TCAD

TCAD milestones for the next 5 years:

- **M1: Comparison of commercial TCAD tools; preparation of a recommendation for parameters and physics models. (Q4/2019)**
- **M2: Development of a reliable radiation damage model covering the HL-LHC fluences for protons and neutrons for a given operation temperature. The model shall be able to reproduce I-V, C-V, CCE and the E-field including double junction effects. (Q4/2020)**
- **M3: Model M1 extended to cover temperature dependence of the bulk-damage related effects from room temperature down to -30 °C. (Q3/2021):**
- **M4: Model from M2 extended to cover annealing effects (Q3/2022):**
- **M5: Model of the donor and acceptor removal (SiPMs, LGAD, CMOS,..) (Q3/2020):**
- **M6: Surface damage model with correct modelling of surface damage in p-type segmented sensors. (Q1/2021)**
- **M7: Evaluation of the possibility of the implementation of cluster related defects in the commercial TCAD device simulators by using a charge carrier occupation dependent energy level distribution. (Q2/2021)**

M1

Synopsys and Silvaco TCAD use different parameterizations and models for band gap, density of states, thermal velocities etc.

- Examples:
  - band gap:

```
##### Synopsys #####
def E_g(T):
    Eg0 = 1.16964  # Bandgap at T=0K
    alpha = 4.73E-4 #
    beta = 636.0
    return Eg0 - alpha * T**2 / (T + beta)
```

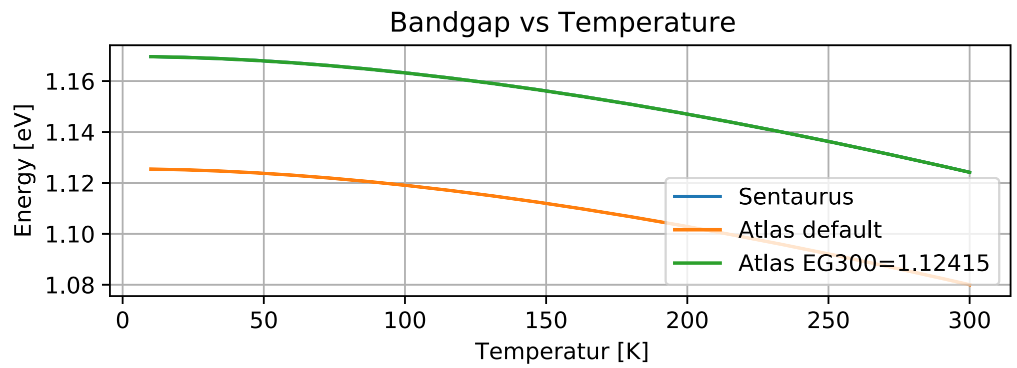
```
#####Silvaco #####
def E_g_Silvaco(T,EG300=1.08):
#    EG300 = 1.08  # Bandgap at T=300K
    EGALPHA = 4.73E-4 #
    EGBETA= 636.0
    return EG300 + EGALPHA*(300**2 /(300.0+EGBETA) - T**2 / (T + EGBETA))
```

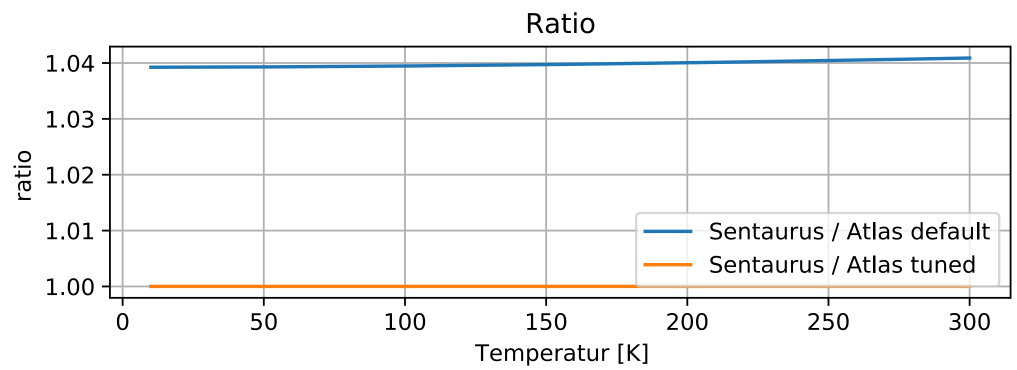
  - hole effective density of state:

