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Understanding Gaps in III-V HBT Modeling and Simulation

(What Silicon Modelers Should Know About III-Vs for TCAD)

Pete Zampardi

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Outline

- General Properties of III-V Material
  - We focus on InGaP/GaAs, but similar issues exist in InP
- Material Design and Specification
- Material Models
- Heterojunctions
- Velocity vs. Field
- Summary

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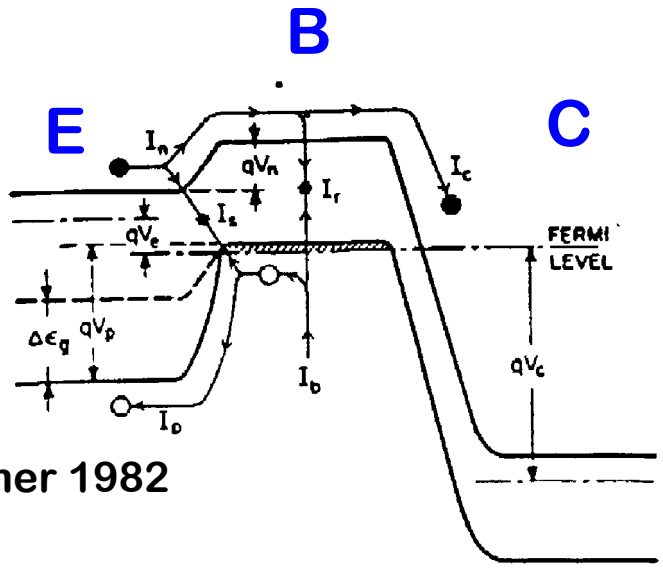
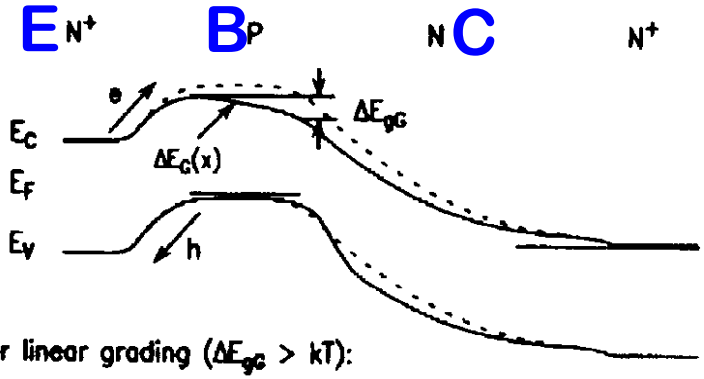
Comparison of Band Diagrams

III-V HBT is compound semiconductor



Kroemer 1982

SiGe is an alloy



For linear grading ($\Delta E_{gG} > kT$):

$$\frac{\tau_{E\,(SiGe)}}{\tau_{E\,(Si)}} = \frac{\beta_{(Si)}}{\beta_{(SiGe)}} \sim \frac{R_{bi\,(Si)}}{R_{bi\,(SiGe)}} \cdot e^{-\Delta E_g(0)/kT} \cdot \frac{kT}{\Delta E_{gG}}$$

$$\frac{\tau_{B\,(SiGe)}}{\tau_{B\,(Si)}} \sim \frac{2kT}{\Delta E_{gG}}\left(1 - \frac{kT}{\Delta E_{gG}}\right)$$

Patton, IEDM, 1990

III-V HBT

Wide Band gap Emitter

Reduces I_p (fewer minority Carriers injected into emitter)

Si/SiGe BJT/HBT

Narrow Band gap Base

Increases I_n (more minority Carriers injected into base)

