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Efficient Band-to-Trap Tunneling Model Including Heterojunction Band Offset

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Traps in Semiconductor Devices

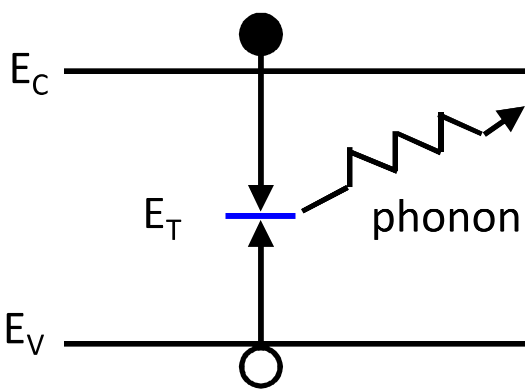
Fabrication processes

Radiation environment

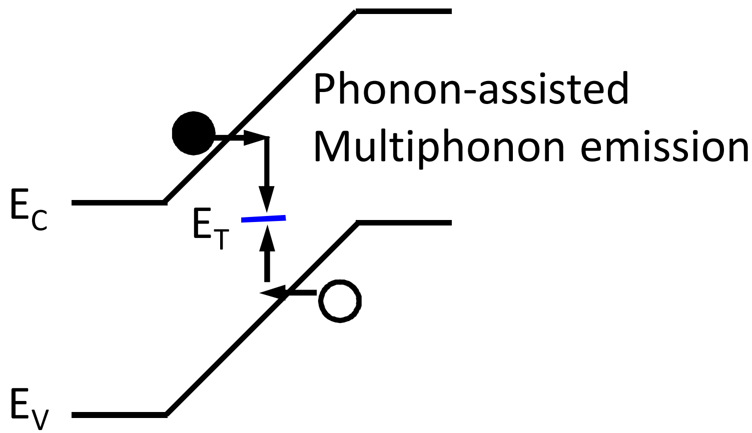
Always traps/defects in semiconductor devices

Other trap-related processes

Shockley-Read-Hall (SRH) Recombination



Band-to-trap tunneling (i.e., trap-assisted tunneling, TAT)



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Modeling of Band-to-Trap Tunneling

Band-to-trap tunneling is widely modeled as field-dependent SRH recombination:

$$R = \frac{np - n_i^2}{\tau_p(n+n_1) + \tau_n(p+p_1)} \qquad \tau_\nu = \frac{\tau_{\nu 0}(T, F=0)}{1 + g_\nu(T,F)}, \nu = n, p$$

Field enhancement factor due to band-to-trap tunneling

$g_\nu(T,F)$ →

- Schenk model [1-2]
- Hurkx model [3]
- Racko model [4]

→

- Schenk and Hurkx exist in TCAD codes
- Contains only field dependence

Assuming **Boltzmann statistics and deep-level** traps, the **Schenk model** is reduced to

Density of states (DOS)

$$g_n(T,F) = \frac{\int_0^{E_t} dE \rho_c(E) I_{E/\hbar\omega_0}(z) \exp\left(\frac{-E}{2k_B T}\right)}{\int_{E_t}^{\infty} dE \rho_c^{F=0}(E) I_{E/\hbar\omega_0}(z) \exp\left(\frac{-E}{2k_B T}\right)}$$

- Contains the field dependence
- Obtained assuming constant field

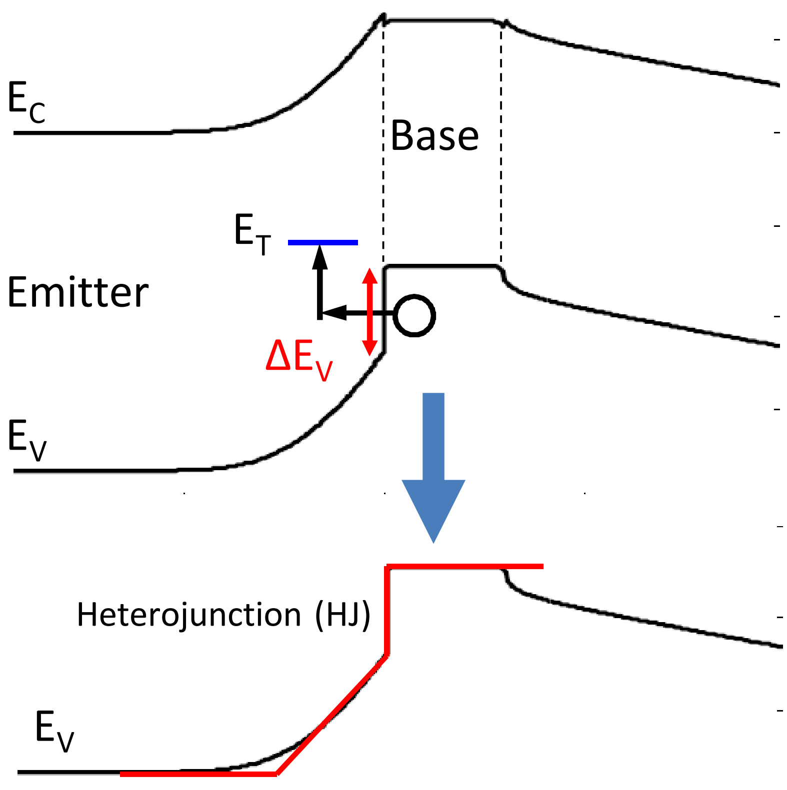
[1] A. Schenk, Journal of Applied Physics **71**, 3339 (1992).
[2] A. Schenk, Solid-State Electronics **35** (11), 1585 (1992).
[3] G. A. M. Hurkx, IEEE Transaction on Electron Devices **39**(2), 331 (1992).
[4] J. Racko et al., RadioEngineering **21**(1), 213 (2012).