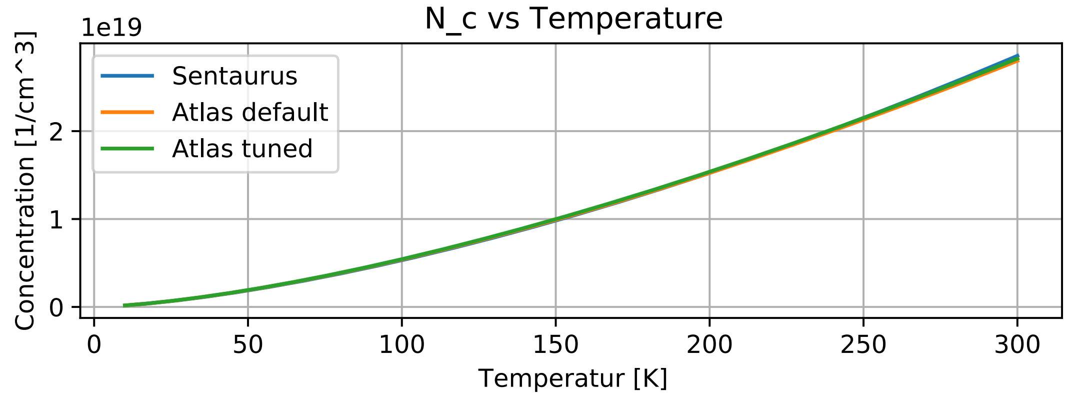
```
##### hole effective mass #####
def mass_p(T):
    a = 0.4435870
    b = 0.3609528E-2
    c = 0.1173515E-3
    d = 0.1263218E-5
    e = 0.3025581E-8
    f = 0.4683382E-2
    g = 0.2286895E-3
    h = 0.7469271E-6
    I = 0.1727481E-8
    return ((a+b * T + c * T**2 + d * T**3 + e * T**4) /
            (1.0+f * T + g * T**2 + h * T**3 + I * T**4))**(2.0/3.0)

##### hole effective density of states ####
def N_v(T):
    return 2.50941675E19 * (mass_p(T))**1.5 * (T / 300.0)**1.5
```

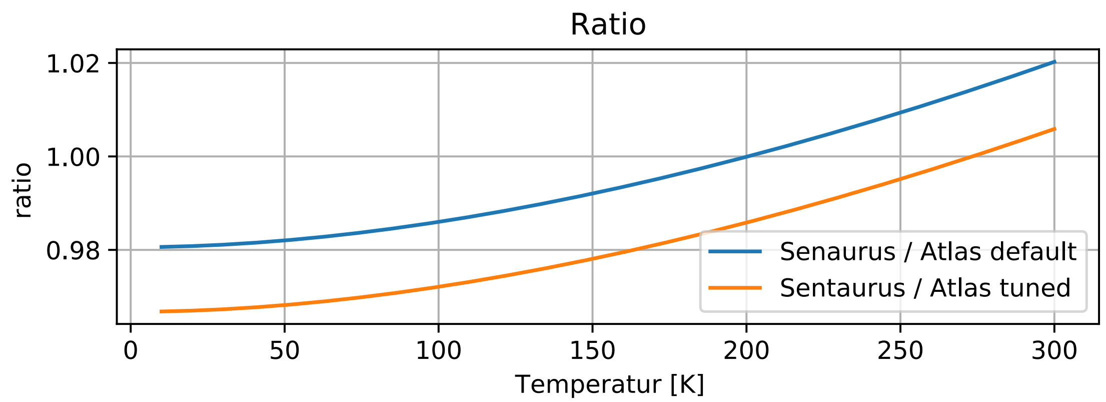
```
#####Silvaco #####
def N_v_Silvaco(T, NV300=1.04e19):
    NVF = 1.5
    return  NV300*(T / 300.0)**NVF
```