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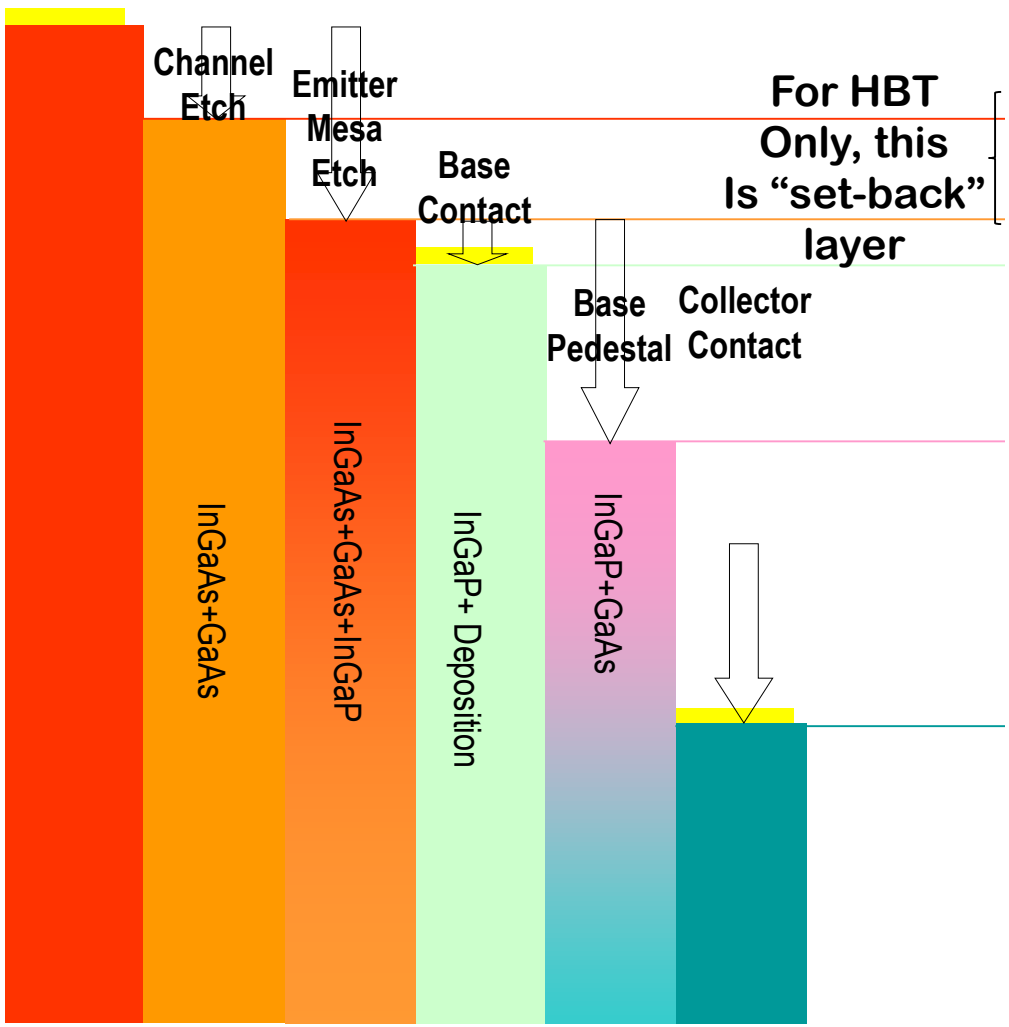
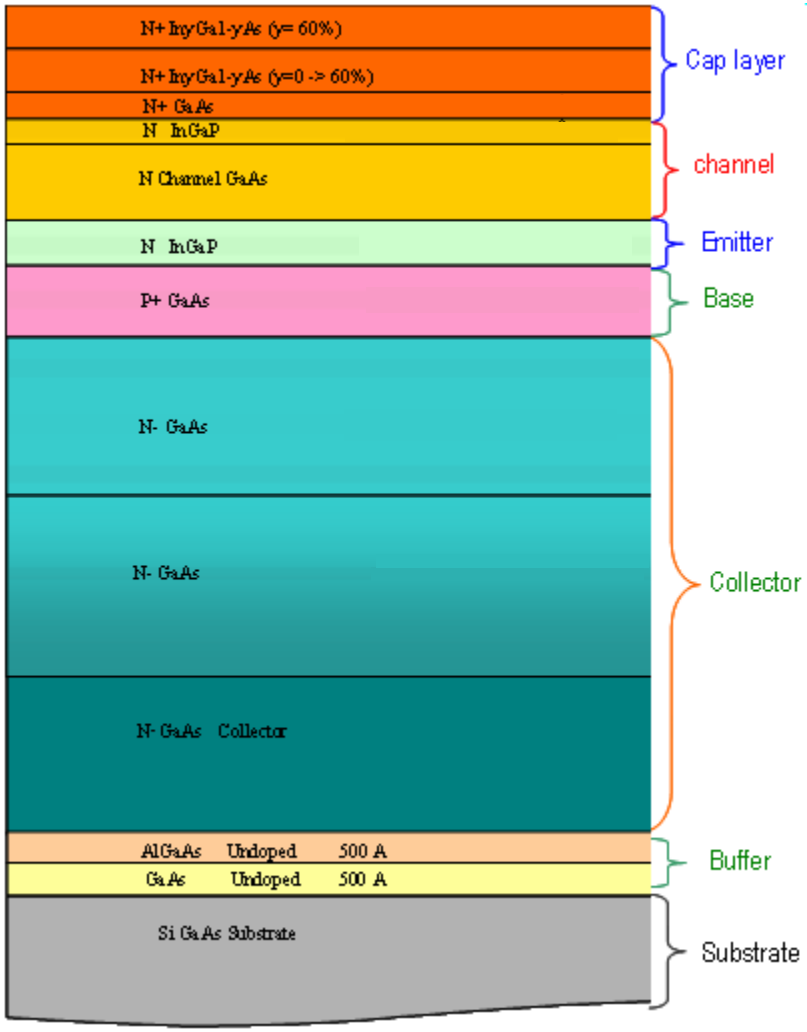
Epi-Layer Example





