ORGANSKI POLUPROVODNIČKI MATERIJALI

Primeri simulacije

S1: Osnovne karakteristike OLED

- Definisanje strukture OLED (Organic Light Emitting Diode)
- Definisanje parametara materijala
- Izbor fizičkog modela OLED
- Gustina struje u zavisnosti od napona na anodi
- Gustina struje u zavisnosti od električnog polja
- Snaga luminiscencije OLED
- Langevin rekombinacija za 10V na anodi

Definisanje strukture OLED

```
# (c) Silvaco Inc., 2017
go atlas
title Device Characteristics of MEH-PPV Polymer Light Emitting Diode

# Change the material thickness here
set MEH_PPV_thick=0.0475
set ITO_thick=0.05
set Cathode_thick=0.05

set total_thick=$MEH_PPV_thick + $Cathode_thick

mesh smooth=1 space.mult=1.0
x.mesh l= 0.0 spacing=1
x.mesh l=10.0 spacing=1

y.mesh l=-$ITO_thick spacing=0.005
y.mesh l=0.0 spacing=0.005
y.mesh l=$MEH_PPV_thick spacing=0.005
y.mesh l=$total_thick spacing=0.005
```

Definisanje kontakata

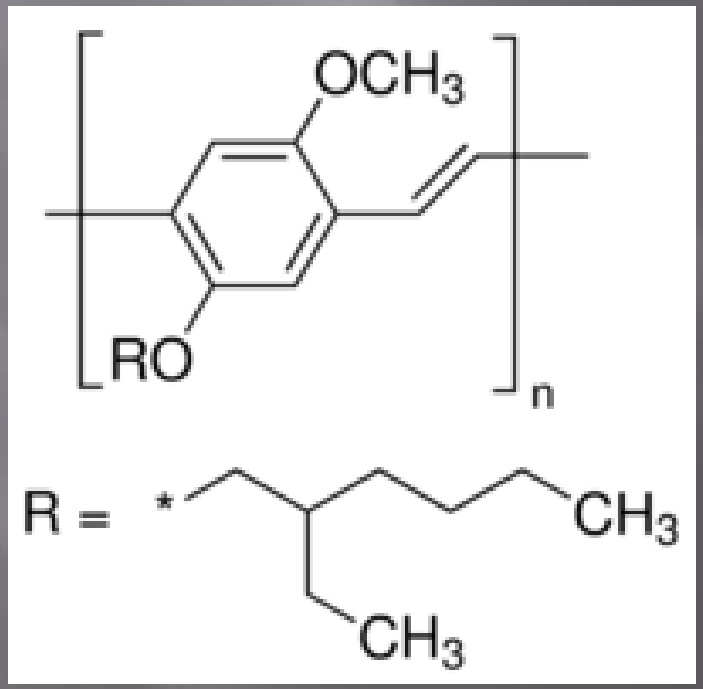
```
region num=1 material=PPV y.max=$MEH_PPV_thick

elec num=1 name=anode x.min=0 x.max=10.0 y.min=-$ITO_thick \
y.max=0 material=ITO
elec num=2 name=cathode x.min=0 x.max=10.0 y.min=$MEH_PPV_thick \
y.max=$total_thick material=Aluminum

doping uniform region=1 conc=1e15 p.type
```

Definisanje parametara materijala

```
# Set parameters for MEH-PPV
material region=1 material=PPV \
eg300=2.1 nc300=2.5e19 nv300=2.5e19 permittivity=3.0 \
taun0=1e-9 taup0=1e-9 affinity=2.8 arichn=120 \
rst.exciton=0.5 taus.exciton=1e-9 lds.exciton=0.01 \
real.index=1.67

# Defining mobility parameters for MEH-PPV
mobility region=1 material=PPV deltaen.pfmob=0.48 deltaep.pfmob=0.48
up=0.5e-4

# Calcium (Cathode)
contact name=cathode workfunc=2.9

# ITO (Anode)
contact name=anode workfunc=4.7

models singlet langevin pfmob print
```

MEH-PPV

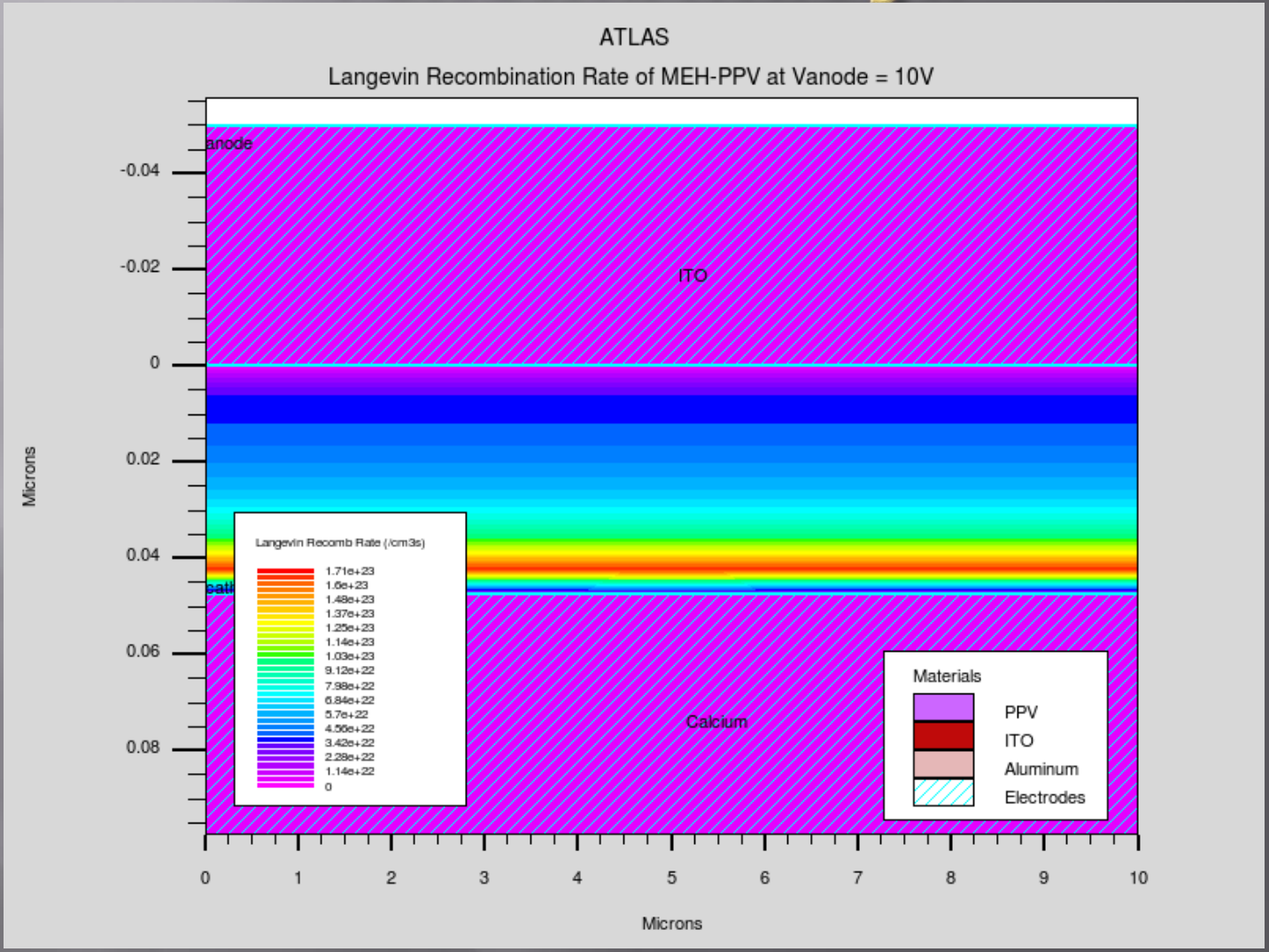
- Poly
- 2-metoxy-5-(2-ethilexyloxy)-1, 4-phenylene vinylene

