# InP Default Parameter Check Up For Sentaurus™ Device

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OUR VOICES WILL DEFINE THE CENTURY

UC SANTA CRUZ

## Overview

- “InP.par” in the TCAD projects directory includes default parameters for InP material.
- The parameter file can be extracted via `sdevice -P:InP` command. This command will spray the parameter information into the system’s standard output interface. Thus, you will save the output by redirecting it to a file.
- `sdevice -P:InP > InP.par`
- Note that the file needs to be assigned as parameter variable in the TCAD input deck to be applied correctly.

# TCAD
# Model Descriptions

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## Epsilon / Epsilon_aniso

Dielectric Constant, aniso means anisometric constant which will be applied to vertical components: i.e. Lombardi's mobility model. But this model will not be used in our simulation yet.

The default dielectric constant of this InP model is 12.4.

$$\varepsilon_r = 12.4$$

## RefractiveIndex / ComplexRefractiveIndex

Only used for optical simulation including ‘raytracing’. Depends on our usecases, but this ‘optical simulation’ literally means ‘optical’ wavelengths. Which only contains the ‘visible’ light wavelengths.

Therefore, those sections are not relevant at the moment.

## SpectralConversion

No default model exists. Also, not being used at the moment.

This is a parameter that simulates scintillators or any similar optical spectral conversion happens.

## EnergyRelaxationTime

Thermo-dynamic model is **not relevant** since we are not simulating Peltier heat generation/consumption. So, this section is also not relevant as well. Regardless, here are energy relaxation time in ps.

$$\tau_{w.elec} = 1\,ps$$

$$\tau_{w.hole} = 0.4\,ps$$

## AvalancheFactors

Avalanche generation modifiers for thermo-hydro factor simulation. Not relevant for now since we are not simulating Peltier contacts.

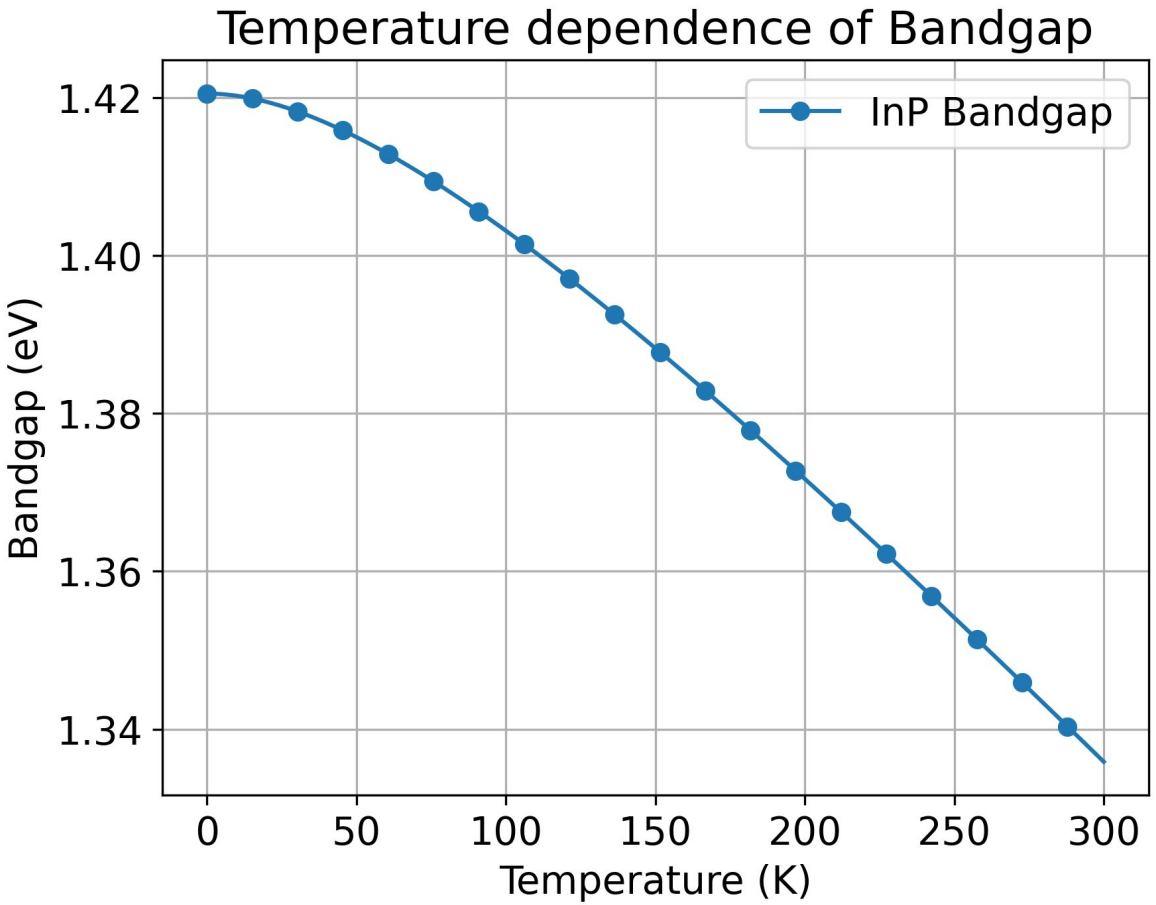
## Bandgap

Classical semiconductor bandgap equation is employed. Additionally, the simulator receives the electron affinity. T par means lattice temperature that will be employed for phonon simulations.

| Equation | Default Parameters |
| --- | --- |
| $$E_g = E_{g0} + \frac{\alpha {T_{par}}^2}{\beta + T_{par}} - \frac{\alpha T^2}{\beta + T}$$ $$\text{where, } \chi_0 = 4.4$$ | $\chi_0 = 4.4\,\text{eV}$<br>$E_{g0} = 1.4205\,\text{eV}$<br>$\alpha = 4.1 \times 10^{-4}\,\text{eV/K}$<br>$\beta = 1.36 \times 10^{2}\,\text{K}$<br>$E_{g.min} = -1 \times 10^{1}\,\text{eV}$<br>$dE_{g.min} = 0.0\,\text{eV}$<br>$T_{par} = 0.0\,\text{K}$ |

Since $T_{par}$ = 0. Default Eg is partly dependent on the ambient temperature.