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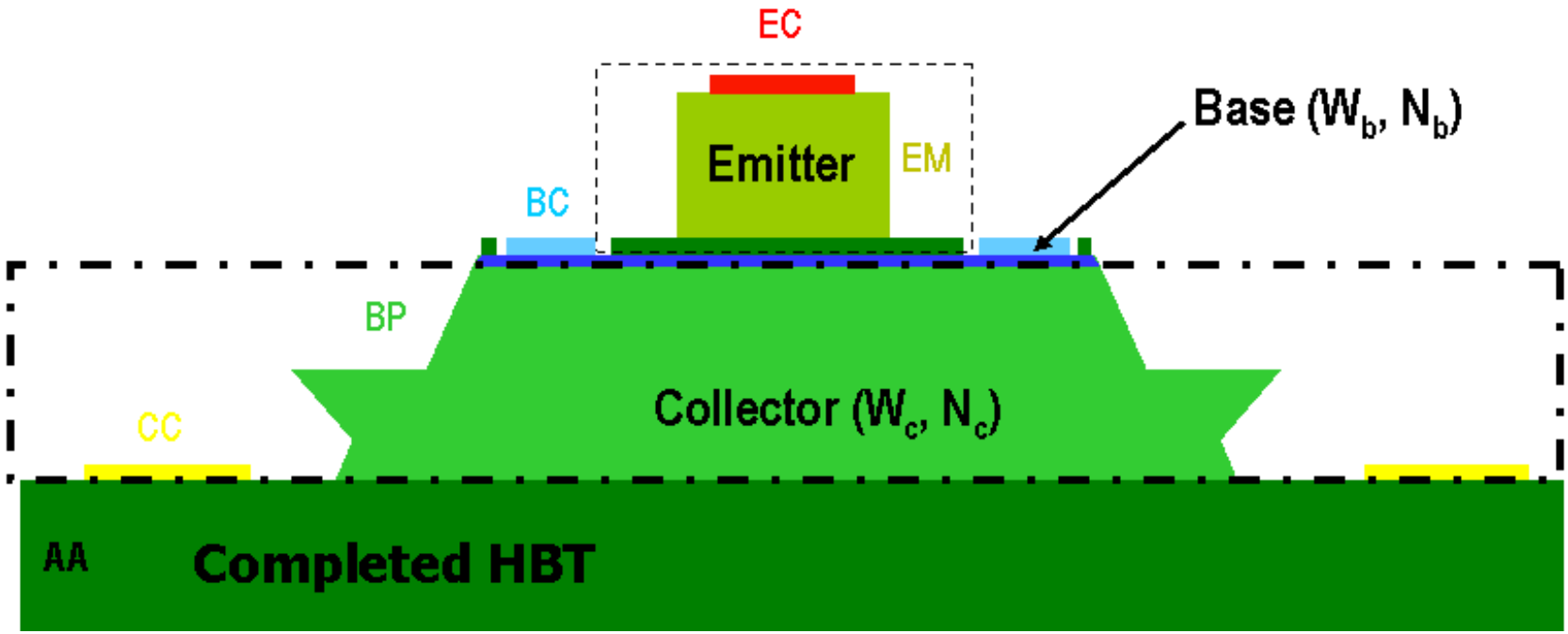
HBT is a vertical device

Sculpted from starting wafer



Zampardi, Mantech 2011

EC Effects Contact Resistance (Emitter)
EM Determines Emitter Size (current density), Emitter Resistance, and is Part of Ledge Definition
BC Part of Base Contact Resistance and Ledge Formation. BC to BP spacing also important for offset
BP Determines Cbc of Device and Defines Part of Passivation Ledge
CC Part of Collector Resistance and Also Defines Part of Cbc (especially reverse bias)
AA Device Isolation (contributes some overlap capacitance)

ALMOST ALL IMPORTANT PARAMETERS SCALE WITH AREA!

