.0 imag.index=0
material material=FTO user.group=semiconductor user.default=ITO eg300=3.5 affinity=2.3
permittivity=9 NC300=2.2e18 NV300=1.8e19 MUN=30 MUP=5 sopra=Ito2.nk taun0=1e-7
taup0=1e-7
```

```
material material=TiO2 user.group=semiconductor  user.default=sio2 eg300=3.2
affinity=2.2 permittivity=9 NC300=2.2e18 NV300=1.8e19 MUN=4.7 MUP=4.7 taun0=1e-7
taup0=1e-7 sopra=Tio2b.nk

material name=MBIperovskite user.group=semiconductor user.default=GaN eg300=1.99
affinity=3.93 permittivity=10.0 NC300=2.2e18 NV300=1.8e19 MUN=20 MUP=20  taun0=1e-
7 taup0=1e-7 sopra = perovskite.nk

material material=HAT6 eg300=3.96 affinity=4 permittivity=8.5 NC300=2.2e18
NV300=1.8e19 MUN=100 MUP=30 sopra=ito2.nk taun0=1e-7 taup0=1e-7

mat mat=Gold sopra=Au.nk

# Defining beams
beam num=1 am1.5g x.o=0 y.o=-1 angle=90 tr.mat
models srh fermi ni.fermi optr auger bgn print
method newton autonr trap maxtrap=10
output con.band val.band band.par e.mobility e.velocity


contact name=anode workf=5.75
contact name=cathode reflect=1 workf=5.2

# Solutions
solve init
solve prev
solve b1=1
log outf=illumination.log
solve name=anode vanode=0 vstep=0.1 vfinal=1.6
log off

tonyplot illumination.log

probe name = "total recombination" RECOMBIN integrate x.min = 0 x.max = 1.0 y.min = 0
y.max = 0.550
probe name = "total generation" PHOTOGEN integrate x.min = 0 x.max = 1.0 y.min = 0
y.max = 0.550


extract init infile="illumination.log"


extract name="Jsc" max(curve(v."anode", i."cathode")) outf="I.log"
extract name="JscmAcm2" $Jsc*1e08*1e03 outf="J.dat"
```

```
extract name="Voc" x.val from curve(v."anode",i."cathode") where y.val=0.0 outf="V.dat"
extract name="Pm" max(curve(v."anode", (v."anode" *i."cathode"*(-1))))
extract name="FF" ($"Pm"/($"Jsc"*$"Voc"))*100
extract name="Opt_int" max(beam."1")
extract name="Eff" (1e8*$Pm/$Opt_int)*100 outf="E.dat"
extract name="Power" curve(v."anode", (v."anode" * i."anode" *(-1))) outf="P.dat"