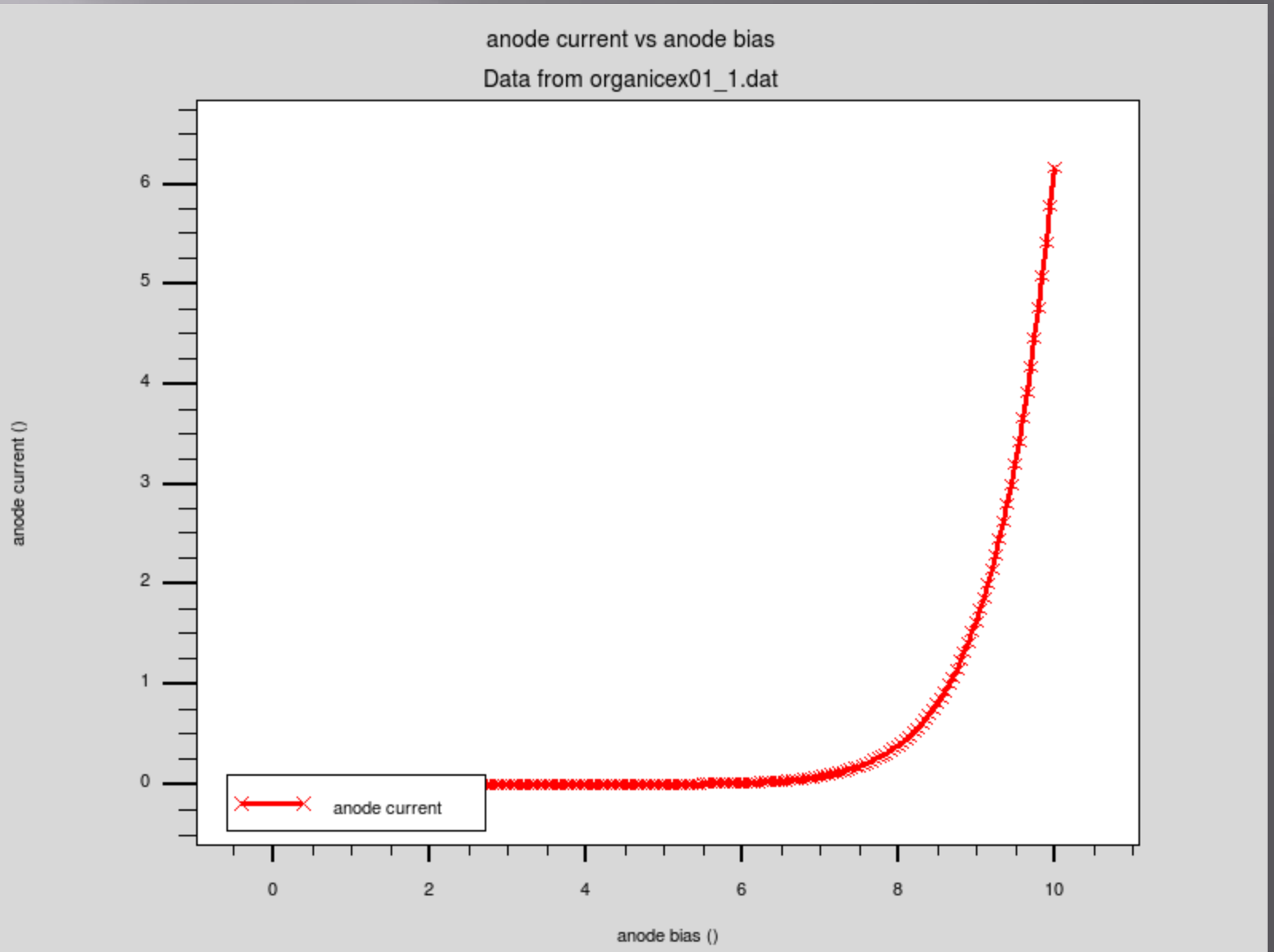


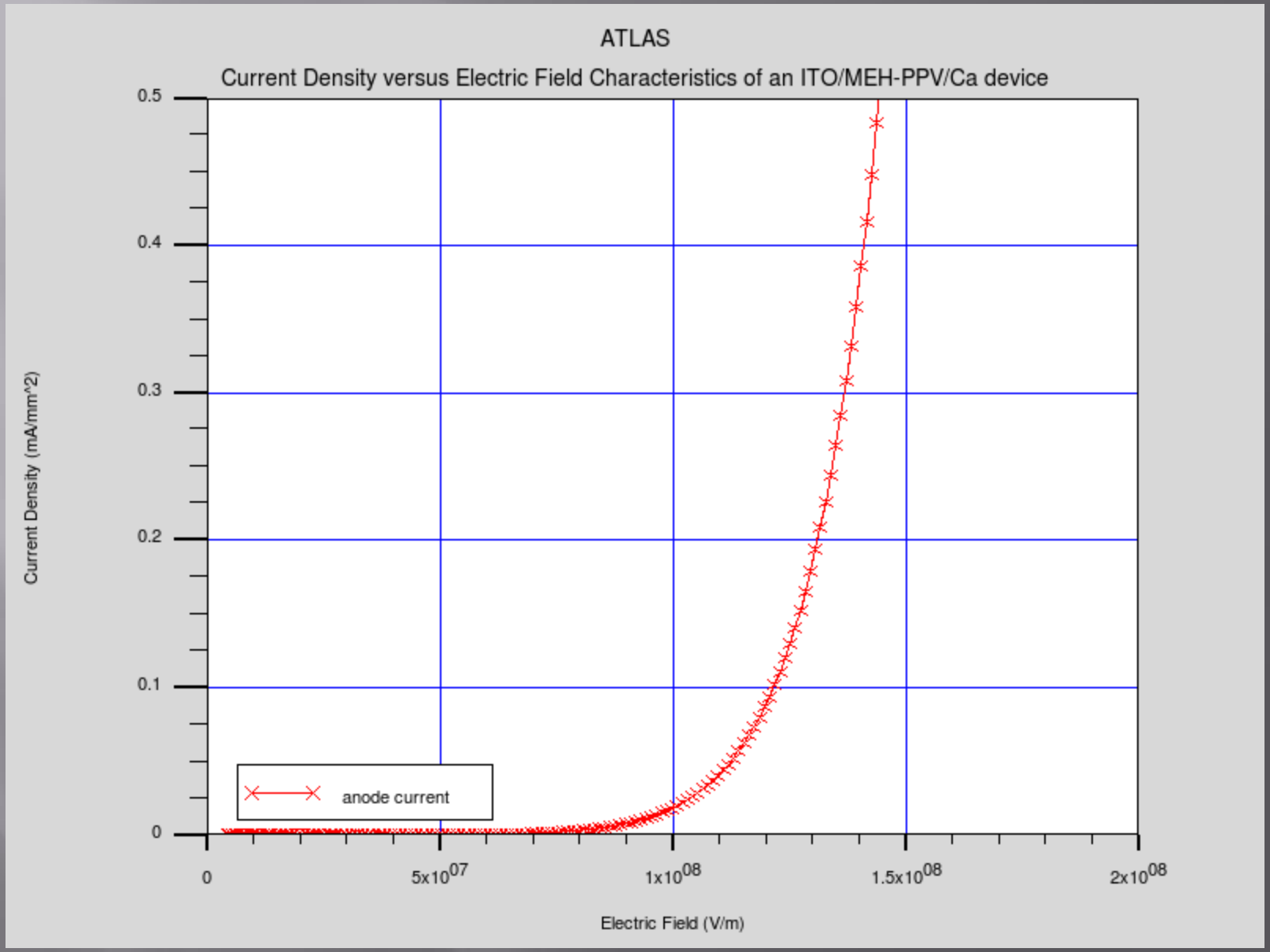
MEH-PPV, Poly: Karakteristike

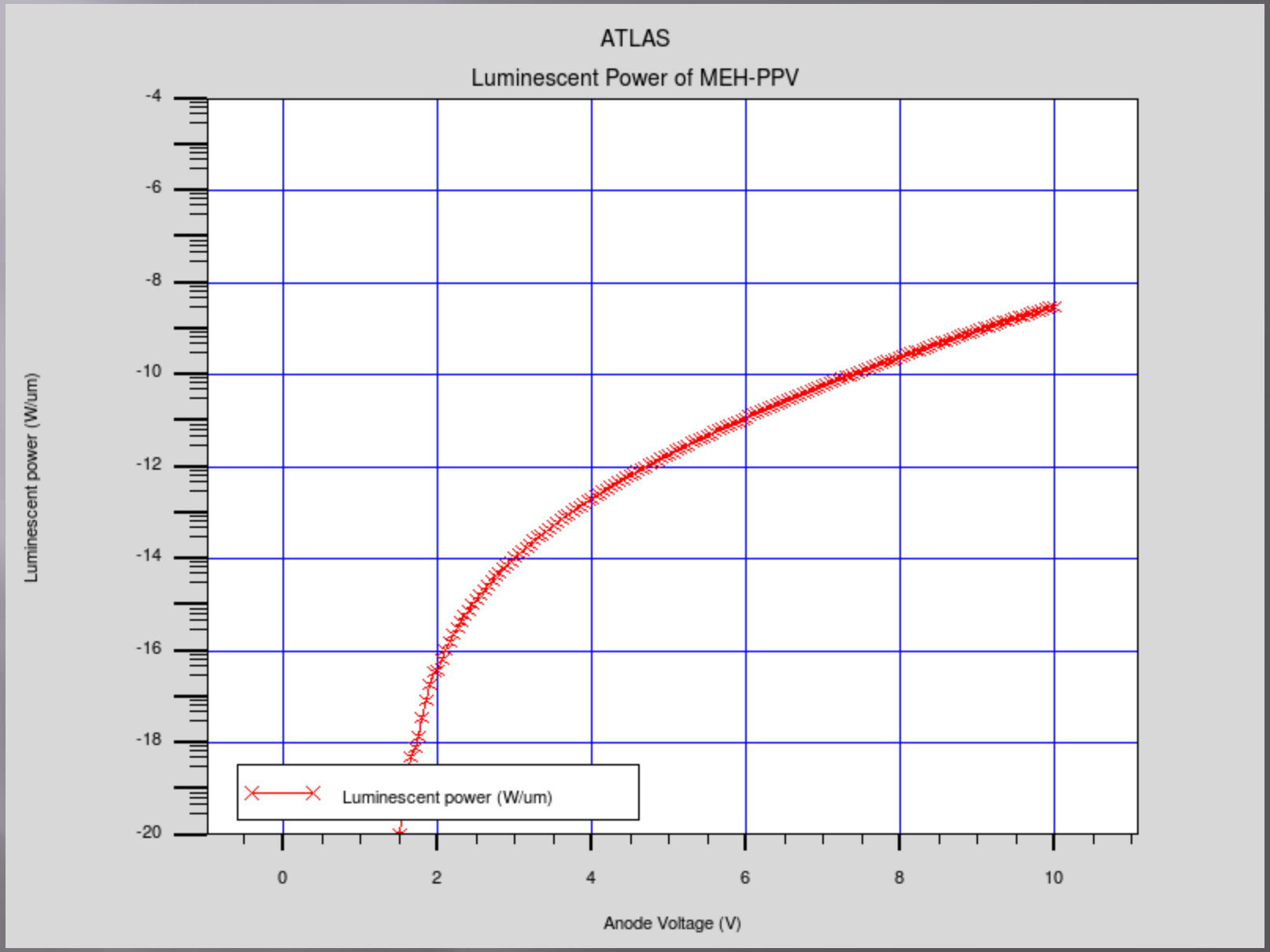
mol wt	average M_n 40,000-70,000
fluorescence	λ_{ex} 493 nm; λ_{em} 554 nm in toluene
Orbital energy	HOMO 5.3 eV
	LUMO 3 eV
OLED Device Performance	ITO/PEDOT:PSS/MEH-PPV/Al[4] • Color: orange-red • Max. Luminance: 220 Cd/m^2 • Max. EQE: 0.3 % • Turn-On Voltage: 3.8 V