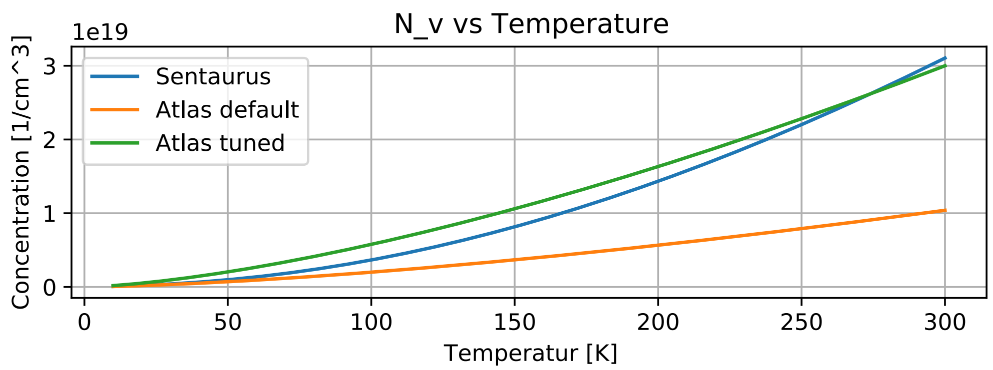
M1

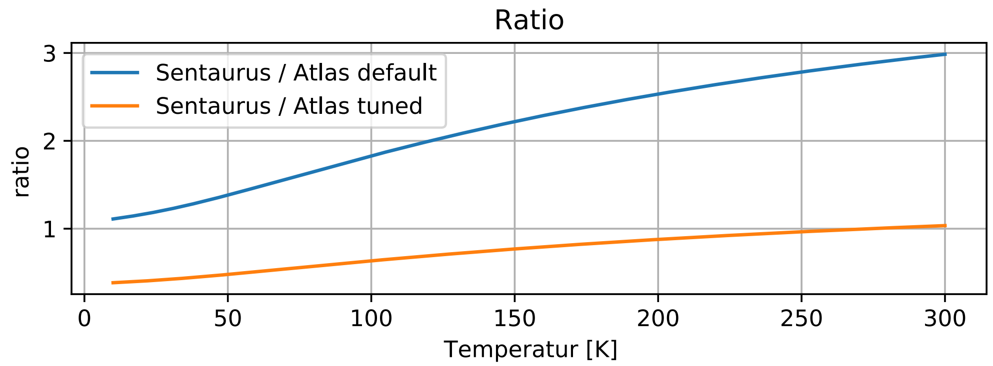

Bandgap vs Temperature
Energy [eV]
Temperatur [K]
Sentaurus
Atlas default
Atlas EG300=1.12415