save outf= struc.str
tonyplot struc.str
tonyplot.IV
tonyplot.JV
tonyplot.PV
quit.
```

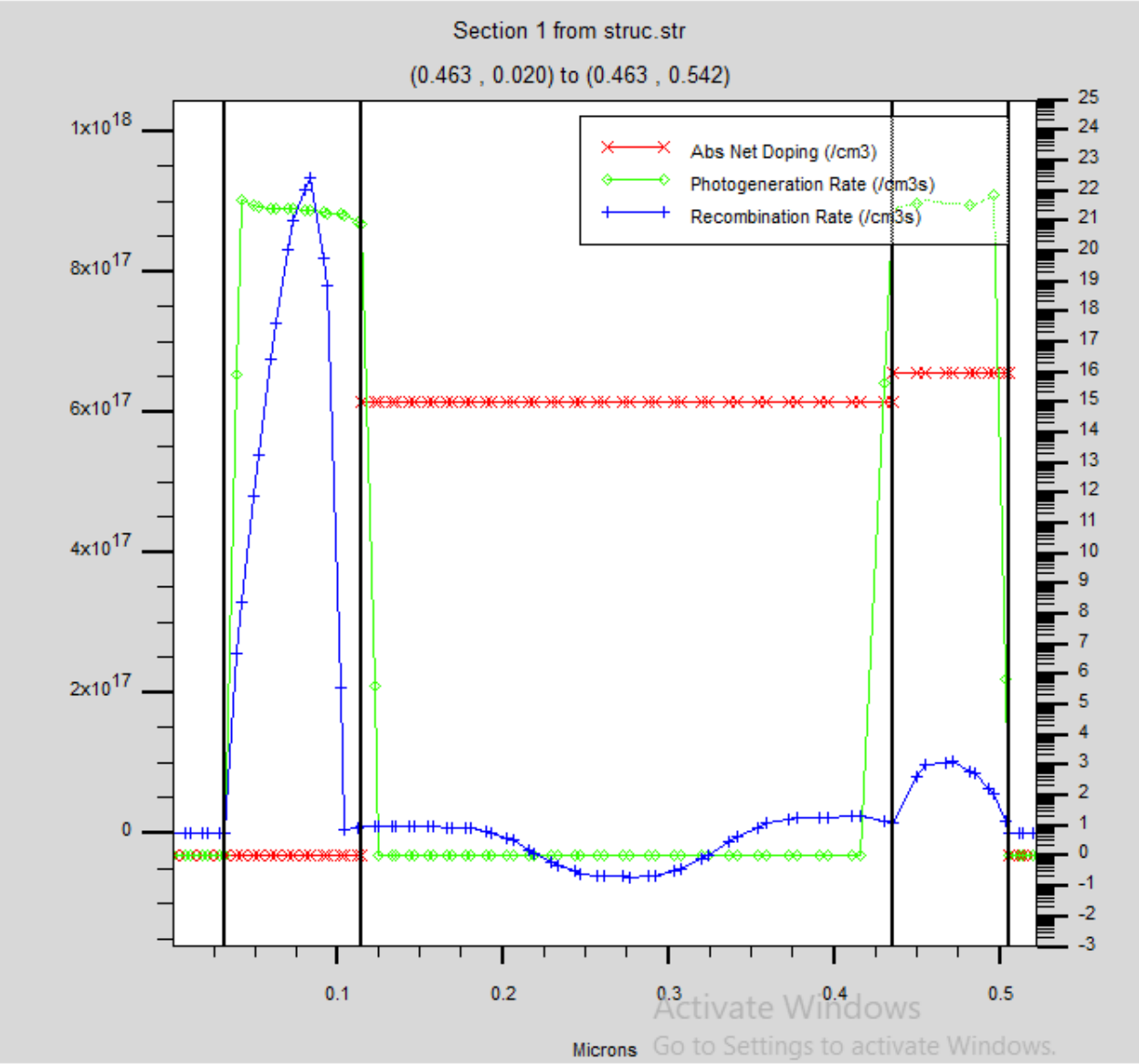
8-Simulation Results:



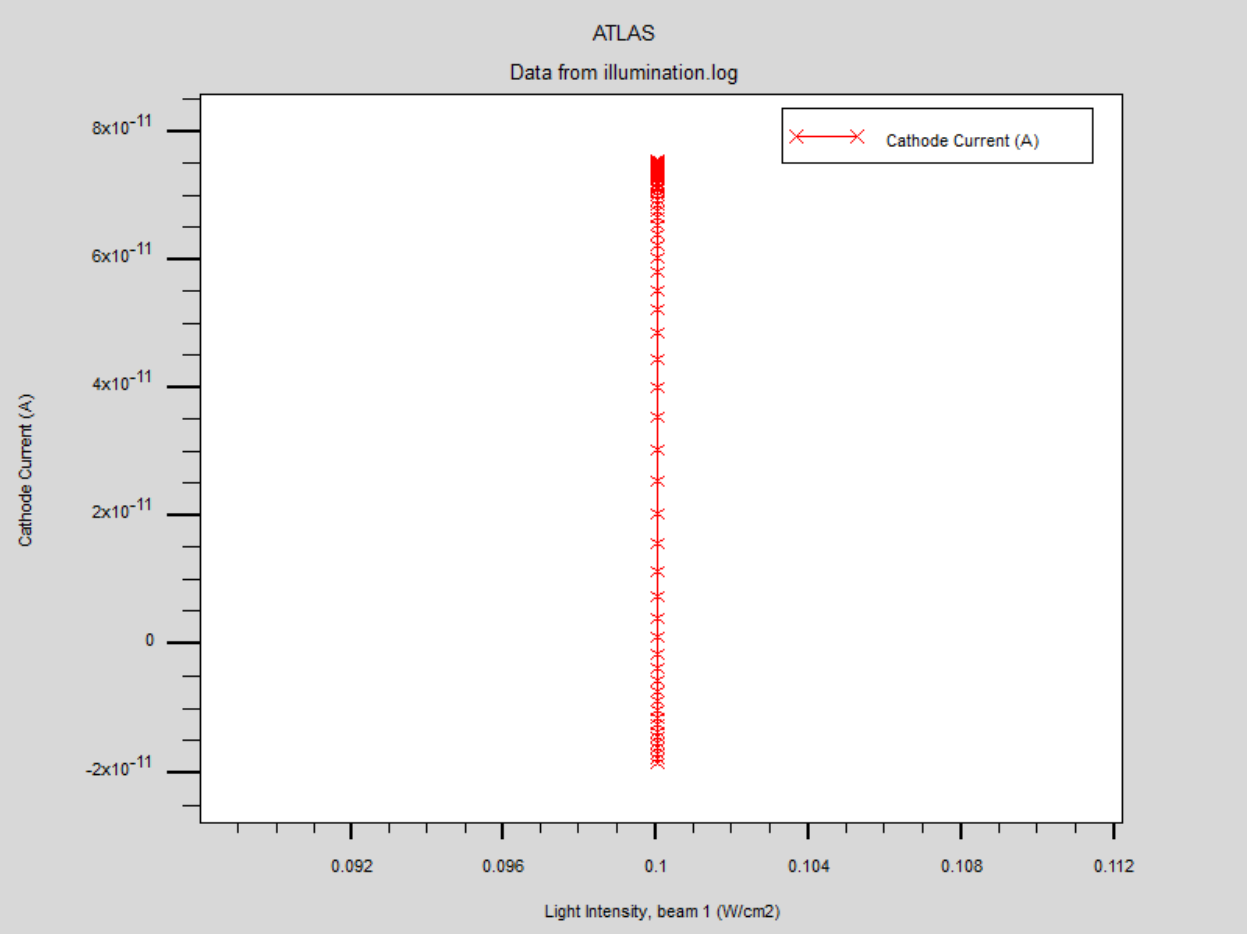
Structure file of the Silvaco TCAD Simulation of MBI Perovskite Solar cell.

Jsc	2.94593502e-11	(# 101)
JscmAcm2	2.94594	(# 103)
Voc	0.719793666785675	(# 105)
Pm	1.09733023872e-10	(# 107)