B-to-T Tunneling in Heterojunction Device

Constant field assumption for the DOS in the Schenk model

- Good for **homojunction** devices
- Not good for **heterojunction** devices

Consider $In_{0.49}Ga_{0.51}As$/GaAs $NP^{+}N$ HBT:



DOS at the trap location is **greatly enhanced** [5] due to the **band offset** ΔE_V, leading to much **higher hole-to-trap tunneling**.

Sam Myers et al. [5] obtained **much higher DOS** than the constant-field DOS by **numerically solving the Schrodinger equation** given the actual E_V band profile.

Trivial – solve 1D Schrod. eqn. numerically once
Inefficient – when solved repeatedly
Difficult – coupled to MPI-parallel PDE-based TCAD code

Goal – find **analytic** DOS model for simplified potential & easy implementation in TCAD code

[5] S. M. Myers et al., J. Appl. Phy. **120**, 134502 (2016).

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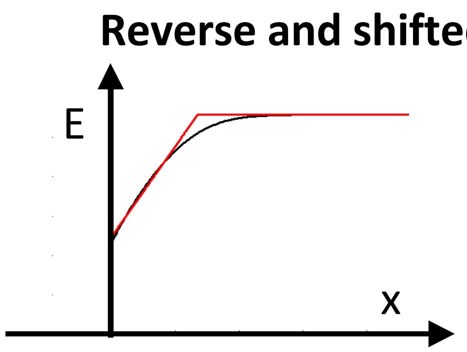
Density of States Method



Goal – find analytic DOS model for simplified potential (red potential) & easy implementation into TCAD code

- Need to compute 3D DOS (used in the Schenk model)
- Non-zero potential in the x direction only
- Three methods to compute the DOS

Method 1 – Numerical approach

$$\rho_{3D}(x,E) = \frac{m}{\pi\hbar^2}\sum_i |\psi_i(x)|^2\theta(E-E_i)$$

$\theta(\cdot)$ – step function

Wave functions normalized to 1 ; Discrete energy spectrum

❖ Require solving the Schrodinger equation **numerically** to obtain ψ_i and E_i

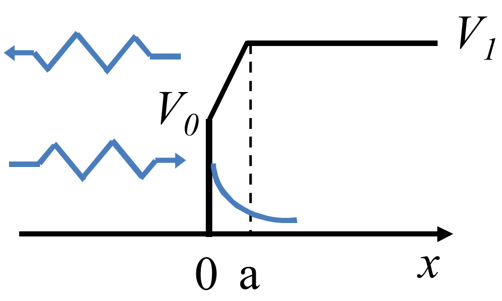
Method 2 – Green's function (GF) approach

$$\rho_{3D}(x,E) = \frac{-2}{\pi}\mathrm{Im}[G^R_{3D}(x,E)] \quad G^R_{3D}(x,E) = \frac{m}{2\pi\hbar^2}\int_0^{+\infty} G^R_{1D}(x,E-E_\perp)dE_\perp\theta(E-E_\perp)$$

❖ Analytic GFs is even harder to obtain than the WFs

Proposed Density of States Method

Method 3 – Proposed scattering approach



Solve the Schrodinger equation with open boundary condition (BC)

- Continuous energy spectrum
- Dirac-delta normalized WF

$$\int_{-\infty}^{+\infty} \psi^*_{E_x}(x)\psi_{E'_x}(x)dx = \delta(E_x - E'_x)$$

$$\rho_{3D}(x,E) = \frac{m}{\pi\hbar^2}\int_0^{+\infty} \left|\psi_{E_x}(x)\right|^2 dE_x \theta(E - E_x)$$