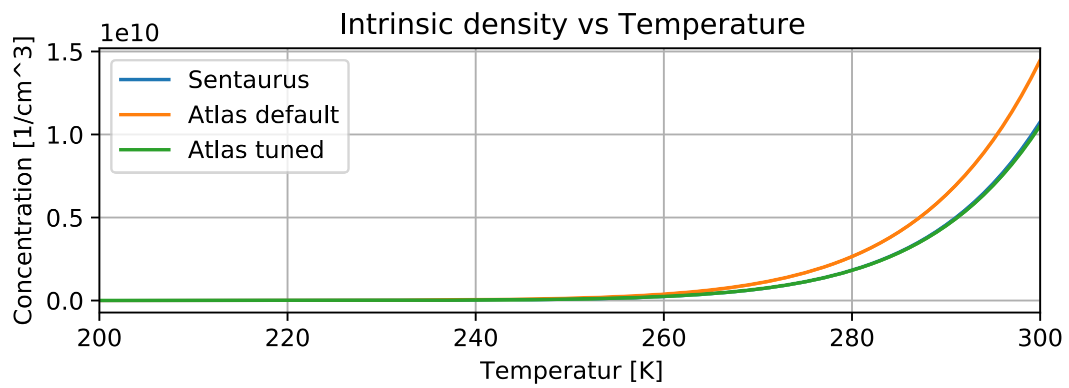

Ratio
ratio
Temperatur [K]
Sentaurus / Atlas default
Sentaurus / Atlas tuned

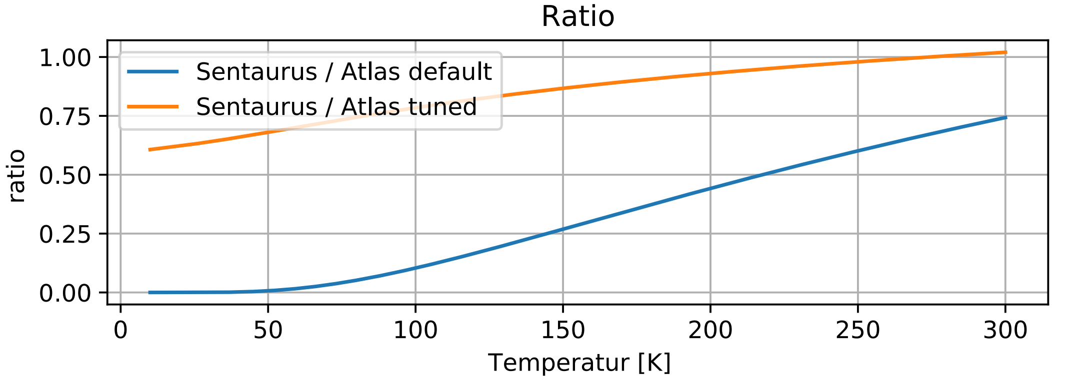

N_c vs Temperature
1e19
Concentration [1/cm^3]
Temperatur [K]
Sentaurus
Atlas default
Atlas tuned


Ratio
ratio
Temperatur [K]
Senaurus / Atlas default
Sentaurus / Atlas tuned


N_v vs Temperature
1e19
Concentration [1/cm^3]
Temperatur [K]
Sentaurus
Atlas default
Atlas tuned


Ratio
ratio
Temperatur [K]
Sentaurus / Atlas default
Sentaurus / Atlas tuned


Intrinsic density vs Temperature
1e10
Concentration [1/cm^3]
Temperatur [K]
Sentaurus
Atlas default
Atlas tuned


Ratio
ratio
Temperatur [K]
Sentaurus / Atlas default
Sentaurus / Atlas tuned

M1

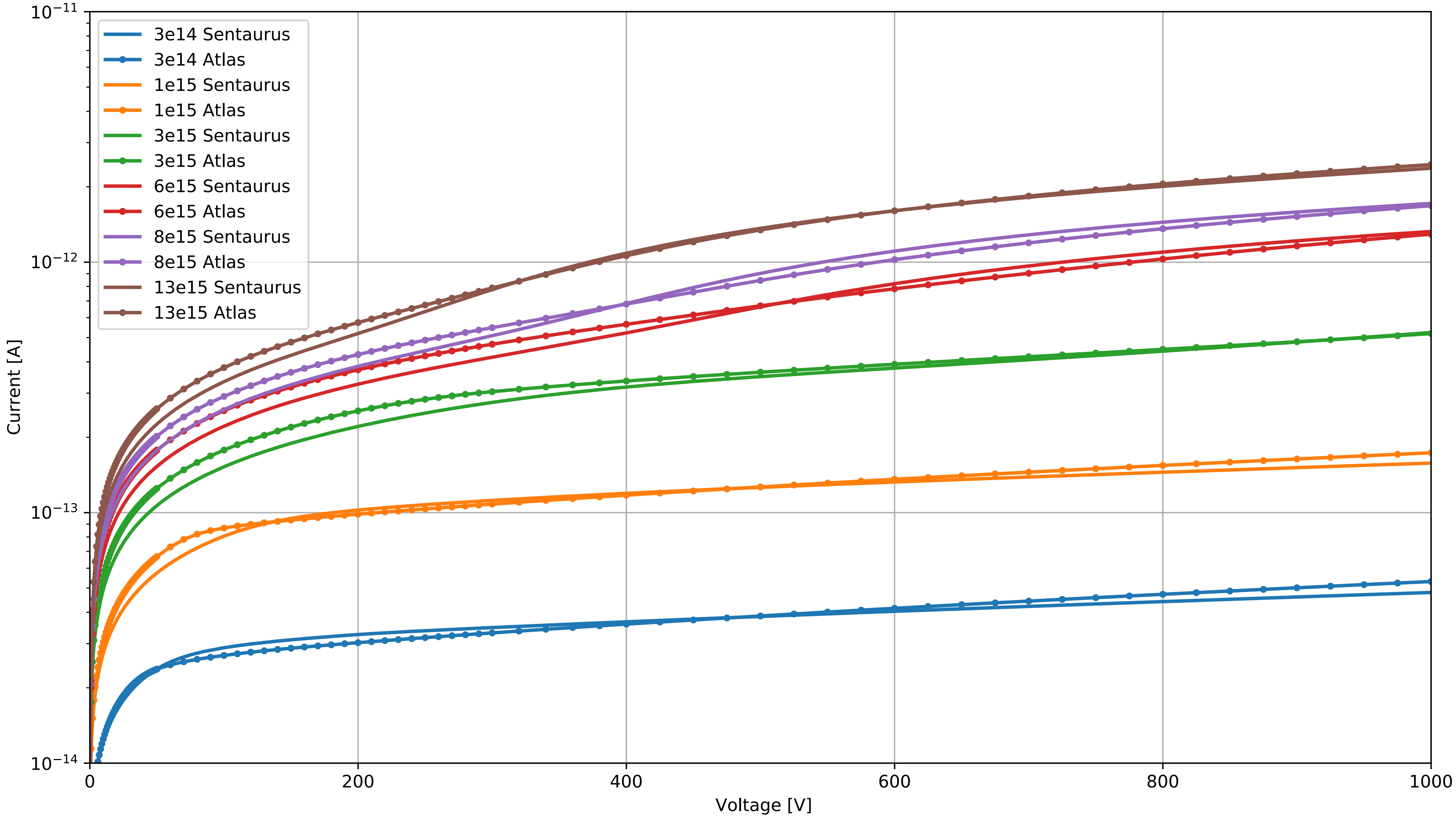
Synopsys and Silvaco TCAD comparison using the HPTM