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Material Design and Specification

- How the material is specified is very important to get what you asked for
- There are added degrees of freedom in III-V HBTs that just don't exists for silicon.
- These degrees of freedom can have a huge impact on parameters important for TCAD!

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Example Layer Specification

What people send to the vendor

(Johnson, Mantech 2013)

Layer	Material	Dopant	Composition	Doping (/cm3)			Thickness (nm)		
				Min.	Target	Max.	Min.	Target	Max.
Contact	InGaAs	Te	--	--	--	--	--	--	--
Emitter cap	GaAs	Si	--	--	--	--	--	--	--
Emitter	InGaP	Si	--	--	--	--	--	--	--
Base	GaAs	C	--	--	--	--	--	--	--
Collector	GaAs	Si	--	--	--	--	--	--	--
Subcollector	GaAs	Si	--	--	--	--	--	--	--
Buffer	--	--	--	--	--	--	--	--	--
Substrate	GaAs	--	--	--	--	--	--	--	--

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Simplified Electrical Spec for Vendor

Measured on Large (75x75 sq. um) Devices

(Johnson, Mantech 2013)

	Min.	Target	Max.
Gain	--	--	--
Vbe	--	--	--
Sheet Resistance			
Base	--	--	--
Emitter	--	--	--
Collector	--	--	--
Capacitance			
Emitter	--	--	--
Collector	--	--	--
Burn-in	--	--	--
Breakdown voltage			
BVcbo	--	--	--
BVebo	--	--	--
Bvceo	--	--	--
Physical			
Particles	--	--	--
Scratches	--	--	--
Surface Haze	--	--	--

Vendors measure these parameters before shipping wafers. Vendors will grow material to match these values, but there is more than one solution (set of growth conditions)!

They are normally correlated to large devices and PCM devices at customer

These specs from customer don't always line up with the layers on previous slide!

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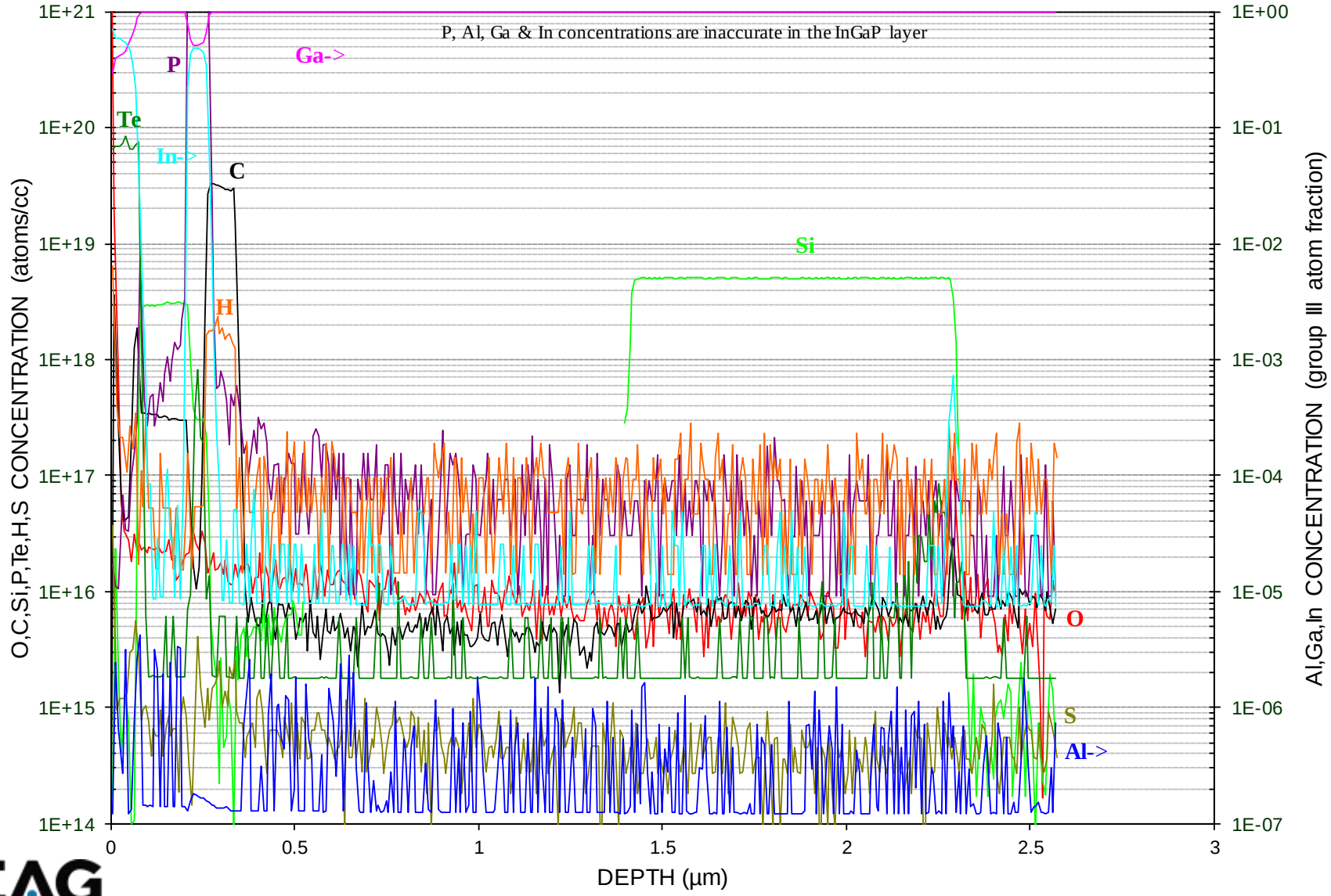
SIMS Example