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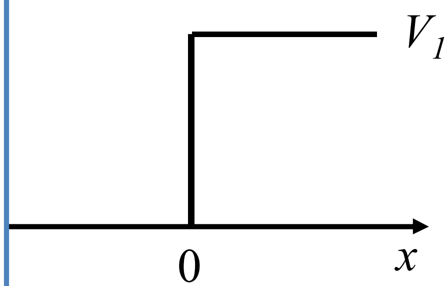
Proposed Density of States Method

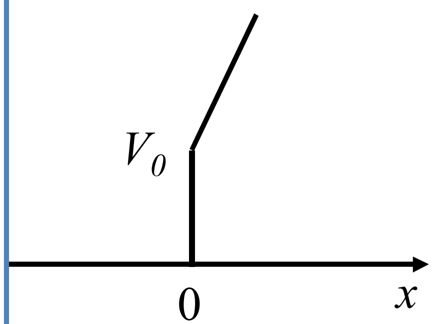
How does the approach work ?

Step 1: Solve the Schrodinger equation with open BC to obtain analytic wave functions



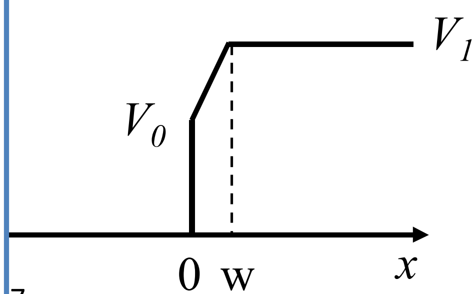
$$\psi(x) = \mathbf{N} \begin{cases} e^{ikx} + a\, e^{-ikx} & x < 0 \\ b\, e^{-\nu x} & x > 0 \end{cases}$$

$$k = \sqrt{\frac{2mE}{\hbar^2}} \qquad \nu = \sqrt{\frac{2m(V_1 - E)}{\hbar^2}}$$



$$\psi(x) = \mathbf{N} \begin{cases} e^{ikx} + a\, e^{-ikx} & x < 0 \\ b\, A_i\,[y(x)] & x > 0 \end{cases}$$

$$y(x) = \left(\frac{2mqF}{\hbar^2}\right)^{1/3} \left(x + \frac{V_0 - E}{qF}\right)$$



$$\psi(x) = \mathbf{N} \begin{cases} e^{ikx} + a\, e^{-ikx} & x < 0 \\ b\, A_i[y(x)] + c\, B_i[y(x)] & 0 < x < w \\ d\, e^{-\nu x} & x > w \end{cases}$$

Consider **0 < E < $\mathbf{V_1}$** and x > 0 (relevant for b-to-t tunneling)

Coefficients (a, b, c, d) depend on E and are determined by continuity of ψ and $d\psi/dx$ at $x = 0$ & w

Proposed Density of States Method

Step 2: Determine the normalization factor

$$\int_{-\infty}^{+\infty} \psi_{E_x}^*(x)\psi_{E_x'}(x)dx = \delta(E_x - E_x')$$ ➡ Determine the normalization factor ***N***

- Challenge task to normalize the WFs to the delta function, even for step barrier
- Discover the same normalization factor for all the three potentials considered
- Believe the same factor is applicable to all other 1D potentials with open BC.

$$|N|^2 = \frac{m}{2\pi\hbar^2 k} \quad \text{with} \quad k = \sqrt{\frac{2mE}{\hbar^2}}$$

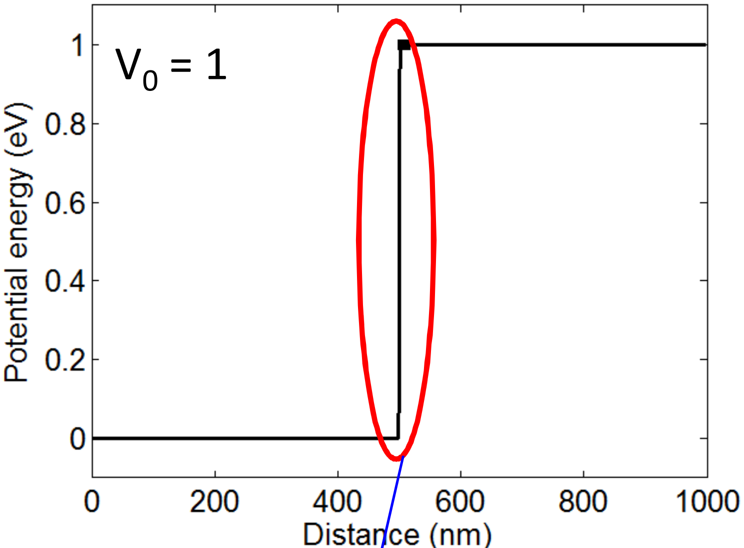
Mathematically prove it for step barrier and linear potential with offset