**Bandgap over Lattice Temperature (Default Parameters)**



## FreeCarrierAbsorption

At this moment, this factor is **not relevant at the moment** since we are not using quantum yield model (QuantumYield) which determines how much of photo-electric energy conversion efficiency. Additionally, this factor can be controlled by ComplexRefractiveIndex model by those coefficients.

$$\mathrm{FCA}_{\alpha.n} = 4.0 \times 10^{-18} \, /\mathrm{cm}$$

$$\mathrm{FCA}_{\alpha.p} = 8.0 \times 10^{-18} \, /\mathrm{cm}$$

## BandstructureParameters / QWStrain

A specific parameter to simulate Wurtzite crystals: for strong coupling of three valence bands: Heavy holes, light holes, and crystal-field split holes.

QWStrain, Quantum-Well Strain, is also related to the specific type of crystal structure.

→ Both LED simulation parameters. **Not relevant!**

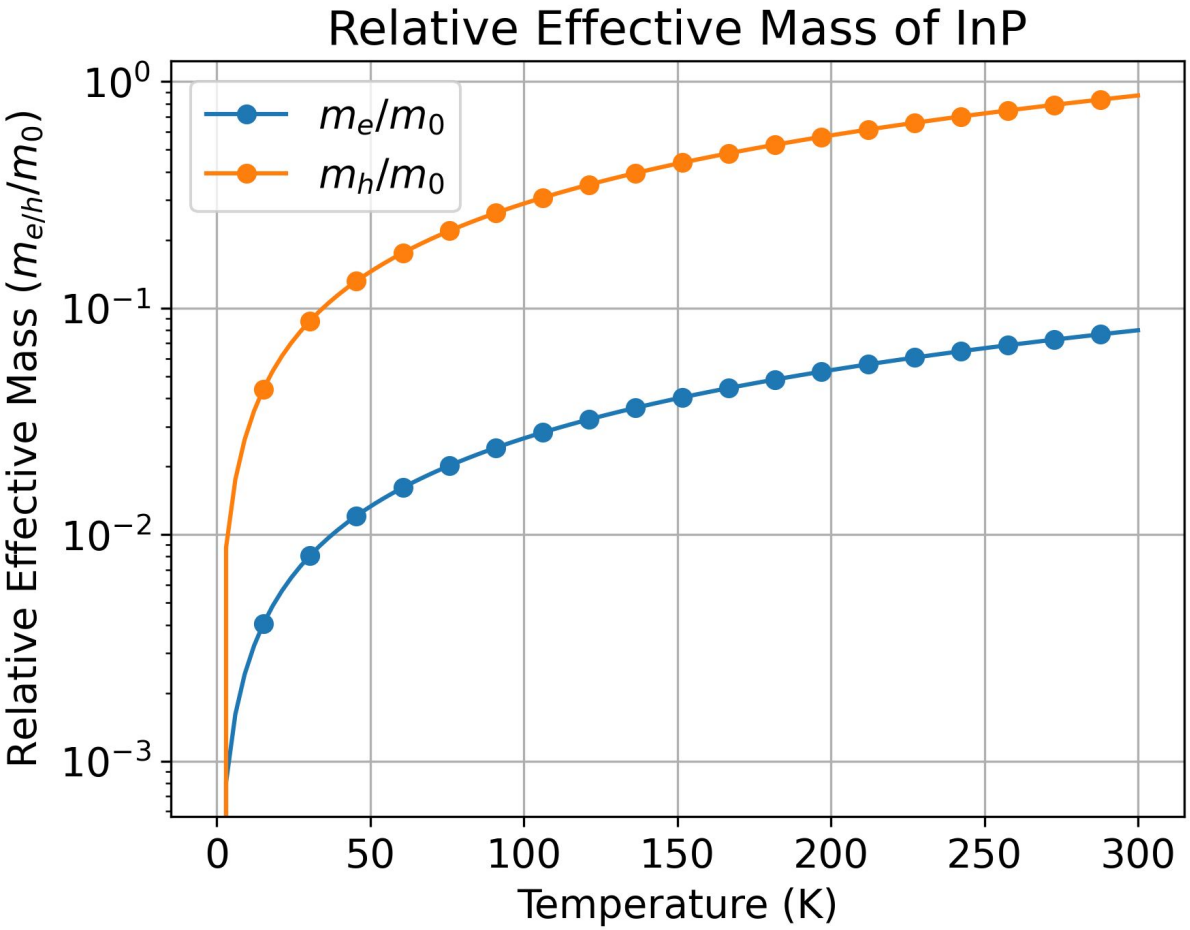
## Effective Mass (eDOSMass/hDOSMass)

Effective mass calculation is based on concentration coefficient method.