PCOR-SIMS℠



EAG LABORATORIES

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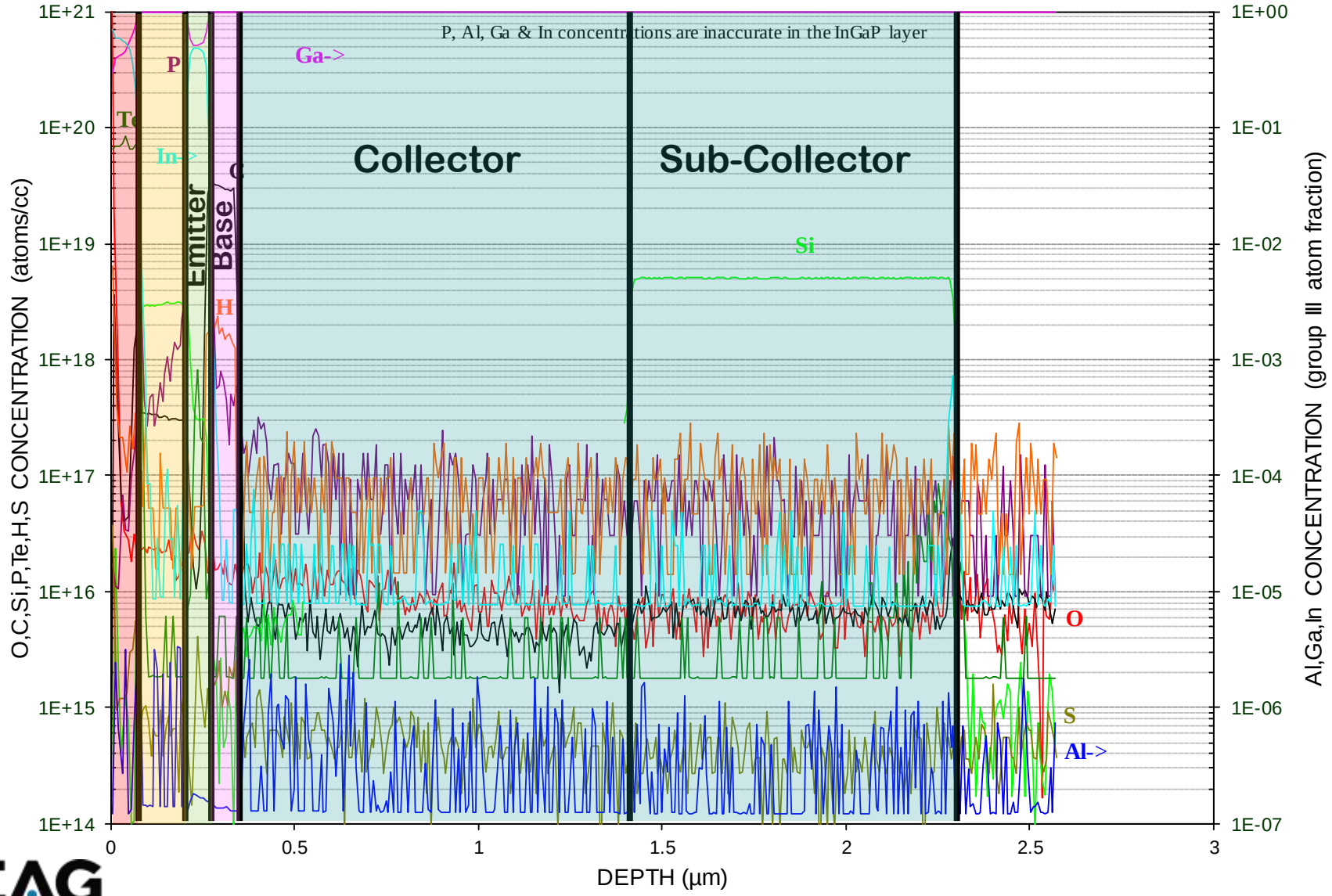
SIMS Example