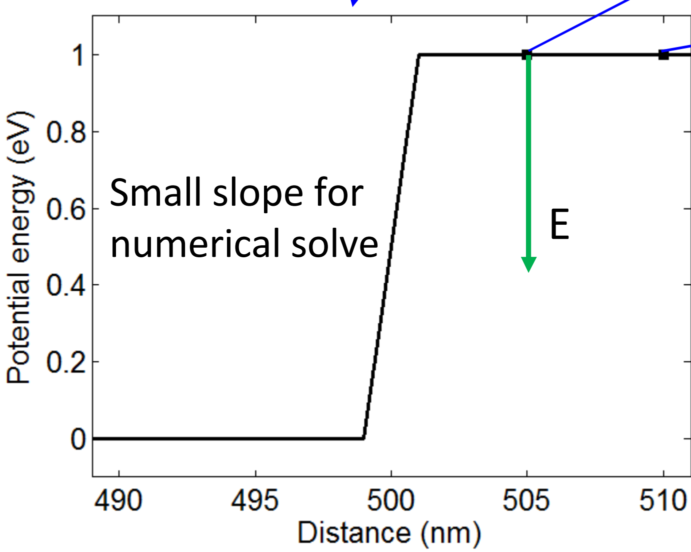
Once **N** is known, ρ_{3D} can be computed !

Pros:
- Analytic wave functions
- Universal normalization factor
- Easy implementation into TCAD

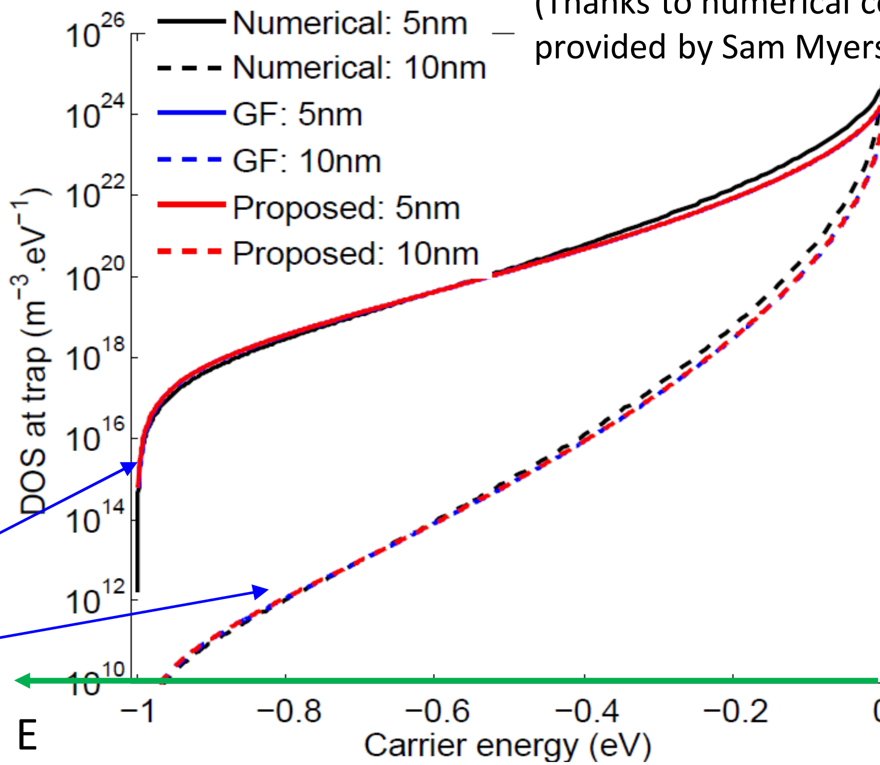
Cons:
- Limited to 1D potentials that lead to piecewise analytic WFs