| Equation | Default Parameters |
| --- | --- |
| $\frac{m_{e/h}}{m_0} = \left( \frac{N_{c/v300}}{2.509 \times 10^{19}} \right)^{\frac{2}{3}}$<br>$N_{c/v}(T) = N_{c/v300} \left( \frac{T}{300} \right)^{\frac{3}{2}}$ | $N_{c300} = 5.66 \times 10^{17}\ /\mathrm{cm}^3$<br>$N_{v300} = 2.03 \times 10^{19}\ /\mathrm{cm}^3$ |

Nc300/Nv300 are concentration coefficients @ 300 K

## Effective Mass of Carriers over Lattice Temperature (Default Parameters)



## SchroedingerParameters

For effective **hole** masses, you can use different formulas. For this InP material, hMass models use Heavy/Light mass models. (Type 2)

$$m_l = 0.0089$$

$$m_h = 0.85$$

$$m_e = 0.0$$

Where $m_e$ is an electron coefficient for refractive index calculation which is not relevant in non-optical simulations.

## ConstantMobility and its aniso

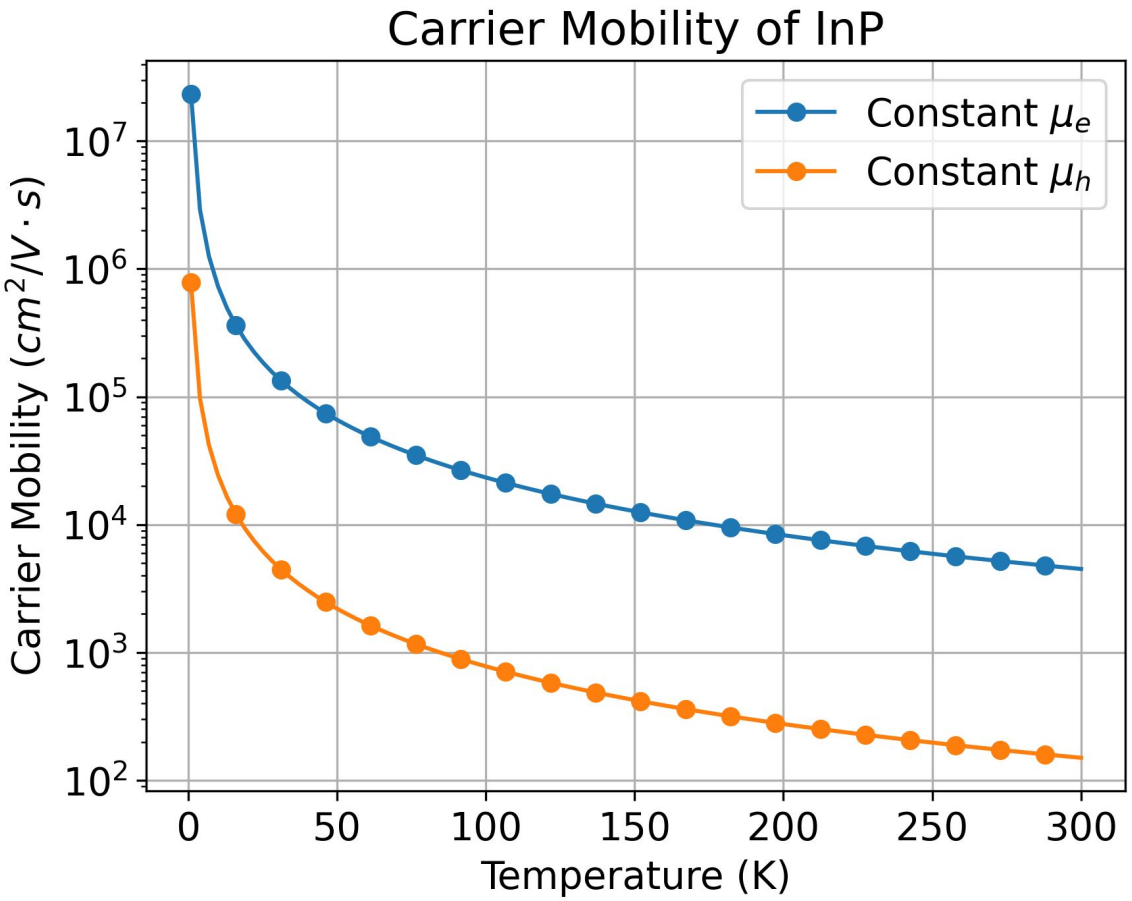
The constant mobility equation from any solid state textbook. Does not distinguish the vertical case.

| Equation | Default Parameters |
| --- | --- |
| $\mu_{e/h.const} = \mu_{e/h.max} \left( \frac{T}{T_0} \right)^{-\alpha_{e/h}}$ | $\mu_{e.max} = 4.5 \times 10^3 \ \mathrm{cm}^2/\mathrm{V} \cdot \mathrm{s}$<br>$\mu_{h.max} = 1.5 \times 10^2 \ \mathrm{cm}^2/\mathrm{V} \cdot \mathrm{s}$<br>$\alpha_e = 1.5$<br>$\alpha_h = 1.5$ |

Note that the alpha is a ‘fitting’ parameter while Mu e/h max are the field effect mobility measured with Hall-effect measurement.