FF	517.493778706279	(# 111)
Opt_int	0.1000370455	(# 113)
Eff	10.9692413806891	(# 115)
Power	9.88131291682493e-324	(# 117)

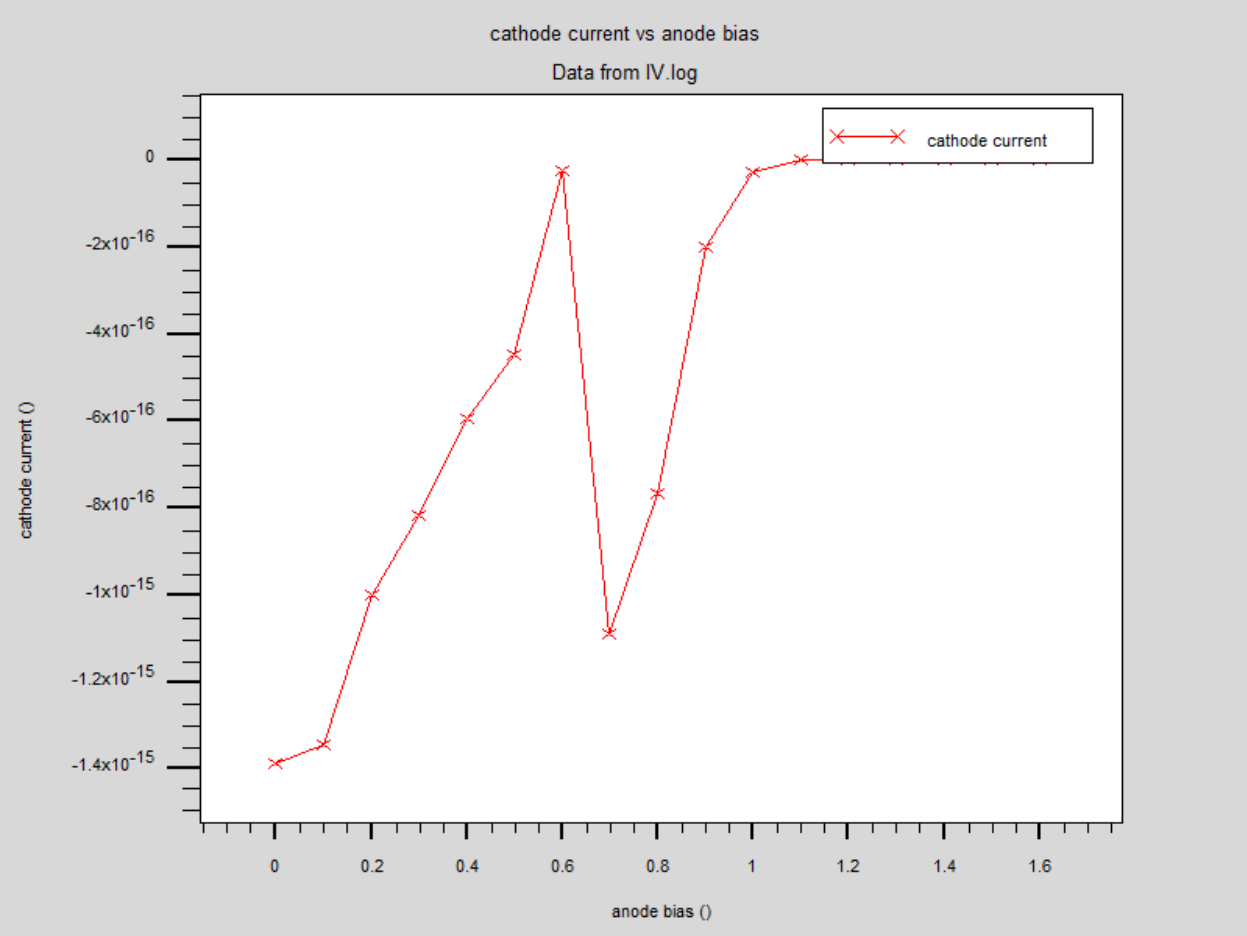
Results of the Silvaco TCAD Simulation of MBI Perovskite Solar cell.



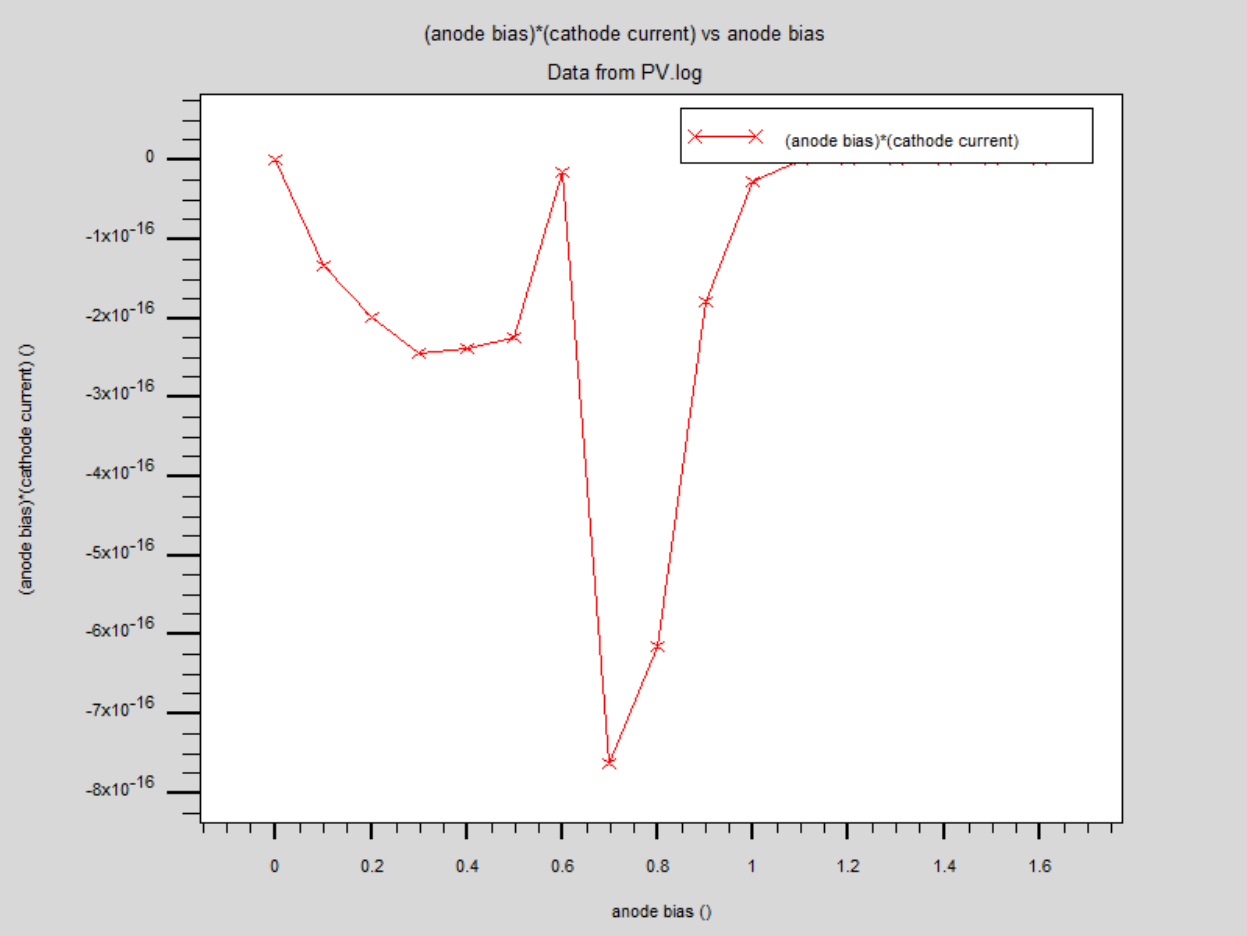
Energy Band Diagram of MBI Perovskite solar cell



Illumination plot of Solar cell


cathode current vs anode bias
Data from IV.log
cathode current
0
-2x10^-16
-4x10^-16
-6x10^-16
-8x10^-16
-1x10^-15
-1.2x10^-15
-1.4x10^-15
cathode current ()
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
anode bias ()

I-V Curve



PV-Curve of Solar Cell

References:

Bertoluzzi, Luca, et al. "Mobile ion concentration measurement and open-access band diagram simulation platform for halide perovskite solar cells." Joule 4.1 (2020): 109-127.

Husainat, A., Ali, W., Cofie, P., Attia, J., & Fuller, J. (2019). Simulation and Analysis of Methylammonium Lead Iodide ($CH_3NH_3PbI_3$) Perovskite Solar Cell with Au Contact Using SCAPS 1D Simulator. *American Journal of Optics and Photonics*, *7*(2), 33. https://doi.org/10.11648/j.ajop.20190702.12

Appendix:

Simulation code:

```
go atlas

mesh space.mult = 1.0

# Meshing

x.mesh loc = 0.00 spac = 1.00

x.mesh loc = 100.00 spac = 1.00

x.mesh loc = 200.00 spac = 1.00


y.mesh loc = 0.00 spac = 1

y.mesh loc = 5.00 spac = 1

y.mesh loc = 25 spac = 0.5

y.mesh loc = 50 spac = 1

y.mesh loc = 130 spac = 0.5

y.mesh loc = 170 spac = 1

y.mesh loc = 200 spac = 1


# Defining Regions

region num = 1 material = Air x.min = 0.00 y.min = 0

region num = 2 user.material = FTO x.min = 0.00 x.max = 200.00 y.min = 0 y.max = 16

region num = 3 material=TiO2 x.min = 0.00 x.max = 200.00 y.min = 16 y.max = 30
```

region num = 4 user.material= MBIperovskite x.min = 0.00 x.max = 200.00 y.min = 30 y.max = 165

region num = 5 user.material=HAT6 x.min = 0.00 x.max = 200.00 y.min = 165 y.max = 195

Defining Electrodes

electrode num=1 name=cathode x.min=0.00 x.max=200.00 y.min=0.0 y.max=16 mat=FTO

electrode num=2 name=anode x.min=0.00 x.max=10.00 y.min=195 y.max=200 mat=Gold

Defining the materials

material material=FTO eg300=3.5 user.group=semiconductor user.default=ITO affinity=4 permittivity=9 NC300=2.2e17 NV300=2.20e19 MUN0=20 MUP0=10 taun0=1e-7 taup0=1e-7 sopra = Ito2.nk

material material=TiO2 eg300=3.2 affinity=4.26 permittivity=50 NC300=2.2e18 NV300=1.8e19 MUN0=2e4 MUP0=1e3 taun0=1e-7 taup0=1e-7 sopra = Tio2.nk