	ITO/PEDOT:PSS/MEH-PPV/PBO/Al[4] • Color: orange-red • Max. Luminance: 970 Cd/m^2 • Max. EQE: 1.9 % • Turn-On Voltage: 2.9 V
	ITO/PEDOT:PSS/MEH-PPV/PBZT/Al[4] • Color: orange-red • Max. Luminance: 1400 Cd/m^2 • Max. EQE: 2.5 % • Turn-On Voltage: 2.8 V

Struktura i Langevin rekombinacija



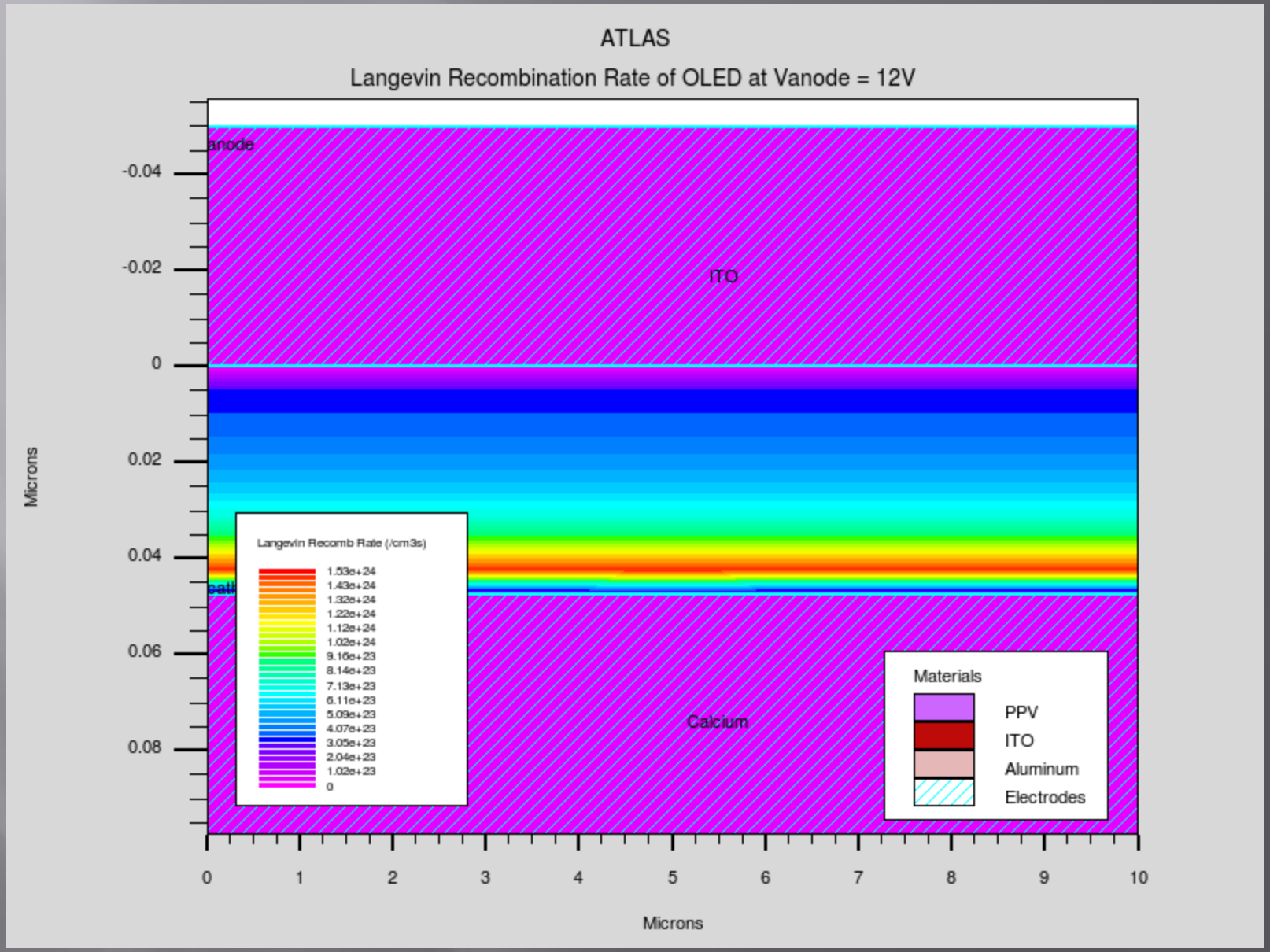

anode current vs anode bias
Data from organicex01_1.dat
anode current ()
anode bias ()
anode current
0
1
2
3
4
5
6
0
2
4
6
8
10