At least, this mobility model dependent on the ambient temperature, T. T0 = 300K

## Constant Mobility over Lattice Temperature (Default Parameters)



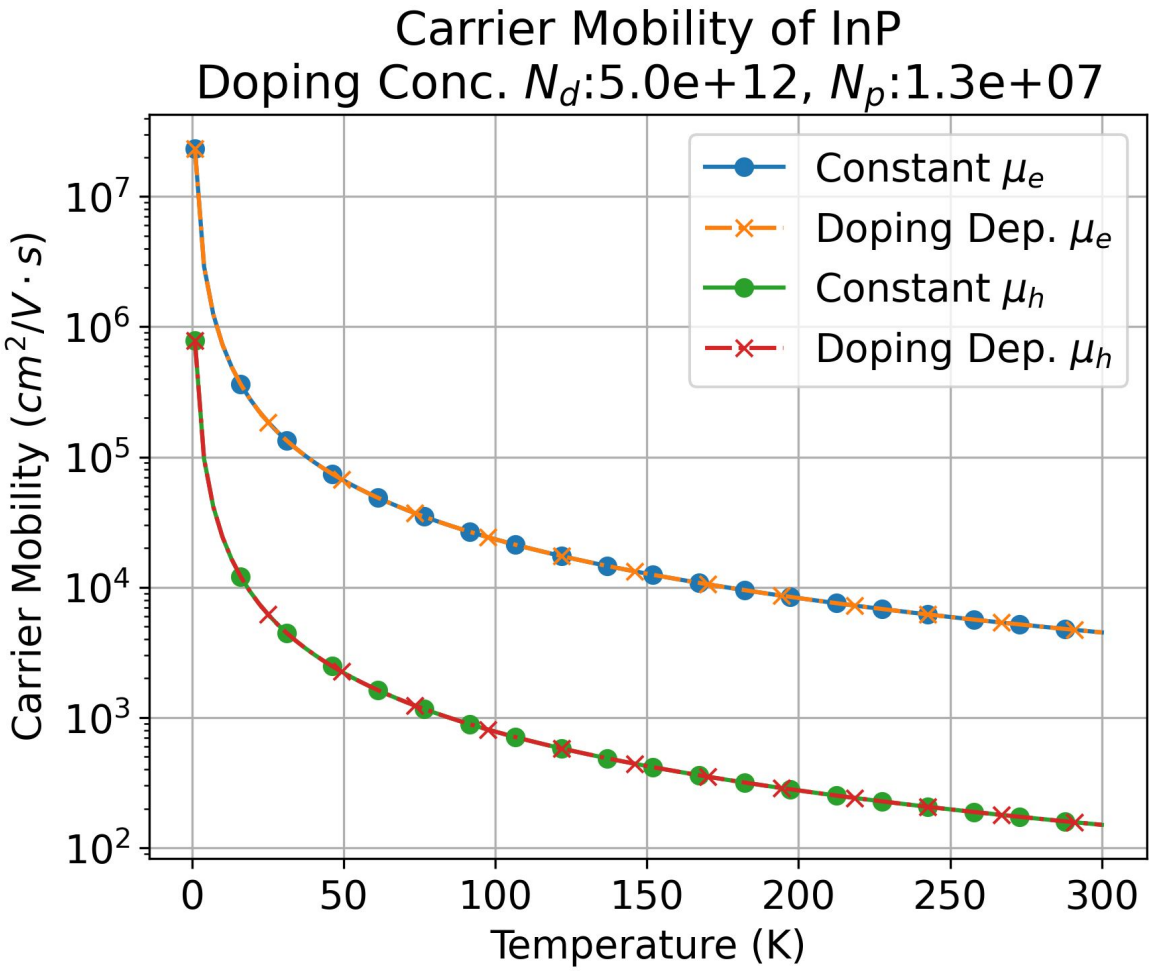
# Doping Dependent Mobility and its aniso

The default model parameter suggests Arora model instead of Masetti. Masetti model is a default model in Silicon but lacks temperature dependency. Thus, Arora seems to be more precise in this case.

| Equation | Default Parameters |
| --- | --- |
| $\mu_{dop} = \mu_{minA} + \frac{\mu_{dA}}{1 + \left(\frac{N}{N_{00}}\right)^{AA}}$ <br> where, <br> $\mu_{minA} = Ar_{\mu_{min}} \left(\frac{T}{T_0}\right)^{Ar_{alm}}$, <br> $\mu_{dA} = Ar_{\mu_d} \left(\frac{T}{T_0}\right)^{Ar_{ald}}$, <br> $N_{00} = Ar_{N_0} \left(\frac{T}{T_0}\right)^{Ar_{alN}}$, <br> $AA = Ar_a \left(\frac{T}{T_0}\right)^{Ar_{ala}}$ | $Ar_{\mu_{min}.e/h} = 4.5 \times 10^3, 1.5 \times 10^2\ \mathrm{cm}^2/\mathrm{V}\cdot\mathrm{s}$ <br> $Ar_{alm.e/h} = -1.5, -1.5$ <br> $Ar_{\mu_d.e/h} = 0.0, 0.0\ \mathrm{cm}^2/\mathrm{V}\cdot\mathrm{s}$ <br> $Ar_{ald.e/h} = 0.0, 0.0$ <br> $Ar_{N_0.e/h} = 1.0 \times 10^{17}, 1.0 \times 10^{17}\ /\mathrm{cm}^3$ <br> $Ar_{alN.e/h} = 0.0, 0.0$ <br> $Ar_{a.e/h} = 0.0, 0.0$ <br> $Ar_{ala.e/h} = 0.0, 0.0$ |

N is the ‘effective’ doping concentration. Also with default parameters, The equation becomes quite similar to the constant mobility. However, since we are not applying excessive doping, this may not factor into seriously…

## Doping Dependent Mobility over Temperature
## (Default Parameters → Same as Constant Mobility at the moment.)




- Note that our doping concentration is of $10^{12}$ /cm$^3$ range.
- Thus, against default Nref of $10^{17}$ /cm$^3$, doping concentration is not relevant.
- We can safely turn off this model at the moment?