PCOR-SIMS℠



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Emitter

Emitter InGaP

- $In_{(1-x)}Ga_{(x)}P$
- Composition, x, changes band-gap
- Details of growth condition (temperature, III/V ratios) can change the atomic scale clustering (ordering).
  - This changes the bandgap
  - Creates an interface polarization charge
- Other III-V materials, such as InAlAs, GaAsSb used for high speed InP-based HBTs have similar behavior

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E_g and λ Dependence on Lattice

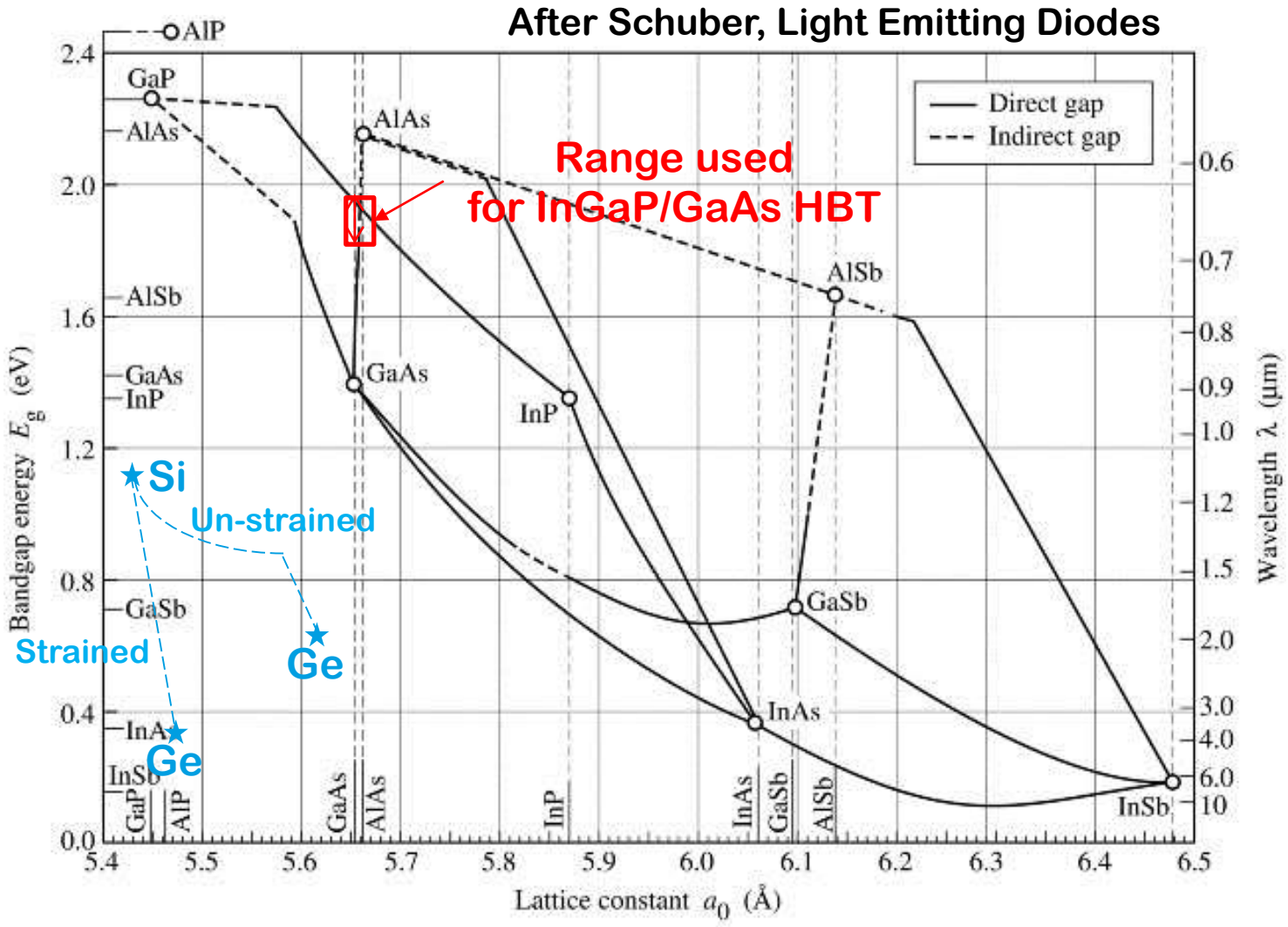

Fig. 7.6. Bandgap energy and lattice constant of various III-V semiconductors at room temperature (adopted from Tien, 1988).

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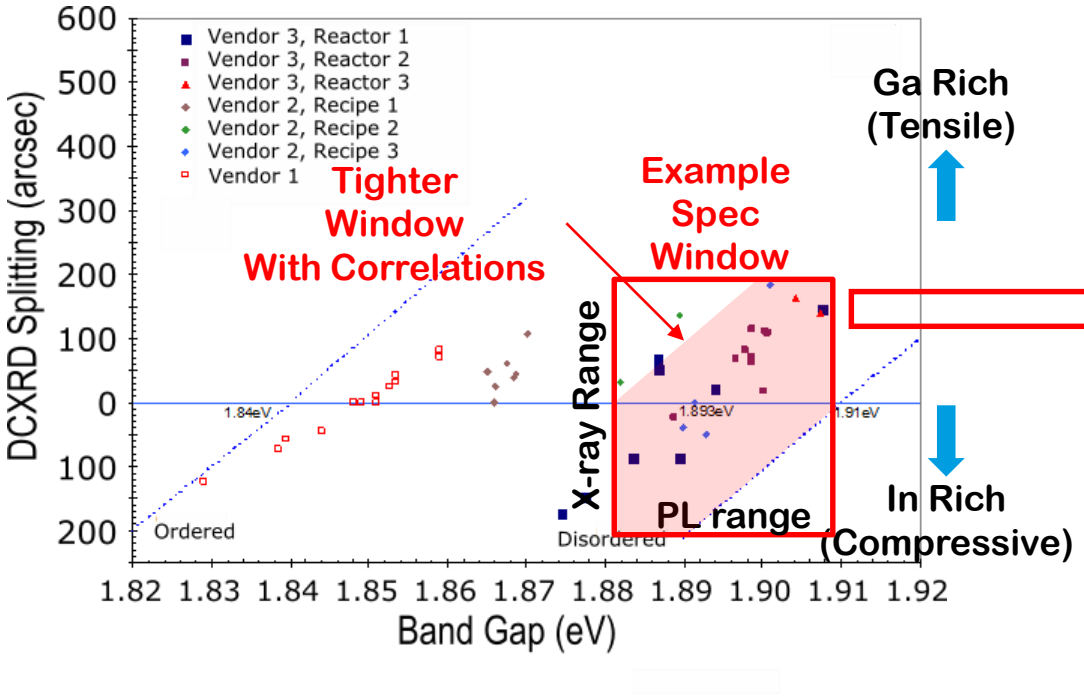
Examples of Possible Vendor Differences

Vendor-vendor and Reactor-reactor differences

$E_g(eV)=1240.8/\lambda_{RTPL}(nm)$



(Calder, Mantech, 1999)