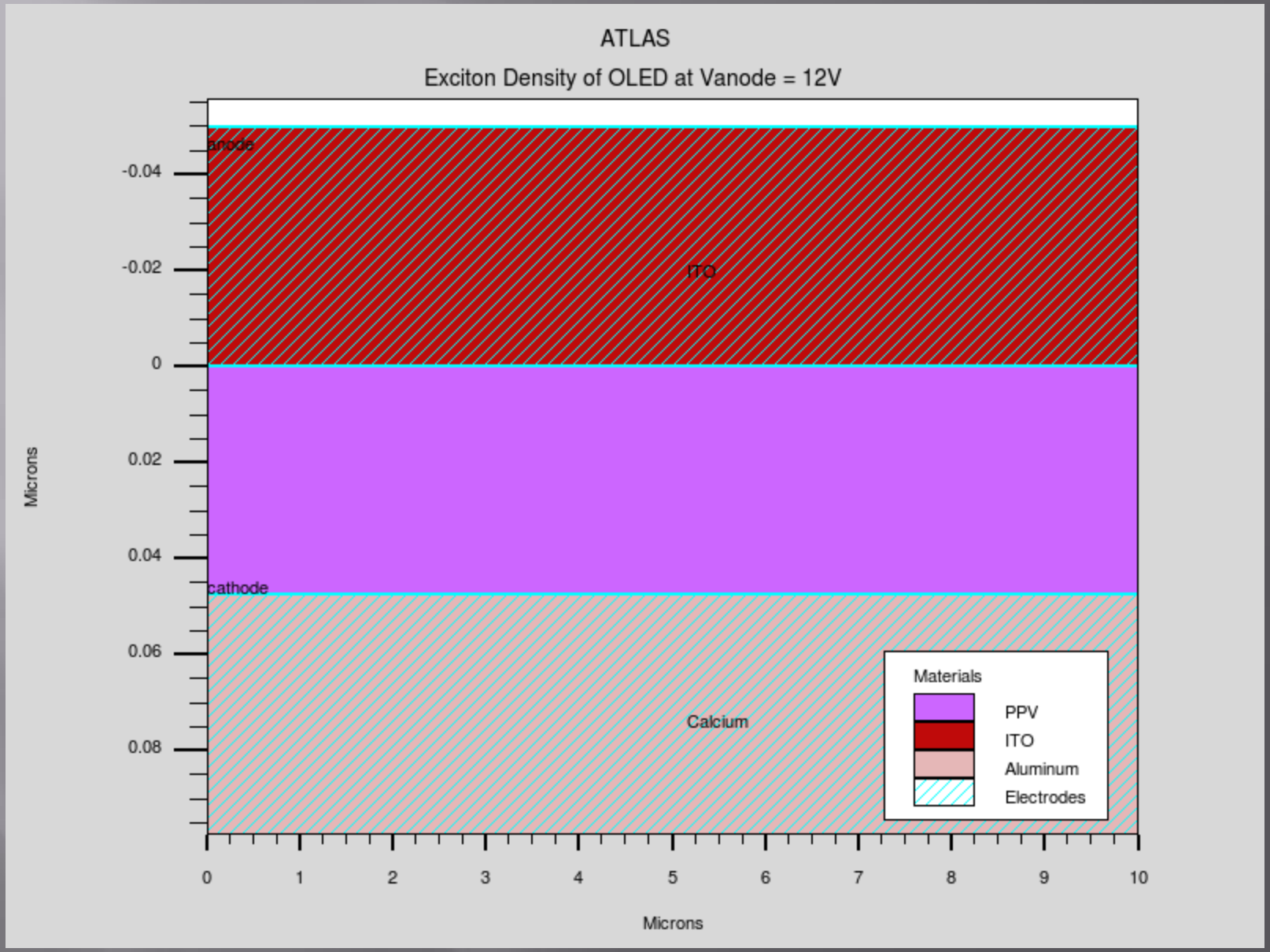

ATLAS
Current Density versus Electric Field Characteristics of an ITO/MEH-PPV/Ca device
Current Density (mA/mm^2)
0.5
0.4
0.3
0.2
0.1
0
anode current
0
5x10^07
1x10^08
1.5x10^08
2x10^08
Electric Field (V/m)

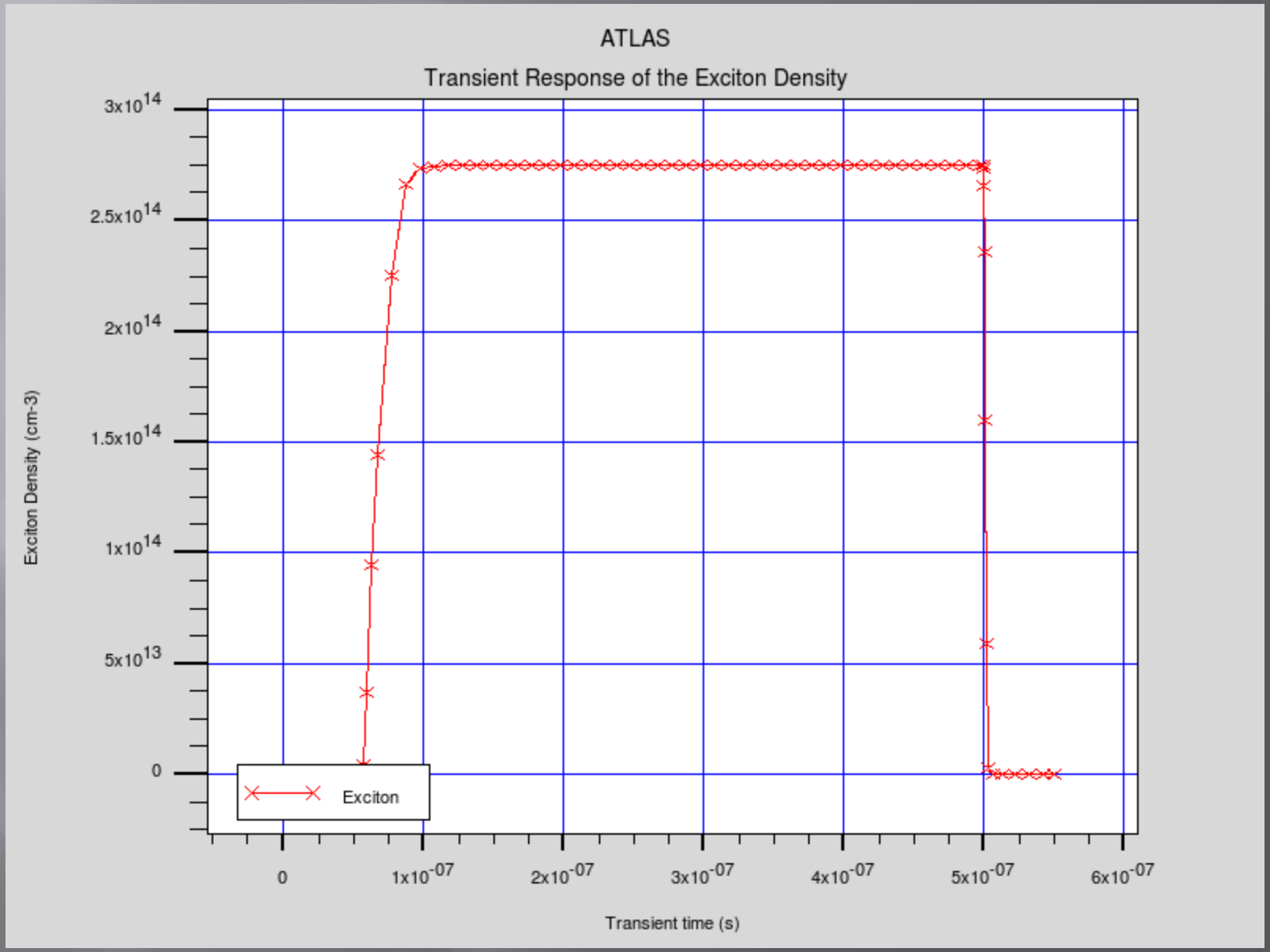

ATLAS
Luminescent Power of MEH-PPV
Luminescent power (W/um)
-4
-6
-8
-10
-12
-14
-16
-18
-20
0
2
4
6
8
10
Anode Voltage (V)
Luminescent power (W/um)

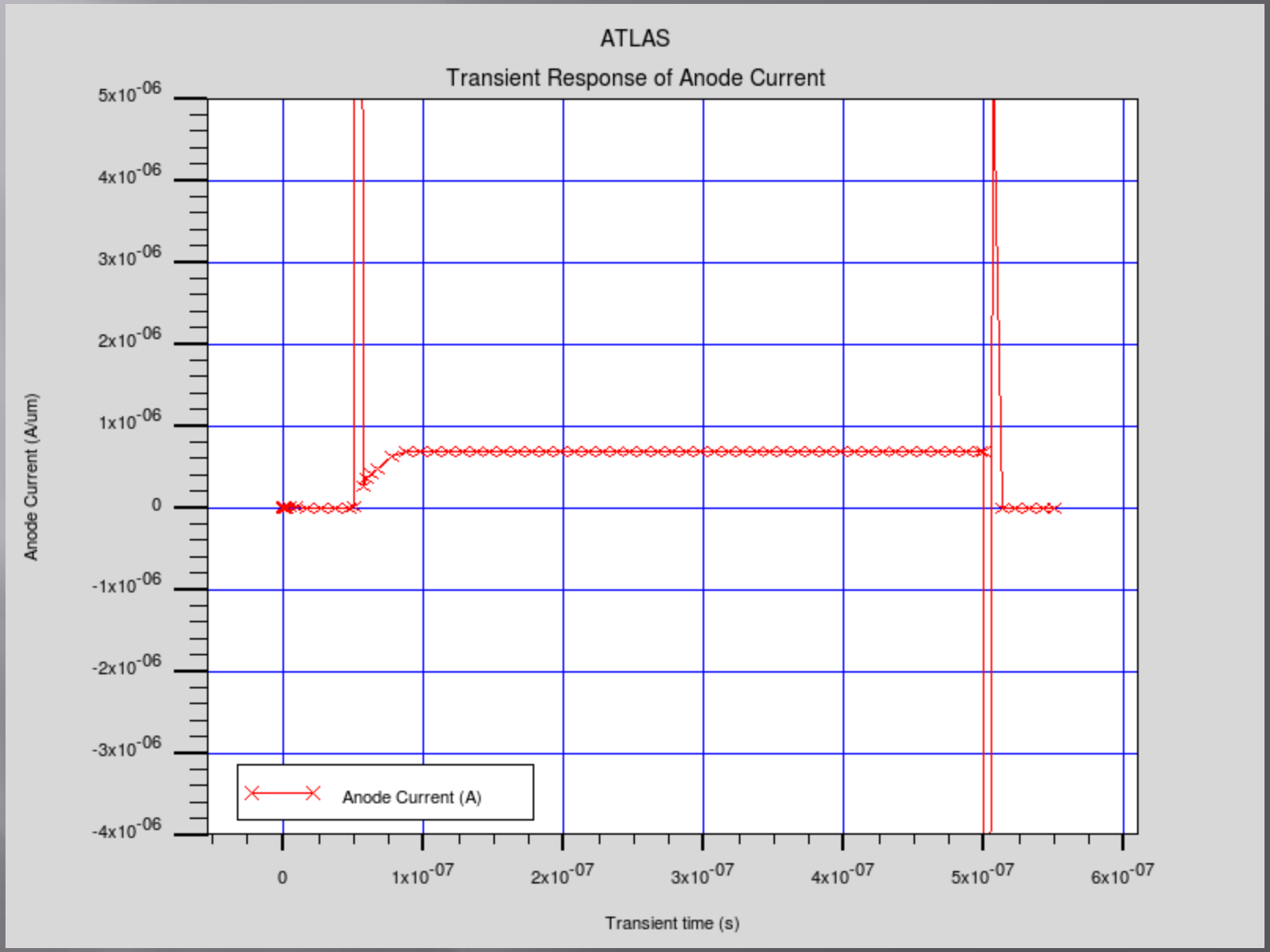
S2: Transient simulacija MEH-PPV polimerne LED