## Mobility - High Field Dependence / aniso (Extended Canali Model)

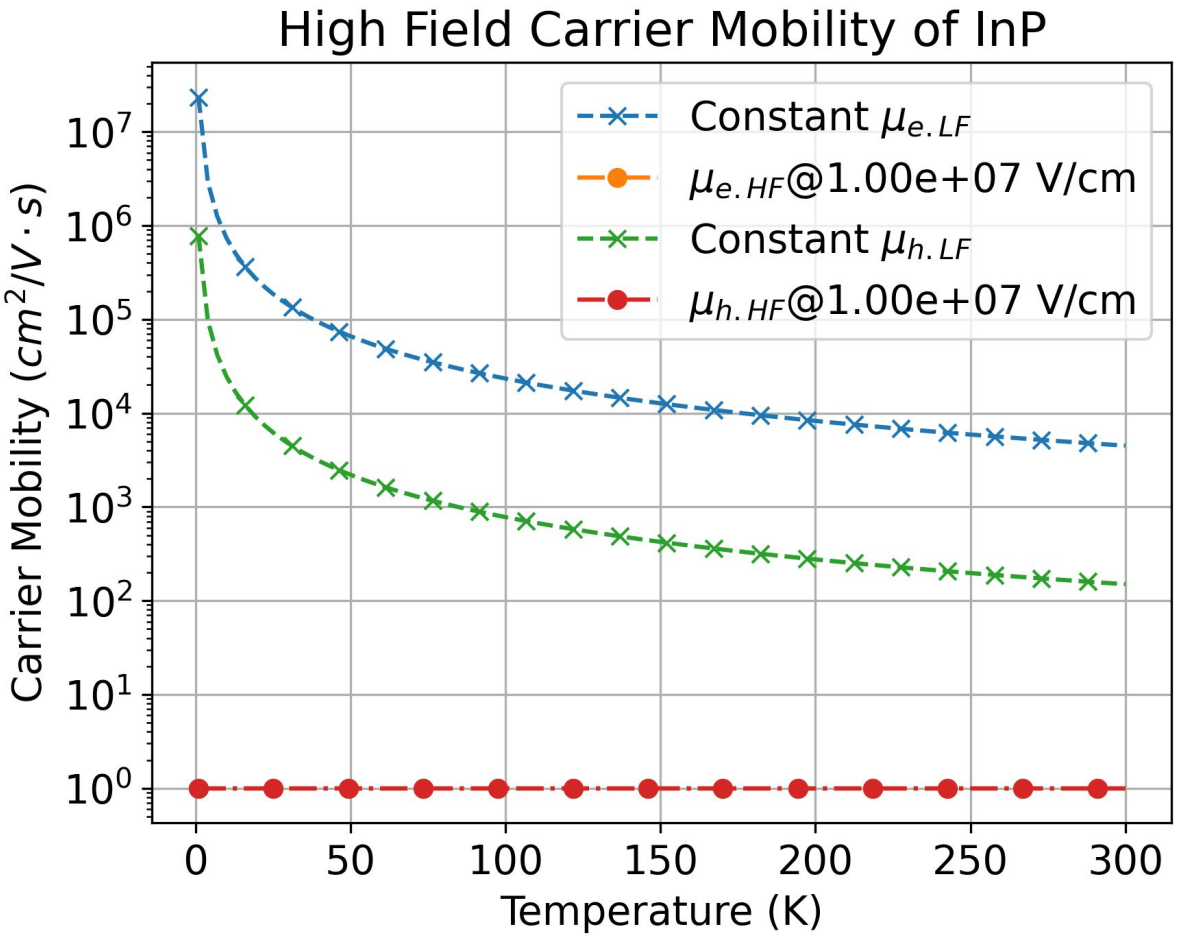
Due to fringing field effects on the pixel/guard ring edges, this might be the most important parameter.

| Equation | Default Parameters |
| --- | --- |
| $$\mu_{HF} = \frac{(\alpha+1)\mu_{LF}}{\alpha + \left[1 + \left(\frac{(\alpha+1)\mu_{LF}E}{v_{sat}}\right)^{\beta}\right]^{1/\beta}}$$ where, $$v_{sat} = A_{v_{sat}} - B_{v_{sat}}\left(\frac{T}{T_0}\right),$$ scale factors : $$\mu_{LF} = k_\mu \times \mu_{LF},$$ $$v_{sat} = k_v \times v_{sat}$$ | $$\beta = \beta_0 \left(\frac{T}{T_0}\right)^{\beta_{exp}}$$ $\beta_{0,e/h} = 2,\ 2$<br>$\beta_{exp,e/h} = 0.0,\ 0.0$<br>$\alpha_{e/h} = 0.0,\ 0.0$<br>$A_{v_{sat},e/h} = 1.0 \times 10^7,\ 1.0 \times 10^7$<br>$B_{v_{sat},e/h} = 0.0,\ 0.0$<br>$v_{sat.min,e/h} = 5.0 \times 10^5,\ 5.0 \times 10^5\ \mathrm{cm/s}$<br>$bs_{0,e/h} = 1.0,\ 1.0$<br>$ns_{0,e/h} = 1.0 \times 10^{50},\ 1.0 \times 10^{50}\ /\mathrm{cm}^3$<br>$k_{\mu,e/h} = 1.0,\ 1.0$<br>$k_{v,e/h} = 1.0,\ 1.0$ |

Hydro-HF parameters are omitted since we are not running phonon simulations yet.