Density of States Comparison



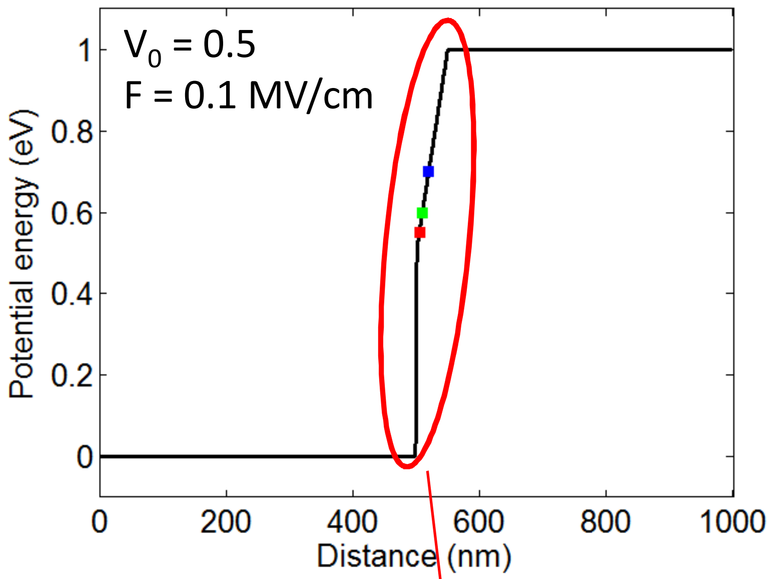


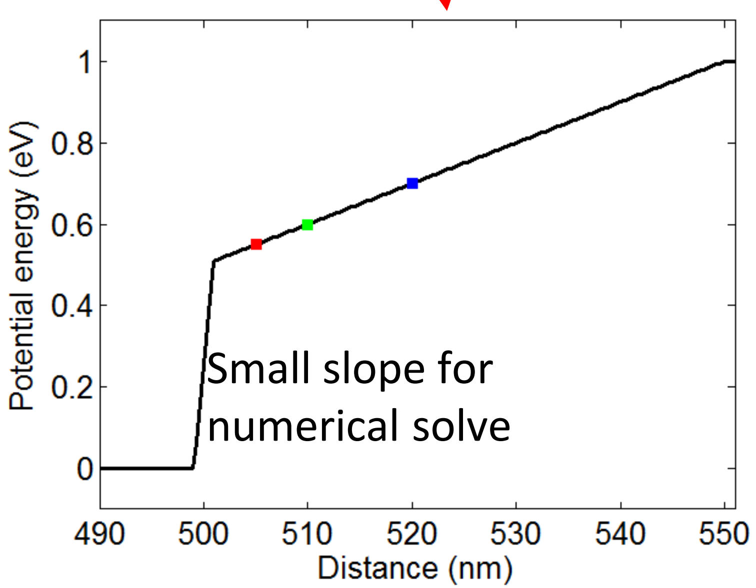
(Thanks to numerical code provided by Sam Myers)