material material=MBIpervoskite user.group=semiconductor user.default=GaN eg300=1.99 affinity=3.9 permittivity=30 NC300=2.2e18 NV300=1.0e18 MUN0=2.20 MUP0=2.2 taun0=1e-7 taup0=1e-7 sopra = perovskite.nk

material material=HAT6 user.group=semiconductor user.default=ZnO eg300=3.96 affinity=4 permittivity=8.5 NC300=2.2e18 NV300=1.8e19 MUN0=100 MUP0=30 taun0=1e-7 taup0=1e-7 sopra = spiroOMeTAD.nk

Doping Concentrations

doping uniform concentration=1E15 n.type region=2

doping uniform concentration=6E19 n.type region=3

doping uniform concentration=9E20 n.type region=4

doping uniform concentration=1E22 p.type region=5

beam and models used

beam num=1 am1.5g x.origin=0.0 y.origin=-1.0 angle=90.0 tr.mat

models srh conmob fermi ni.fermi bgn optr auger print

method newton trap

output val.band con.band qfn qfp e.field j.electron j.hole j.conduction j.total ex.field ey.field flowline e.mobility h.mobility qss e.temp h.temp j.disp

Defining contacts

contact name=cathode workfun=4.4

contact name=anode workfun=5.1

Solving the Recurssive relation

solve init

solve prev

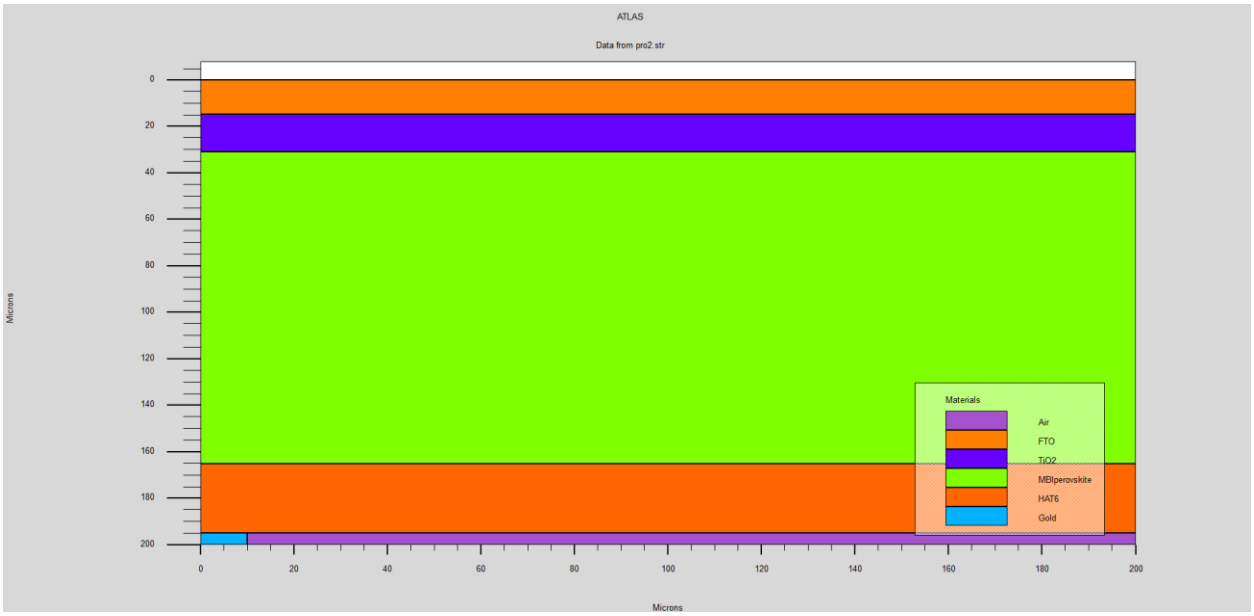
solve b1=1

log outf=illumination.log

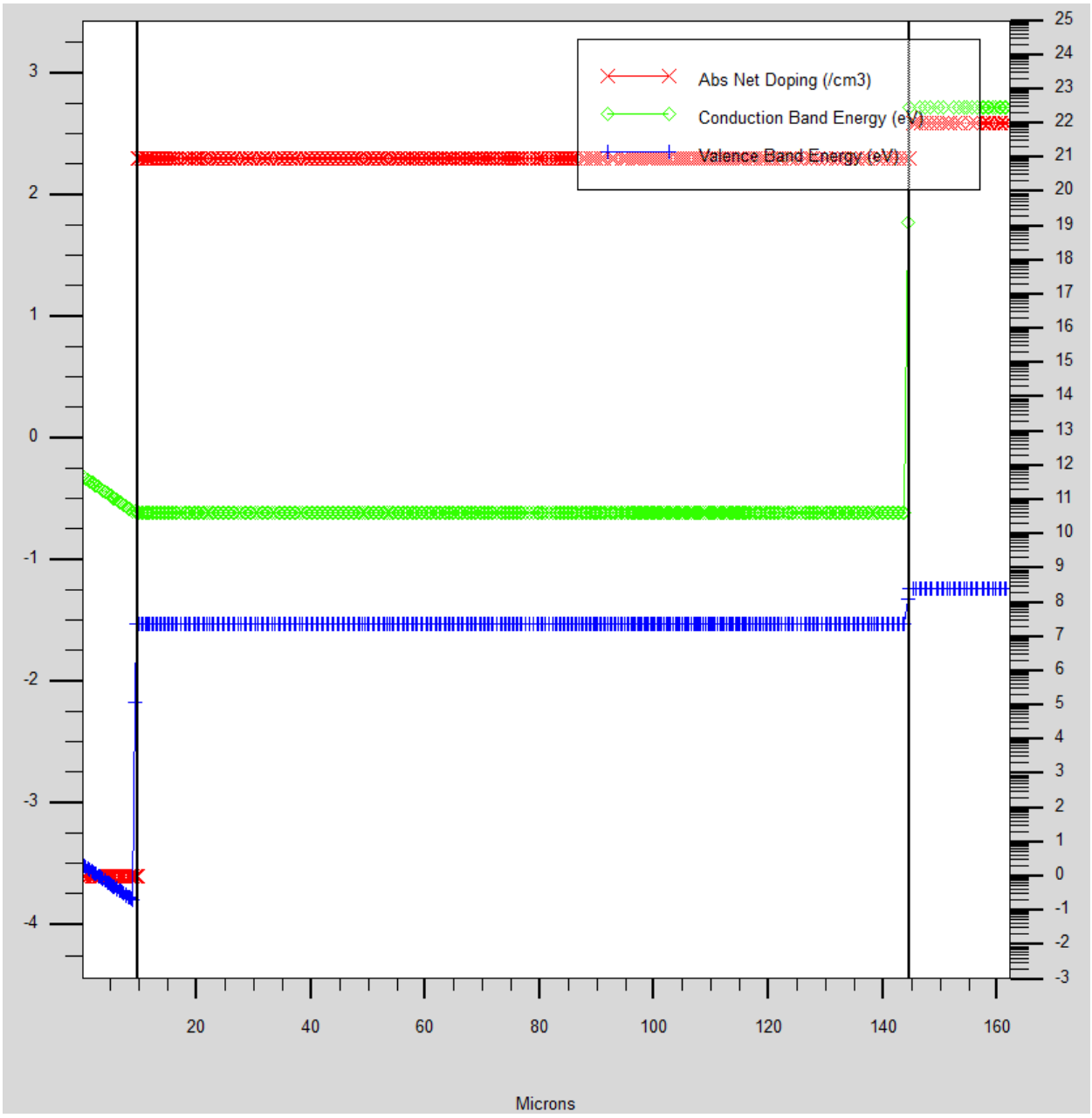
```
# Defining Recombinations vs Photogeneration graph