Again, this parameter is omitting the temperature dependence with default values.

**Mobility - High Field Dependence**
**(Default Parameters) → Not valid yet. EField = 1.29e5 V/cm @ 450V bias**

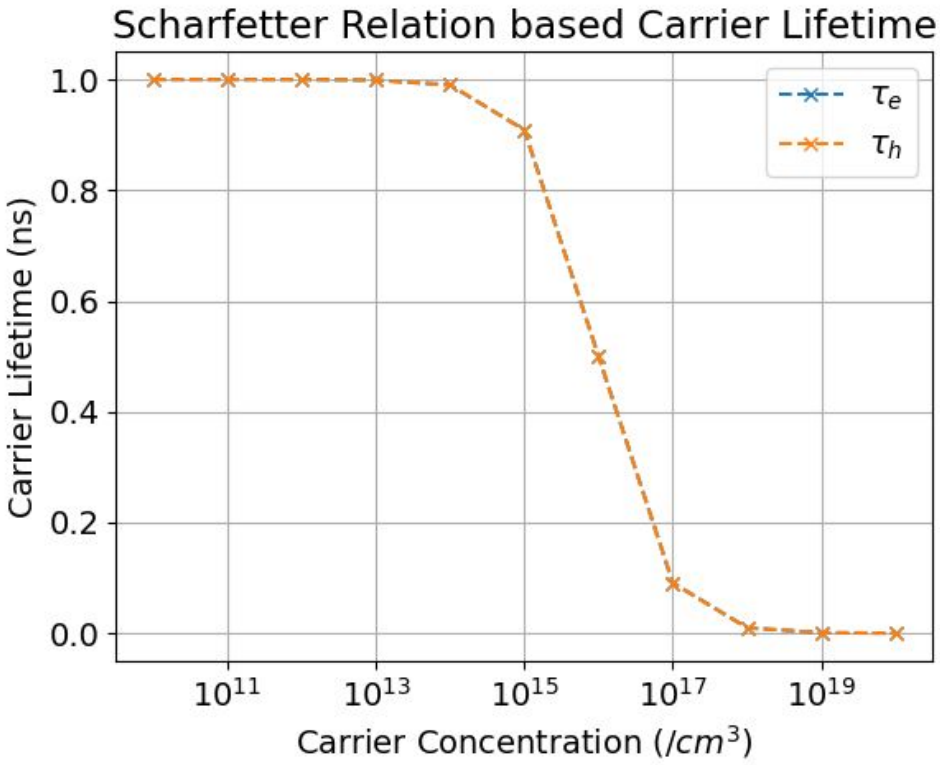


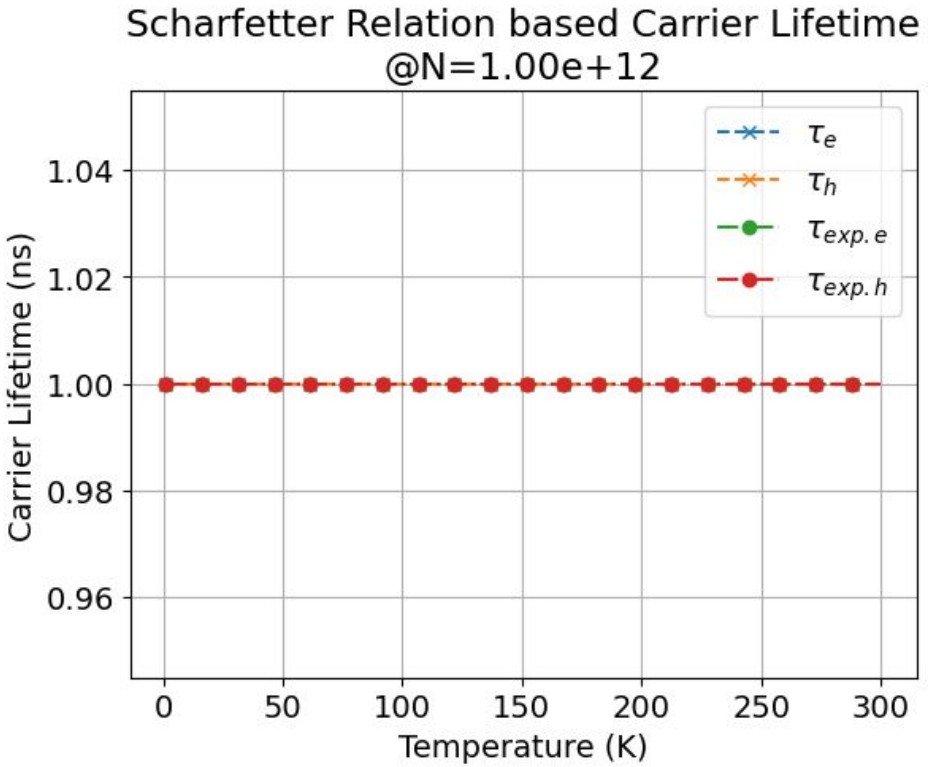
## Carrier Lifetime
## (Scharfetter relation and traps for SRH recombination)