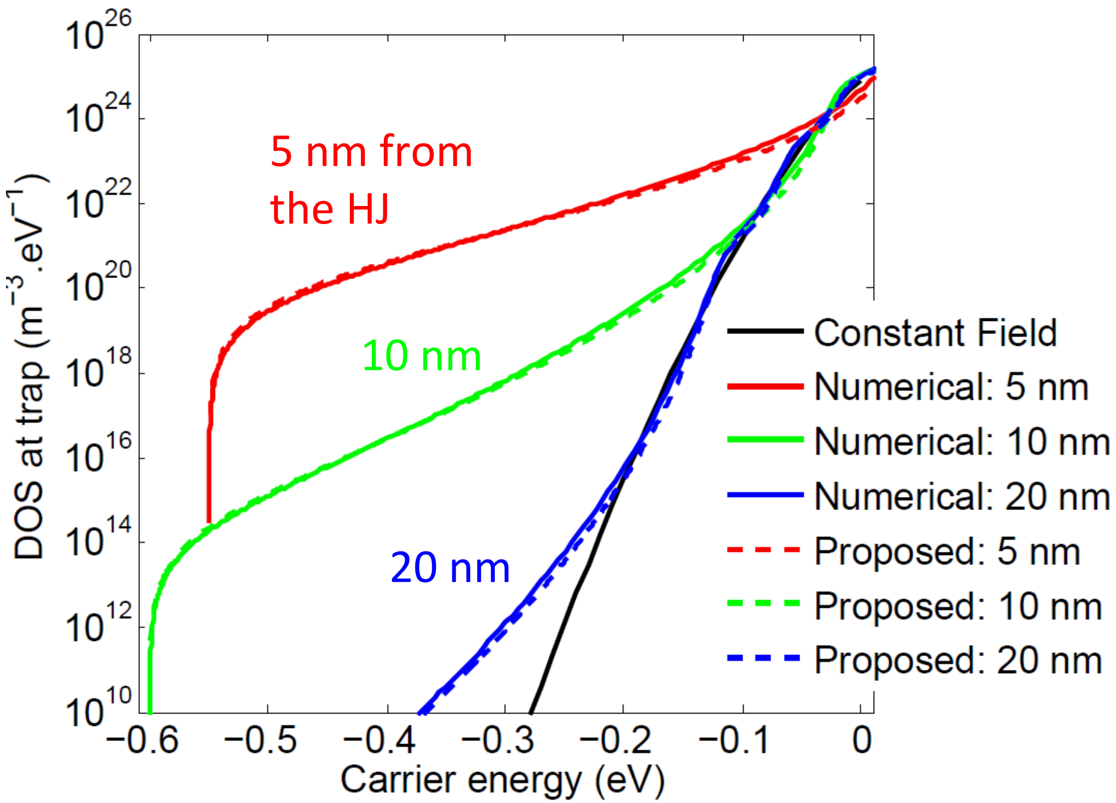


- The Green's function and proposed methods produce **the same DOS**
- Small difference between the numerical and proposed methods is due to the **non-ideal step** used in the numerical code

Density of States Comparison

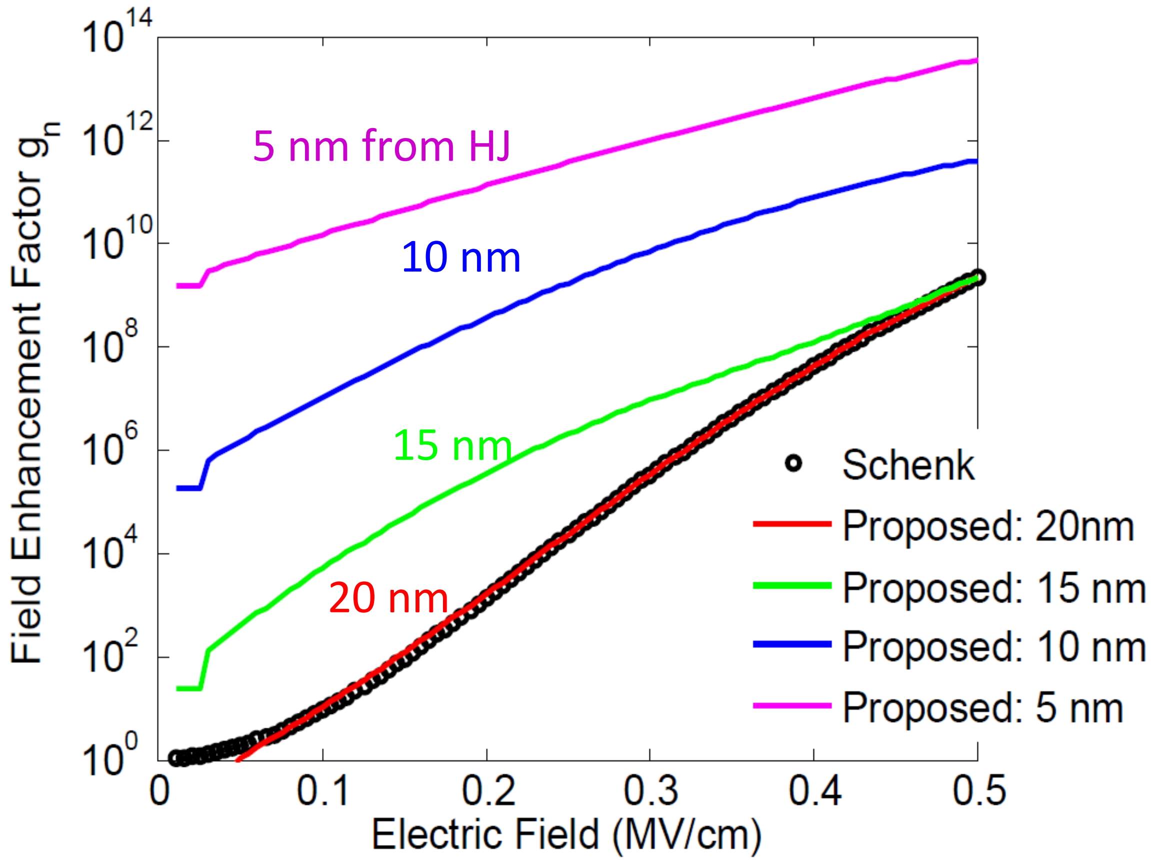






- The constant-field DOS is **valid only for more than 20 nm** away from the heterojunction (HJ)
- The DOS computed using the proposed method **agree well** with numerical results
- The **band offset has a strong effect** on the DOS for distances within 20 nm from the HJ