- Definisanje strukture OLED (Organic Light Emitting Diode)
- Definisanje parametara materijala
- Izbor fizičkog modela OLED
- Langevin rekombinacija za 12V na anodi
- Transient odziv gustine eksitacije
- Transient odziv anodne struje


ATLAS
Langevin Recombination Rate of OLED at Vanode = 12V
anode
ITO
Calcium
Langevin Recomb Rate (/cm3s)
1.53e+24
1.43e+24
1.32e+24
1.22e+24
1.12e+24
1.02e+24
9.16e+23
8.14e+23
7.13e+23
6.11e+23
5.09e+23
4.07e+23
3.05e+23
2.04e+23
1.02e+23
0
Materials
PPV
ITO
Aluminum
Electrodes
-0.04
-0.02
0
0.02
0.04
0.06
0.08
Microns
0
1
2
3
4
5
6
7
8
9
10
Microns


ATLAS
Exciton Density of OLED at Vanode = 12V
anode
ITO
cathode
Calcium
Materials
PPV
ITO
Aluminum
Electrodes
-0.04
-0.02
0
0.02
0.04
0.06
0.08
Microns
0
1
2
3
4
5
6
7
8
9
10
Microns


ATLAS
Transient Response of the Exciton Density
Exciton Density (cm-3)
3x10^14
2.5x10^14
2x10^14
1.5x10^14
1x10^14
5x10^13
0
Exciton
0
1x10^-07
2x10^-07
3x10^-07
4x10^-07
5x10^-07
6x10^-07
Transient time (s)

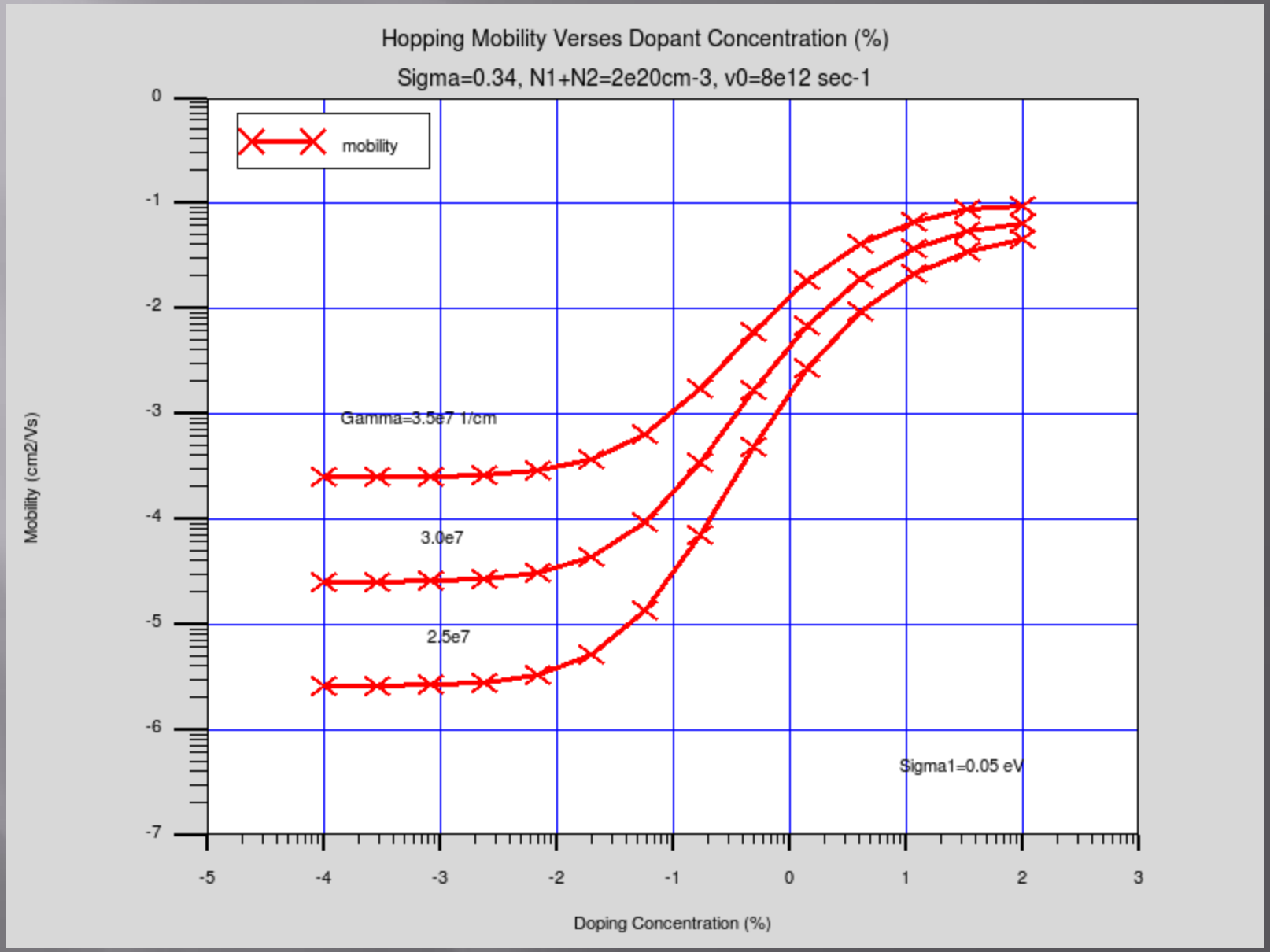

ATLAS
Transient Response of Anode Current
Anode Current (A/um)
5x10-06
4x10-06
3x10-06
2x10-06
1x10-06
0
-1x10-06
-2x10-06
-3x10-06
-4x10-06
Anode Current (A)
0
1x10-07
2x10-07
3x10-07
4x10-07
5x10-07
6x10-07
Transient time (s)

S3: Zavisnost Hopping pokretljivosti od nivoa dopiranja

- Definisanje jednog sloja organskog materijala
- Definisanje modela Hopping pokretljivosti
- Definisanje parametara materijala
- Definisanje pokretljivosti
- Definisanje kontakata
- Nivo dopiranja se menja od 1E17 do 1E23
- gamma: 2.5E7 – 3.5E7