| Equation | Default Parameters |
| --- | --- |
| $$\tau = \tau_{min} + \frac{\tau_{max} - \tau_{min}}{1 + \left(\frac{N}{N_{ref}}\right)^{\gamma}}$$ $$\tau(T) = \tau \left(\frac{T}{300}\right)^{T_\alpha} \quad \text{(TempDep)}$$ $$\tau(T) = \tau e^{T_c\left[\left(\frac{T}{300}\right)-1\right]} \quad \text{(ExpTempDep)}$$ | $\tau_{min,e/h} = 0.0,\ 0.0$ seconds<br>$\tau_{max,e/h} = 1.0 \times 10^{-9},\ 1.0 \times 10^{-9}$ seconds<br>$N_{ref,e/h} = 1.0 \times 10^{16},\ 1.0 \times 10^{16}\ /\text{cm}^3$<br>$\gamma_{e/h} = 1.0,\ 1.0$<br>$T_{\alpha,e/h} = 0.0,\ 0.0$<br>$T_{c,e/h} = 0.0,\ 0.0$<br>$E_{trap} = 0.0$ eV<br>$\tau_{0,e/h} = 1.0 \times 10^{-9},\ 1.0 \times 10^{-9}$ seconds |

Default parameter concludes that the tau is gently affected by the net doping concentration. With N_ref in 16th order, our defect based doping concentration may not affect too much on the default lifetime of 1 ns.

# Carrier Lifetime (Scharfetter Relation) (Defaut Parameter)



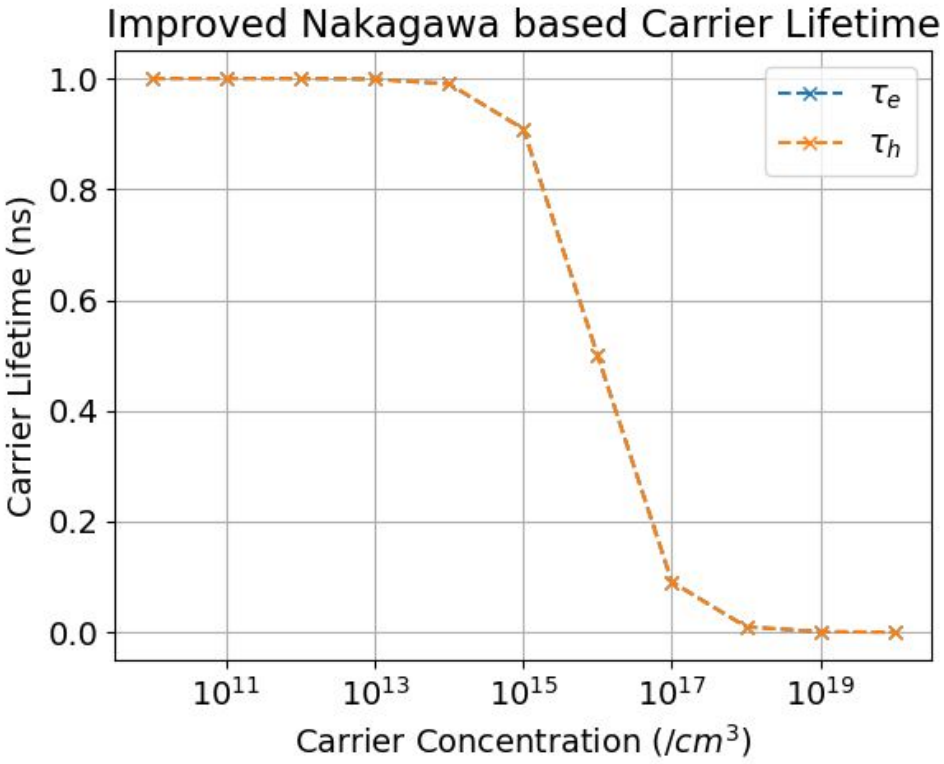



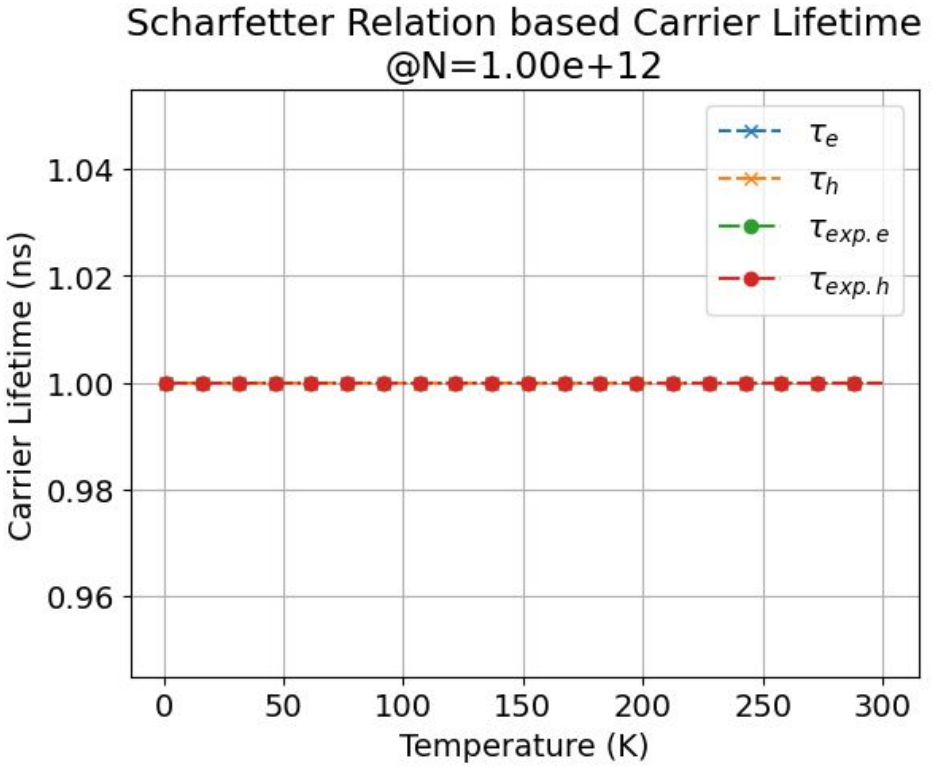
## Carrier Lifetime
## (Scharfetter relation and traps for SRH recombination - Improved Nakagawa)