Field Enhancement Factor g_n



- For locations **>= 20 nm** from the HJ, proposed & Schenk models produces **similar g_n**
- g_n by the proposed model **increases with decreasing distance** from the HJ
- Field dep. of g_n by the proposed model **reduces with decreasing distance** from the HJ

Charon Device Simulator

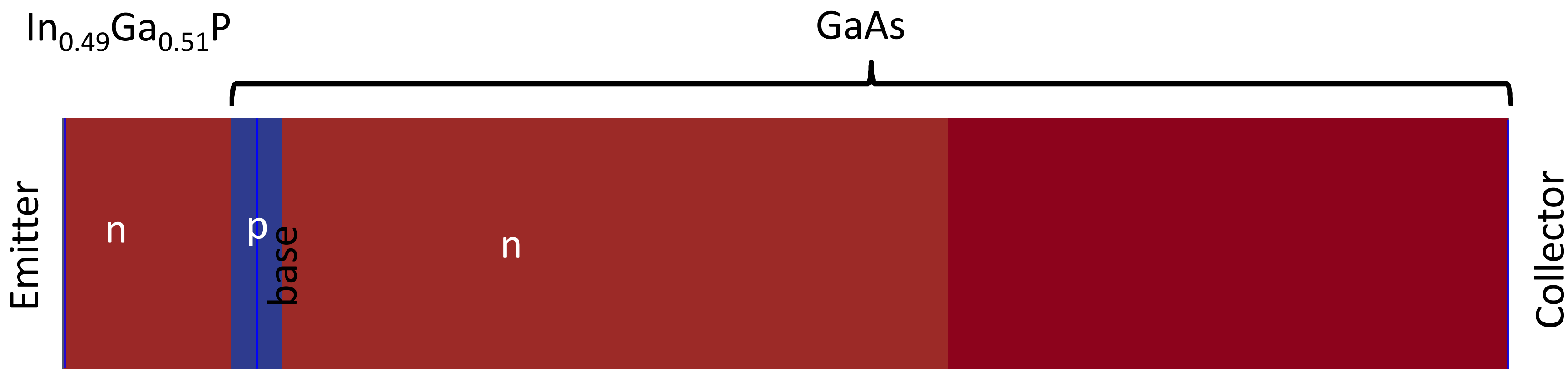
The proposed band-to-trap tunneling model is implemented in Charon.

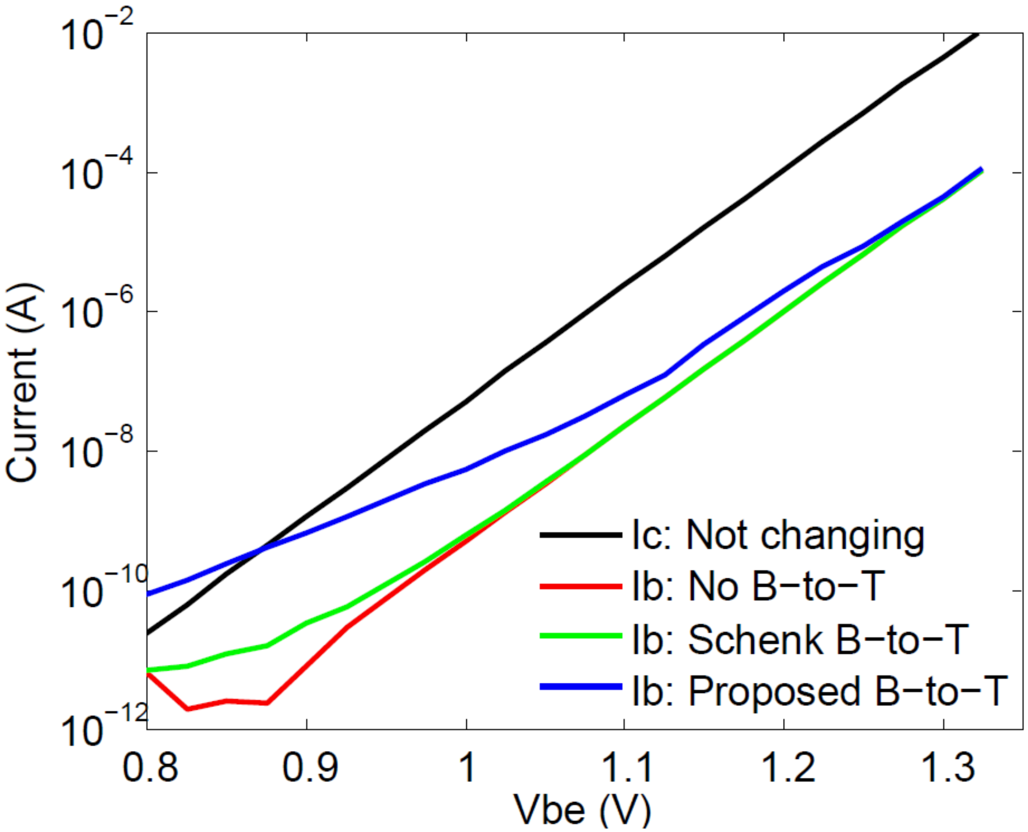
Sandia-developed TCAD code with support for radiation effects modeling