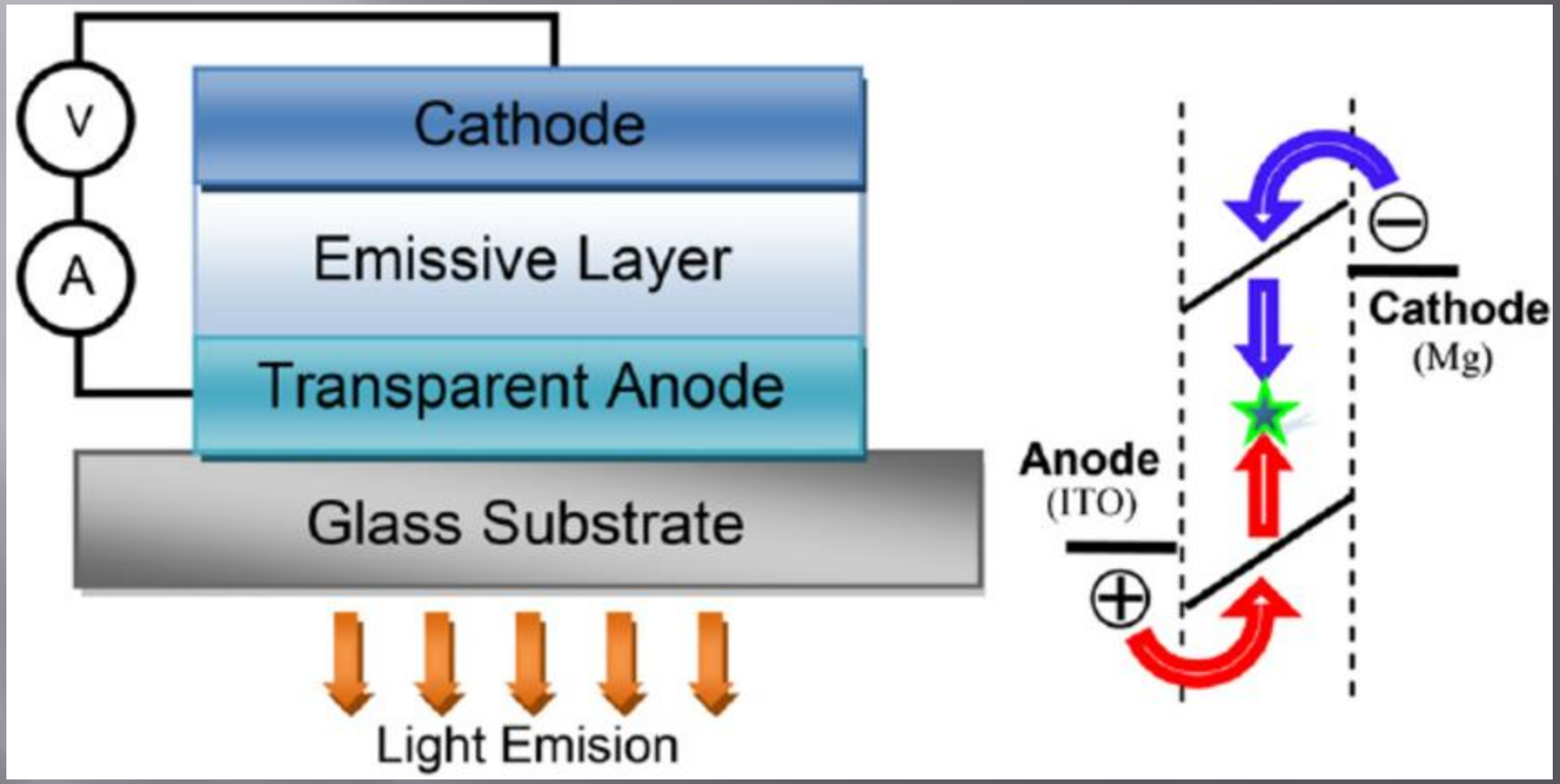
```
go atlas

set doping=1e18
set sigma=0.34
set gamma=3.3e7

mesh

x.mesh l=0 s=0.5
x.mesh l=1 s=0.5

y.mesh l=0   s=0.002
y.mesh l=0.1 s=0.002

region num=1 material=Alq3

electrode name=anode   top
electrode name=cathode bottom

doping uniform n.type conc=$doping

odefects cont hopping \
         ea=0 na=$doping nia=1e20 sigmaia=0.05 sigmaa=$sigma \
         ed=0 nd=$doping nid=1e20 sigmaid=0.05 sigmad=$sigma

models hopmob langevin print
```

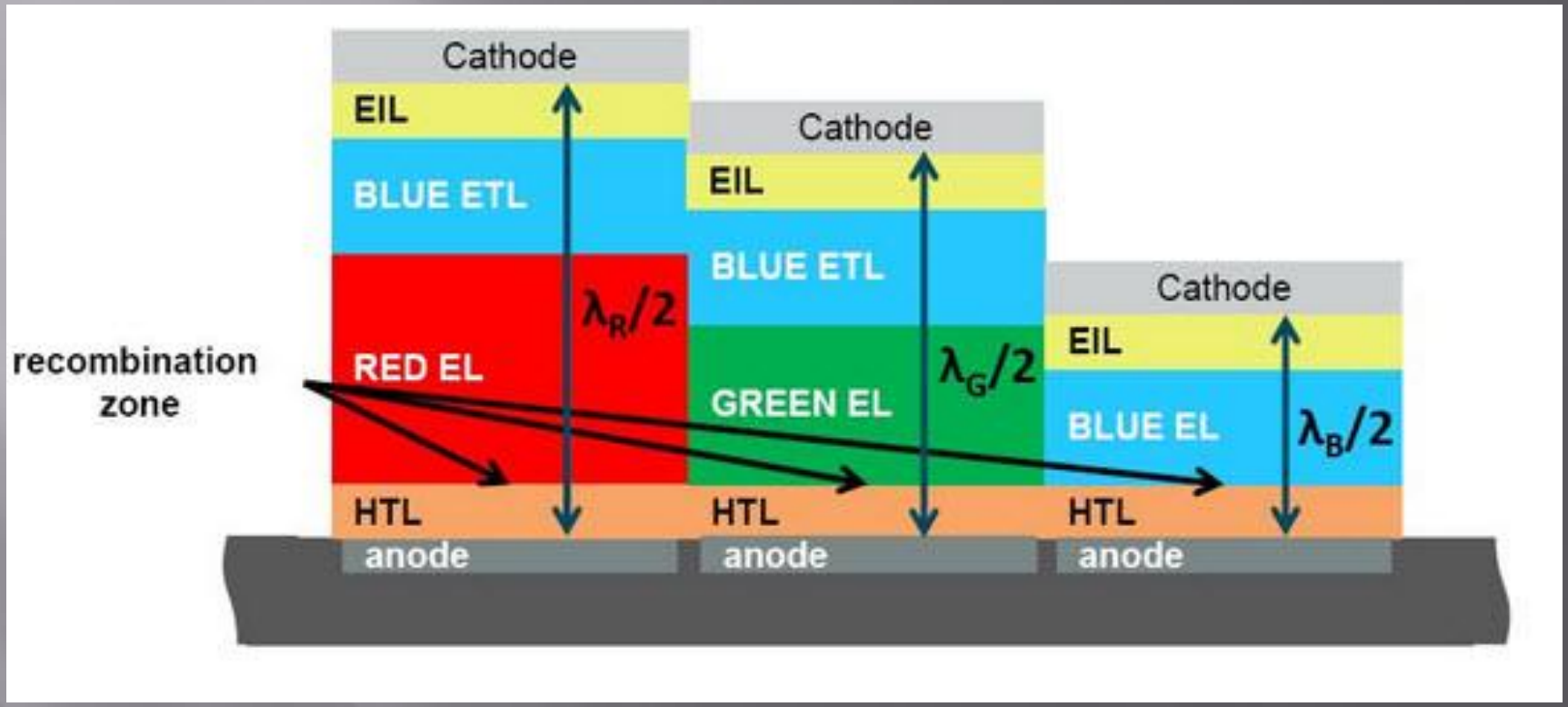
```
material material=Alq3 hopn.gamma=$gamma hopp.gamma=$gamma
material material=Alq3 hopn.beta=2.5 hopp.beta=2.5
material material=Alq3 hopn.v0=8e12 hopp.v0=8e12
material material=Alq3 affinity=3.2 eg300=2.8 nc300=1e21 nv300=
1e21 \
         permi=3.0

mobility material=Alq3 hopmob.n hopmob.p

contact name=anode   workf=5.8
contact name=cathode workf=5.4

solve init
solve prev

output con.band val.band e.mobility h.mobility

save outf=organicex03_0.str

solve vstep=0.2 vfinal=1.0 name=anode

save outf=organicex03_1.str
```


Hopping Mobility Verses Dopant Concentration (%)
Sigma=0.34, N1+N2=2e20cm-3, v0=8e12 sec-1
mobility
Gamma=3.5e7 1/cm
3.0e7
2.5e7
Sigma1=0.05 eV
Mobility (cm2/Vs)
Doping Concentration (%)
0
-1
-2
-3
-4
-5
-6
-7
-5
-4
-3
-2
-1
0
1
2
3

S4: Poređenje dvoslojnih i troslojnih OLED

- 2-slojna OLED:
  - HTL – hole transport layer
  - ETL (EIL) – electron transport (injection) layer
- Dobra OLED struktura zahteva dovoljnu injekciju nosilaca, tako da dobijamo veću gustinu exciton, kada se nosioci rekombinuju.
- Ova struktura ima male struje zbog loših karakteristika spoja metal/organski materijal pa su zbog toga i efikasnosti manje.
- Komercijalne OLED strukture su višeslojne!!!