| Equation | Default Parameters |
|---|---|
| $$\tau = \frac{\tau_{max} + \tau_{min}\left(\frac{N}{N_{ref}}\right)^{\gamma}}{1 + \frac{\tau_{max}}{\tau_0}\left(\frac{N}{N_{ref}}\right)^{\gamma}}$$ where, $$\tau(T) = \tau\left(\frac{T}{300}\right)^{T_\alpha} \quad \text{(TempDep)}$$ $$\tau(T) = \tau e^{T_c\left[\left(\frac{T}{300}\right)-1\right]} \quad \text{(ExpTempDep)}$$ | $\tau_{min,e/h} = 0.0,\ 0.0$ seconds<br>$\tau_{max,e/h} = 1.0\times10^{-9},\ 1.0\times10^{-9}$ seconds<br>$N_{ref,e/h} = 1.0\times10^{16},\ 1.0\times10^{16}\ /\text{cm}^{-3}$<br>$\gamma_{e/h} = 1.0,\ 1.0$<br>$T_{\alpha,e/h} = 0.0,\ 0.0$<br>$T_{c,e/h} = 0.0,\ 0.0$<br>$E_{trap} = 0.0$ eV<br>$\tau_{0,e/h} = 1.0\times10^{-9},\ 1.0\times10^{-9}$ seconds |

Carrier lifetime with default parameter is just tau_max with carrier concentration modifier. Sine N_ref is order of 16, our trap density of 12th order is not affecting the lifetime too much.

# Carrier Lifetime - Improved Nakagawa (Default Parameters)



# Auger Recombination

Auger Recombination model is valid when the carrier density is high. → Recombination generates heat.

Also, the second part of the equation is the mass action law… so it will be zero?

| Equation | Default Parameters |
| --- | --- |
| $R_{auger} = (C_n \times n + C_p \times p)(np - n_i^2)$ where, $C_{n/p} = \left[A + B\left(\frac{T}{T_0}\right) + C\left(\frac{T}{T_0}\right)^2\right] \times \left(1 + He^{-\frac{N_{n/p}}{N_0}}\right)$ | $A_{e/h} = 1.0 \times 10^{-30},\ 1.0 \times 10^{-30}\ \mathrm{cm}^6/\mathrm{s}$<br>$B_{e/h} = 0.0,\ 0.0\ \mathrm{cm}^6/\mathrm{s}$<br>$C_{e/h} = 0.0,\ 0.0\ \mathrm{cm}^6/\mathrm{s}$<br>$H_{e/h} = 0.0,\ 0.0$<br>$N_{0.e/h} = 1.0 \times 10^{18},\ 1.0 \times 10^{18}\ /\mathrm{cm}^3$ |

Note that the default H is zero: No Auger effect is simulated by default.

## PooleFrenkel

Typically, Poole-Frenkel recombination happens when trap states are extremely high (over $10^{19}$ /cm$^3$) and electric field is strong enough to admit thermionic emission. Since we are introducing traps as dopants, this effect may have some effect.

| Equation | Default Parameters |
| --- | --- |
| $$\sigma^{enh} = \sigma_0(1+\Gamma_{pf})$$ where, $$\Gamma_{pf} = \frac{1+(\alpha-1)e^{\alpha}}{\alpha^2} - \frac{1}{2},$$ $$\alpha = \frac{1}{kT}\sqrt{\frac{q^3F}{\pi\varepsilon_{pf}}}$$ | $$\sigma = < \text{CrossSection} > /\text{cm}^2$$ $$\sigma^{enh} = \text{Enhanced by Thermionic Emission}$$ $$\sigma_0 = \text{Constant CrossSection}$$ $$\varepsilon_{pf.e/h} = 12.4,\ 12.4$$ $$F = < \text{Electric Field} > \text{V/cm}$$ |

## RadiativeRecombination

Simply put, LED-recombination. Not happening very often in our devices. We are not simulating SiPM at the moment.

| Equation | Default Parameters |
| --- | --- |
| $R_{rad} = C \left( \frac{T}{T_{par}} \right)^{\alpha} (np - n_i^2)$ | $C = 0.0\ \mathrm{cm}^3/\mathrm{seconds}$<br>$\alpha = 0.0$<br>$T_{par} = 3.0 \times 10^2\ \mathrm{K}$ |

## Conclusions on the Model Descriptions

- Most of default parameters are either simply too simple or not characterized at all.
- Carrier lifetime factors seem to have temperature dependence. But in fact, the fitting parameters in the model nullifies the temperature parameters.
- The only meaningful parameters are Dielectric Constant, Energy Bandgap, and Constant Mobility model parameters.
- At the moment, we are ‘artificially’ pushing in the carriers for trap states and those carriers are the main driving factors for IV-sweep current results.
- Thus, we will have to manipulate the carrier occupancy model for traps to match the dark current models to the experimental data first.