Unique Capabilities provided by Charon

- Open source (just approved)
- Two & three dimensional + MPI parallel capability
- Various governing PDEs (Poisson, drift-diffusion for e/h/ions, lattice heating)
- Different discretization schemes (e.g., finite volume, finite element)
- Advanced physics models (Fermi-Dirac, transport across heterojunction, band-to-trap tunneling, etc.)
- Numerous devices (diodes, BJTs, HBTs, MOSFETs, GaN devices, memristors, etc.)

Application of B-to-T Model to NPN HBT



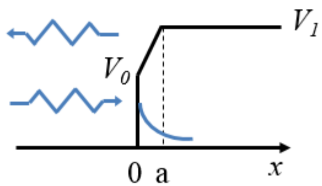


- Mid-band gap traps in the emitter
- τ_{n0} = 1 ns, τ_{p0} = 0.1 us
- Only hole-to-trap tunneling

The proposed b-to-t tunneling model **produces much larger base current** than the original Schenk model, due to the **hole-to-trap tunneling** enhanced by the emitter-base band offset.

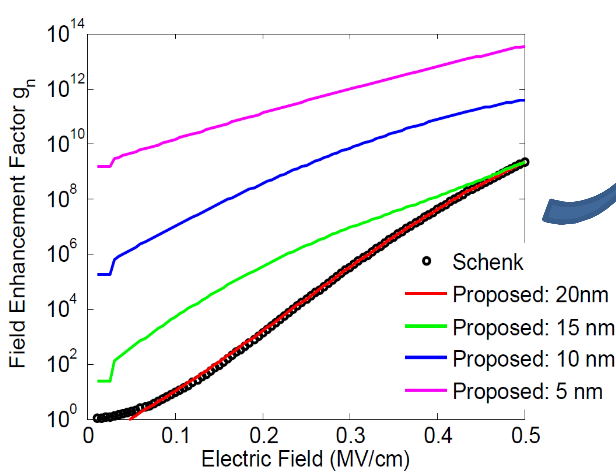
Conclusion

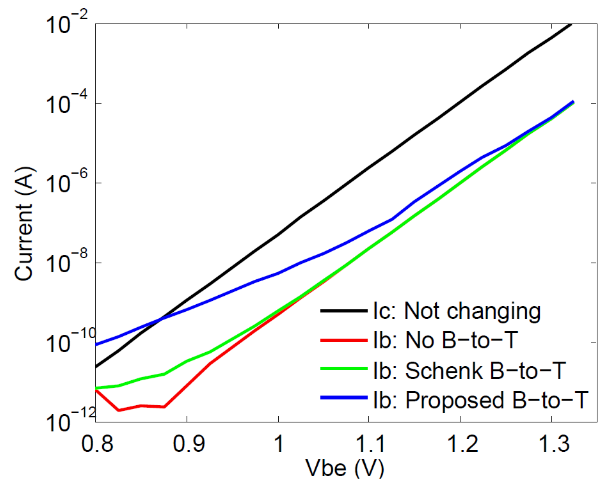
- Develop an analytic DOS model that includes the effects of both electric field and HJ band offset based on the open boundary scattering approach



$$\rho_{3D}(x,E) = \frac{m}{\pi\hbar^2}\int_0^{+\infty}\left|\psi_{E_x}(x)\right|^2 dE_x\theta(E-E_x)$$

- The proposed band-to-trap tunneling model can be easily implemented into TCAD codes thanks to its analytic form
- Demonstrate the dramatically increased band-to-trap tunneling strength (via the field enhancement factor) at locations close to the HJ using the proposed model





- Demonstrate the dramatically increased base current in a InGaP/GaAs NPN HBT due to the hole-to-trap tunneling enhanced by the emitter-base junction band offset

Backup Slides

Charon Device Simulator

Sandia TCAD code

CHARON

Trilinos

ParaView

Cubit for geometry and mesh creation (arbitrary 2D/3D geometry)

https://cubit.sandia.gov/

Open-source suite:

- Discretization (FE, FV)
- Nonlinear & linear solvers
- MPI parallel
- Automatic differentiation
- Many more…

http://trilinos.org/

Data analysis and visualization

http://www.paraview.org/