V
A
Cathode
Emissive Layer
Transparent Anode
Glass Substrate
Light Emision
Cathode
(Mg)
Anode
(ITO)


Cathode
EIL
BLUE ETL
RED EL
HTL
anode
Cathode
EIL
BLUE ETL
GREEN EL
HTL
anode
Cathode
EIL
BLUE EL
HTL
anode
recombination zone
λR/2
λG/2
λB/2

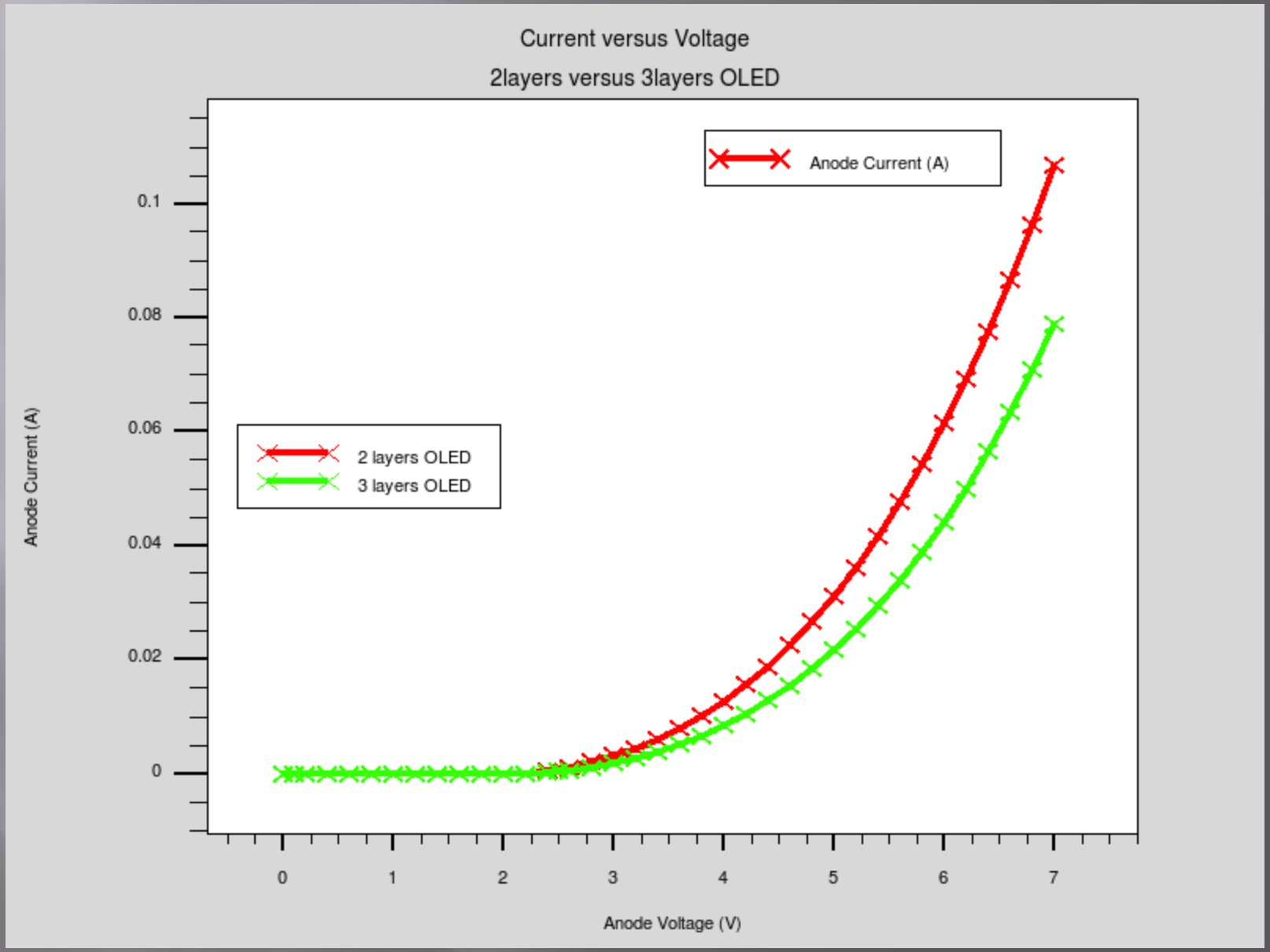
```
#####################################
# 2 Layers
#####################################

go atlas

mesh width=1e8

x.m l=0 s=0.5
x.m l=1 s=0.5

y.m l=0 s=0.002
y.m l=0.06 s=0.0001
y.m l=0.1 s=0.001


region num=1 user.mat=HIL y.min=0 y.max=0.06
region num=2 user.mat=ETL y.min=0.06 y.max=0.1

elec num=1 name=anode top
elec num=2 name=cathode bottom

interface s.s thermionic tunnel y.min=0.059 y.max=0.061 \
dd.tunnel=0.01 dy.tunnel=0.001

contact name=anode workf=5.01 surf.rec
contact name=cathode workf=3.08 surf.rec

ointdefect s.s cont y.min=0.058 y.max=0.062 numa=24 numd=24 ha=1.4e10 hd=1.4e10 tca=5500 \
tcd=5500 afile=organicex04_0_ointaccep.dat dfile=organicex04_0_ointdon.dat \
sigae=1e-16 sigah=1e-14 sigde=1e-14 sigdh=1e-16
```

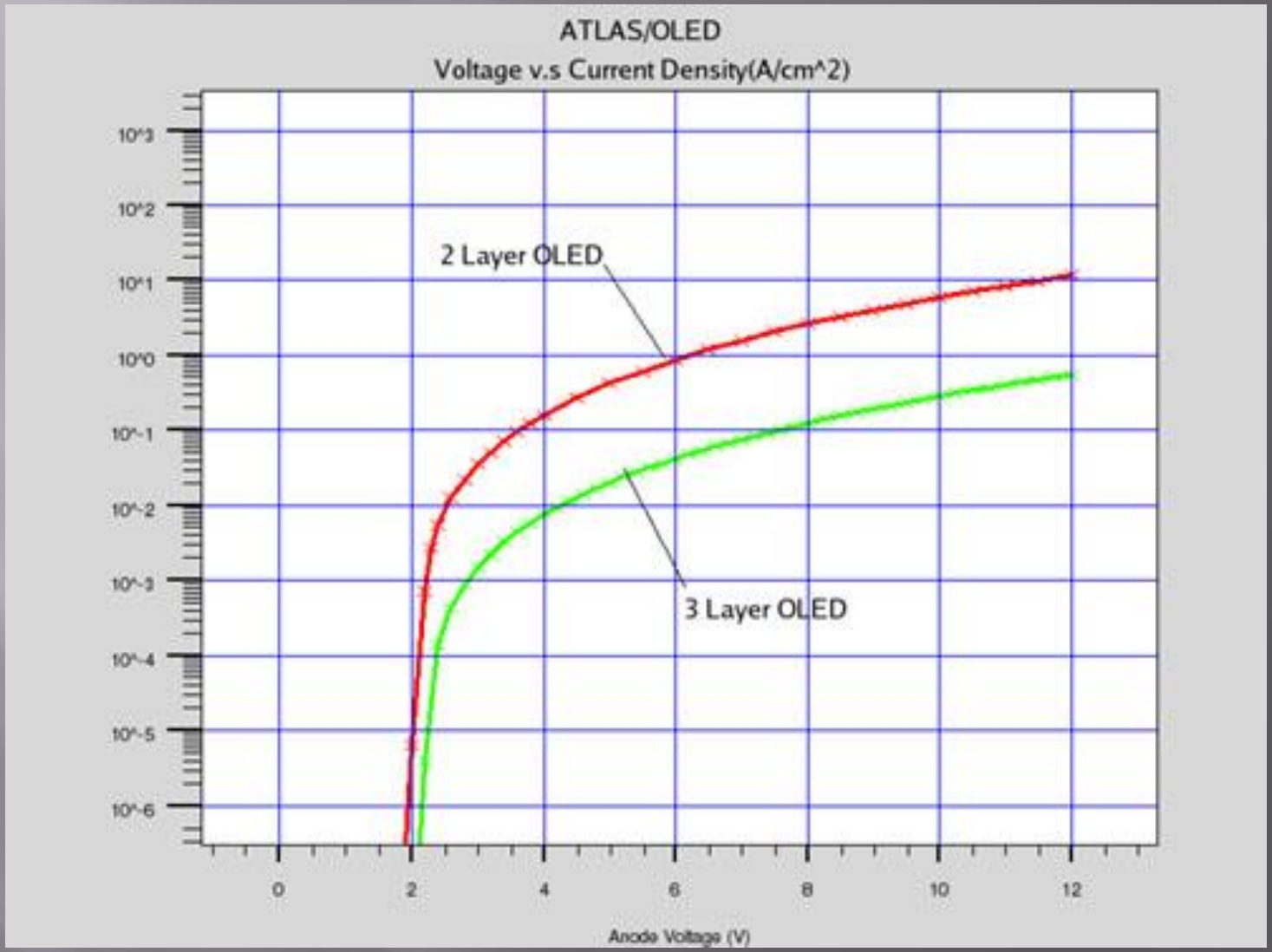
```
odefects region=1 cont ha=2e16 hd=2e16 tca=2700 tcd=2700 numa=30 numd=30
odefects region=2 cont ha=2e16 hd=2e16 tca=2700 tcd=2700 numa=30 numd=30

set LUMO1=2.31
set HOMO1=5.31
set eg300_1=$HOMO1-$LUMO1

set LUMO3=2.98
set HOMO3=5.68
set eg300_3=$HOMO3-$LUMO3

material region=1 user.default=organic user.group=semiconductor \
eg300=$eg300_1 affinity=$LUMO1 permi=3.5 nv300=2e19 nc300=2e19

material region=2 user.default=organic user.group=semiconductor \
eg300=$eg300_3 affinity=$LUMO3 permi=3.5 nv300=2e19 nc300=2e19

material region=1 rst.exciton=0.25 lds.exciton=0.01 taus.exciton=10e-9
material region=2 rst.exciton=0.25 lds.exciton=0.01 taus.exciton=10e-9


mobility region=1 mun0=1.1e-4*2 mup0=8.83e-5*2 e0n.pfmob=5e4 e0p.pfmob=5e4
mobility region=2 mun0=5.52e-06*2 mup0=3.68e-7*2 e0n.pfmob=1.5e6 e0p.pfmob=1.5e6

models pfmob langevin singlets

output u.langevin band.param con.band val.band \
charge e.field e.mobility h.mobility traps
```