probe name="total recombination" RECOMBIN integrate x.min=0 x.max=200 y.min=0
y.max=200

probe name="total photogeneration" PHOTOGEN integrate x.min=0 x.max=200
y.min=0 y.max=200

solve vanode=0.0 name=anode vstep=0.1 vfinal=1.6

log off

#Extract parameters

extract init infile="illumination.log"

extract name="Isc" y.val from curve(v."anode", i."anode") where x.val=0.0

extract name="JscmAcm2" $Isc*1e08*1e03/$length

extract name="Voc" x.val from curve(v."anode", i."anode") where y.val=0.0

extract name="P" curve(v."anode", i."anode") outf="IV.LOG"

extract name="P" curve(v."anode",(i."anode" *1e08*1e03/$length)) outf="JV.LOG"

extract name="P" curve(v."anode", (v."anode" * i."anode")) outf="PV.log"

extract name="Pm" max(curve(v."anode", (v."anode" * i."anode"*(-1))))

extract name="FF" ($"Pm"/($"Isc"*$"Voc"))

extract name="Opt_int" max(beam."1")
```

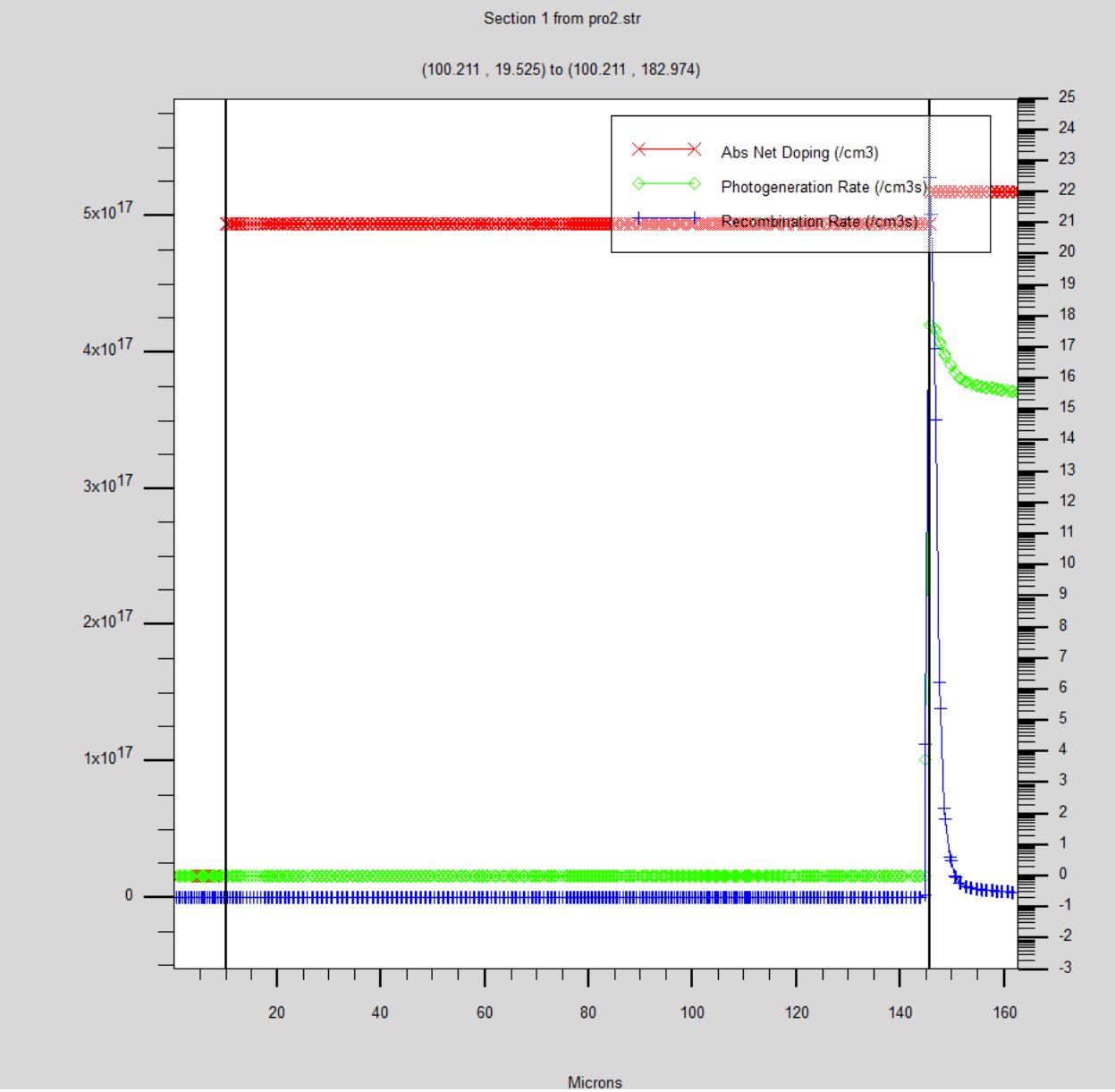
```
extract name="Eff" (1e8*$Pm/$Opt_int)*100


save outf=pro2.str

tonyplot pro2.str

tonyplot illumination.log

tonyplot IV.log

tonyplot JV.log

tonyplot PV.log

quit
```

Simulation Results:



Isc	2.217028671e-17	(# 67)
Voc	0.500002043186251	(# 69)
P	9.88131291682493e-324	(# 72)
Pm	7.623752591e-16	(# 73)
FF	68.7741663858584	(# 74)
Opt_int	0.1000370455	(# 75)
Eff	7.62093025580535e-05	(# 76)


Abs Net Doping (/cm3)
Conduction Band Energy (eV)
Valence Band Energy (eV)
3
2
1
0
-1
-2
-3
-4
25
24
23
22
21
20
19
18
17
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
20
40
60
80
100
120
140
160
Microns


Section 1 from pro2.str
(100.211 , 19.525) to (100.211 , 182.974)
Abs Net Doping (/cm3)
Photogeneration Rate (/cm3s)
Recombination Rate (/cm3s)
5x10^17
4x10^17
3x10^17
2x10^17
1x10^17
0
20
40
60
80
100
120
140
160
Microns