- 1D diode, n⁺-p, thichness 200 µm

TABLE I
HAMBURG PENTA TRAP MODEL (HPTM) PARAMETER

Defect	Type	Energy	g_{int} [cm^{-1}]	σ_e [cm^2]	σ_h [cm^2]
E30K	Donor	E_C-0.1 eV	0.0497	2.300E-14	2.920E-16
V_3	Acceptor	E_C-0.458 eV	0.6447	2.551E-14	1.511E-13
I_p	Acceptor	E_C-0.545 eV	0.4335	4.478E-15	6.709E-15
H220	Donor	E_V+0.48 eV	0.5978	4.166E-15	1.965E-16
C_iO_i	Donor	E_V+0.36 eV	0.3780	3.230E-17	2.036E-14

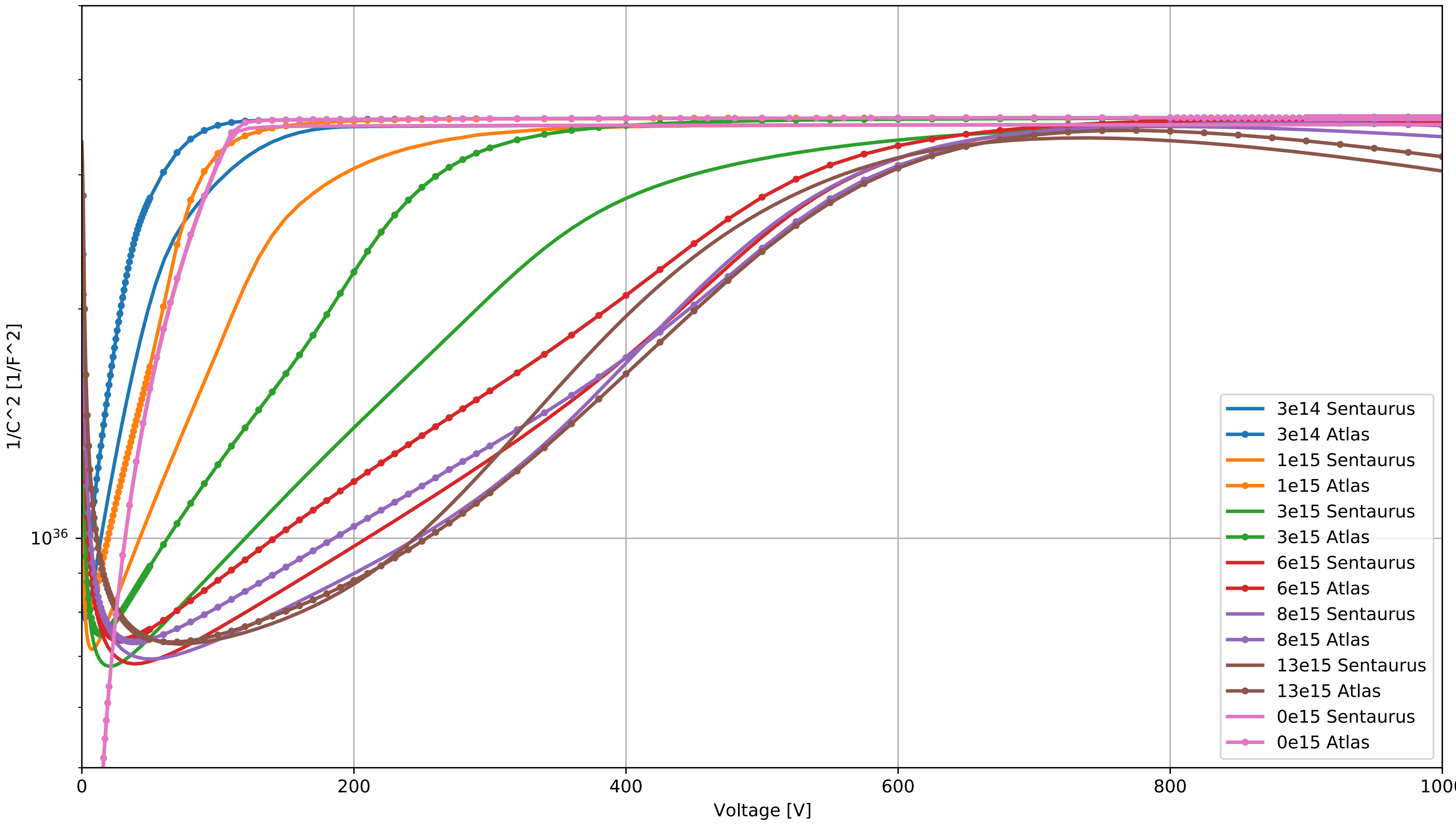
I-V at T = -20°C



All Silvaco TCAD simulations done by Marco Bomben

M1

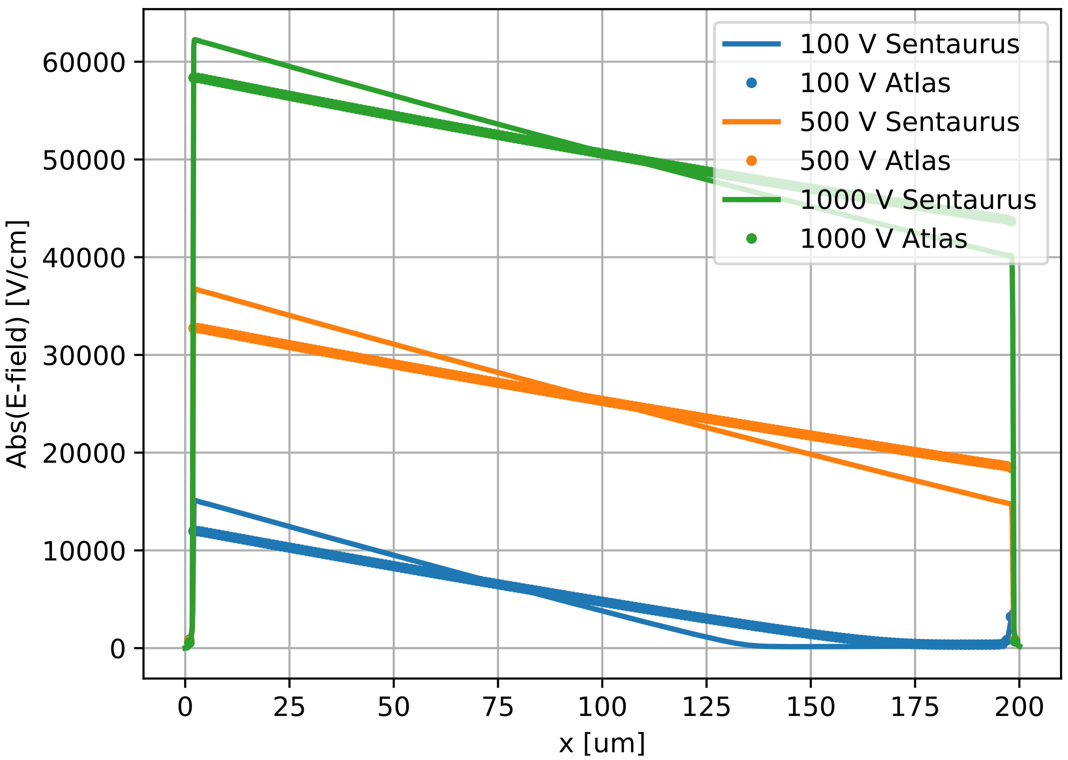
1/C^2-V at 1kHz and T = -20°C



M1

E-Field at different voltages

$\Phi_{eq} = 3{\cdot}10^{14}\ cm^{-2}$



$\Phi_{eq} = 3{\cdot}10^{15}\ cm^{-2}$