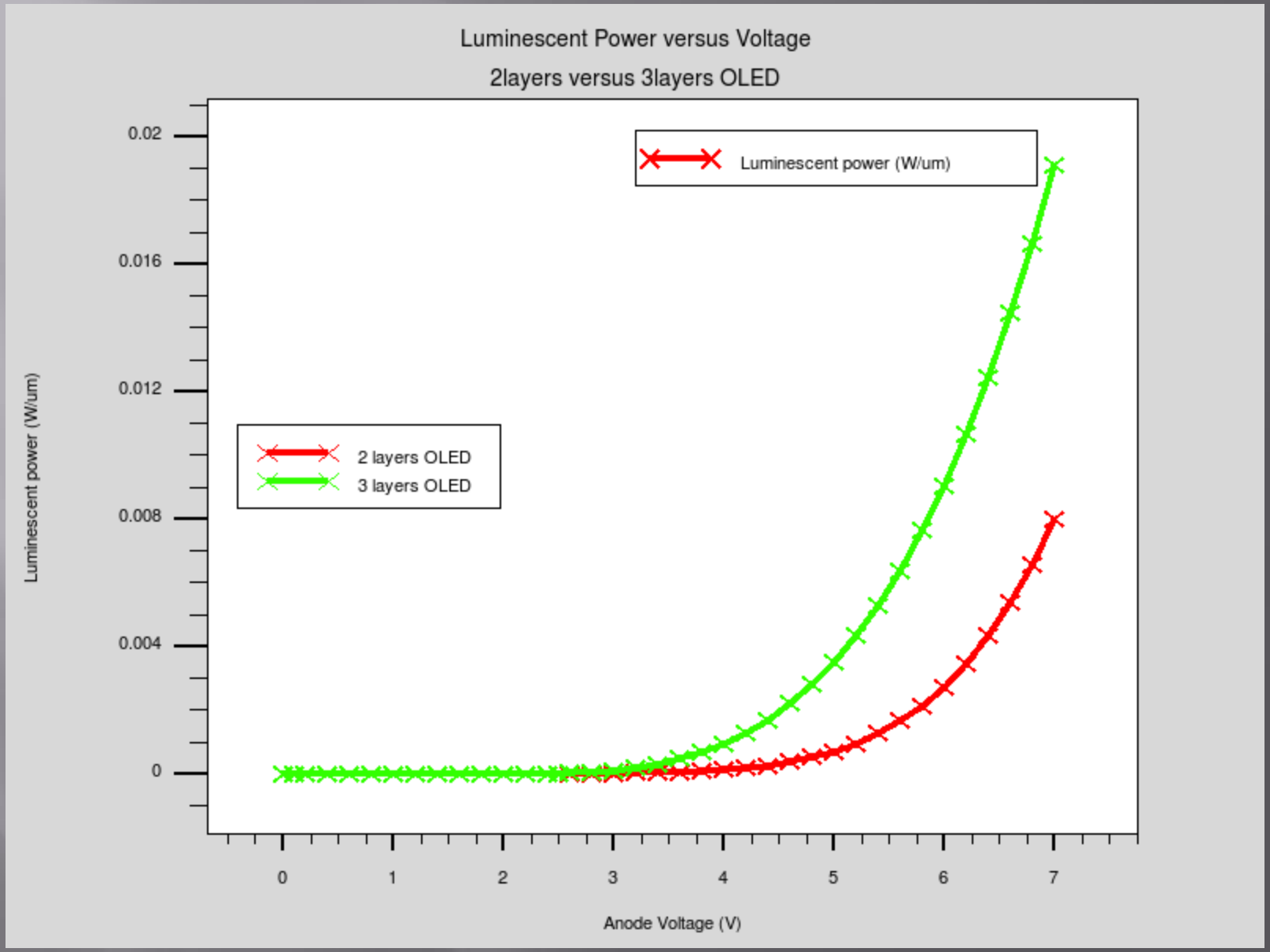
```
####################################
# 3 Layers
####################################


go atlas

mesh width=1e8

x.m l=0 s=0.5
x.m l=1 s=0.5

y.m l=0 s=0.002
y.m l=0.06 s=0.0001
y.m l=0.07 s=0.0005
y.m l=0.08 s=0.0001
y.m l=0.10 s=0.001

region num=1 user.mat=HIL y.max=0.06
region num=2 user.mat=HTL y.min=0.06 y.max=0.08
region num=3 user.mat=ETL y.min=0.08 y.max=0.10

elec num=1 name=anode top
elec num=2 name=cathode bottom

interface s.s thermionic tunnel y.min=0.059 y.max=0.061 \
dd.tunnel=0.01 dy.tunnel=0.001

interface s.s thermionic tunnel y.min=0.079 y.max=0.081 \
dd.tunnel=0.01 dy.tunnel=0.001


contact name=anode workf=5.01 surf.rec barrier
contact name=cathode workf=3.08 surf.rec barrier
```

```
ointdefect s.s cont y.min=0.058 y.max=0.062 numa=24 numd=24 ha=1.4e10 hd=1.4e10 tca=5500 \
tcd=5500 afile=organicex04_0_ointaccep.dat dfile=organicex04_0_ointdon.dat \
sigae=1e-16 sigah=1e-14 sigde=1e-14 sigdh=1e-16


ointdefect s.s cont y.min=0.079 y.max=0.081 numa=24 numd=24 ha=2.2e8 hd=2.2e8 tca=3000 \
tcd=3000 afile=organicex04_1_ointaccep.dat dfile=organicex04_1_ointdon.dat \
sigae=1e-16 sigah=1e-14 sigde=1e-14 sigdh=1e-16

odefects region=1 cont ha=2e16 hd=2e16 tca=2700 tcd=2700 \
afile=acep1.dat dfile=don1.dat numa=30 numd=30
odefects region=2 cont ha=2e16 hd=2e16 tca=2700 tcd=2700 \
afile=acep2.dat dfile=don2.dat numa=30 numd=30
odefects region=3 cont ha=2e16 hd=2e16 tca=2700 tcd=2700 \
afile=acep3.dat dfile=don3.dat numa=30 numd=30


set LUMO1=2.31
set HOMO1=5.31
set eg300_1=$HOMO1-$LUMO1

set LUMO2=2.48
set HOMO2=5.44
set eg300_2=$HOMO2-$LUMO2

set LUMO3=2.98
set HOMO3=5.68
set eg300_3=$HOMO3-$LUMO3
```

```
material region=1 user.default=organic user.group=semiconductor \
eg300=$eg300_1 affinity=$LUMO1 permi=3.5 nv300=2e19 nc300=2e19

material region=2 user.default=organic user.group=semiconductor \
eg300=$eg300_2 affinity=$LUMO2 permi=3.5 nv300=2e19 nc300=2e19

material region=3 user.default=organic user.group=semiconductor \
eg300=$eg300_3 affinity=$LUMO3 permi=3.5 nv300=2e19 nc300=2e19


material region=1 rst.exciton=0.25 lds.exciton=0.01 taus.exciton=10e-9
material region=2 rst.exciton=0.25 lds.exciton=0.01 taus.exciton=10e-9
material region=3 rst.exciton=0.25 lds.exciton=0.01 taus.exciton=10e-9

mobility region=1 mun0=1.1e-4*2 mup0=8.83e-5*2 e0n.pfmob=5e4 e0p.pfmob=5e4
mobility region=2 mun0=2.13e-05*2 mup0=5.15e-6*2 e0n.pfmob=2.5e5 e0p.pfmob=1.5e5
mobility region=3 mun0=5.52e-06*2 mup0=3.68e-7*2 e0n.pfmob=1.5e6 e0p.pfmob=1.5e6

models pfmob langevin singlet print

output u.langevin band.param con.band val.band \
charge e.field e.mobility h.mobility

probe name="int_exciton" exciton integr

solve init
```


Current versus Voltage
2layers versus 3layers OLED
Anode Current (A)
2 layers OLED
3 layers OLED
Anode Current (A)
0.1
0.08
0.06
0.04
0.02
0
0
1
2
3
4
5
6
7
Anode Voltage (V)


ATLAS/OLED
Voltage v.s Current Density(A/cm^2)
10^3
10^2
10^1
10^0
10^-1
10^-2
10^-3
10^-4
10^-5
10^-6
2 Layer OLED
3 Layer OLED
0
2
4
6
8
10
12
Anode Voltage (V)


Luminescent Power versus Voltage
2layers versus 3layers OLED
Luminescent power (W/um)
2 layers OLED
3 layers OLED
Luminescent power (W/um)
0.02
0.016
0.012
0.008
0.004
0
0
1
2
3
4
5
6
7
Anode Voltage (V)