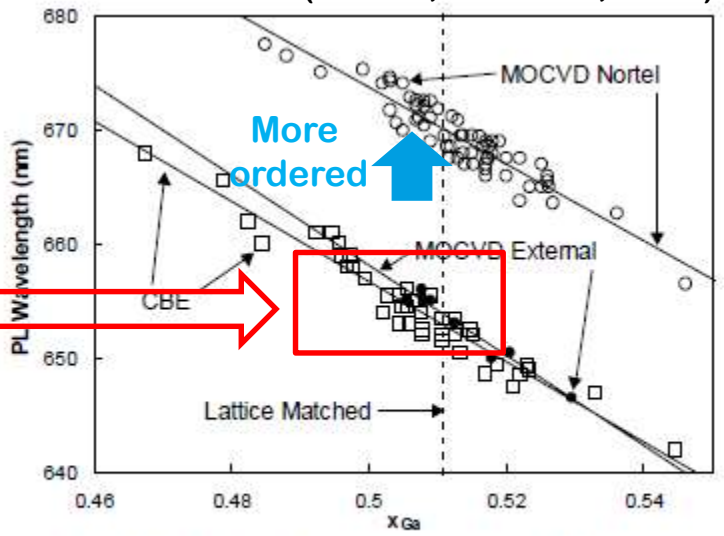


Figure 6. Bulk GaInP sample correlation for material grown in house-MOCVD Nortel, CBE, and externally—MOCVD external.

Double Crystal X-ray Diffraction (DCXRD) determines the composition
Photo-luminescence (PL) Wavelength is combination composition and ordering

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Ordering Induced Polarization Charge

- Changes bandgap
- *Creates accumulation charge at interface*

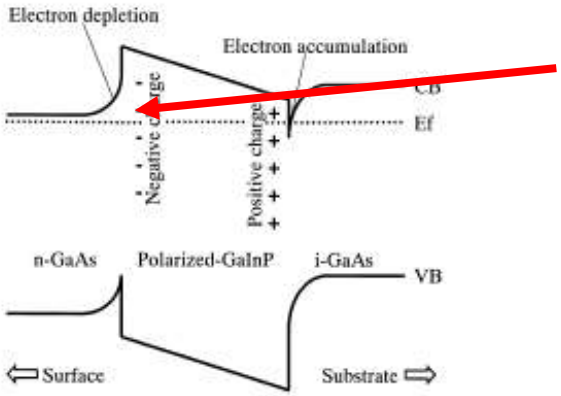

Fig. 6. Estimated band alignment of n-GaAs/polarized-GaInP/i-GaAs hetero structure, where CB, Ef and VB stand for conduction band, Fermi-level energy and valence band, respectively.

The sign of the polarization charge is OPPOSITE To that expected from the quasi-electric field due to conduction band discontinuity (dEc)!

$$J_n = q\mu_n n\left(-\frac{dV}{dx}+\frac{1}{q}\frac{d\Delta E_c}{dx}\right)+qD_n\left(\frac{dn}{dx}-\frac{n}{N_c}\frac{dN_c}{dx}\right)$$

$$J_p = q\mu_p p\left(\frac{dV}{dx}+\frac{1}{q}\frac{d\Delta E_v}{dx}\right)-qD_p\left(\frac{dp}{dx}-\frac{p}{N_v}\frac{dN_v}{dx}\right)$$

Ordering-induced electron accumulation at GaInP/GaAs hetero-interfaces

Takeshi Tanaka*, Kazuto Takano, Tadayoshi Tsuchiya, Harunori Sakaguchi

Advanced Research Center, Hitachi Cable Ltd., 3550 Kidamari, Tsuchiura, Ibaraki, 300-0026, Japan

Numerical Simulation of GaAs/GaAlAs Heterojunction Bipolar Transistors

P. M. ASBECK, MEMBER, IEEE, D. L. MILLER, R. ASATOURIAN, AND C. G. KIRKPATRICK, SENIOR MEMBER, IEEE

Presence of this charge will modify turn-on and C(V) curve

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Emitter Sheet Resistance

Resistance Components

- Emitter sheet resistance may be specified
- The sheet resistance (measured by horizontal current flow) is the sum of the emitter layers in parallel. Changes to layers other than the InGaAs or Emitter Cap (GaAs above InGaP), that do not carry much current, don't contribute much.
- The InGaAs layer is so heavily strained, the mobility is degraded. does not impact vertical current flow (as in HBT), but does change sheet resistance.

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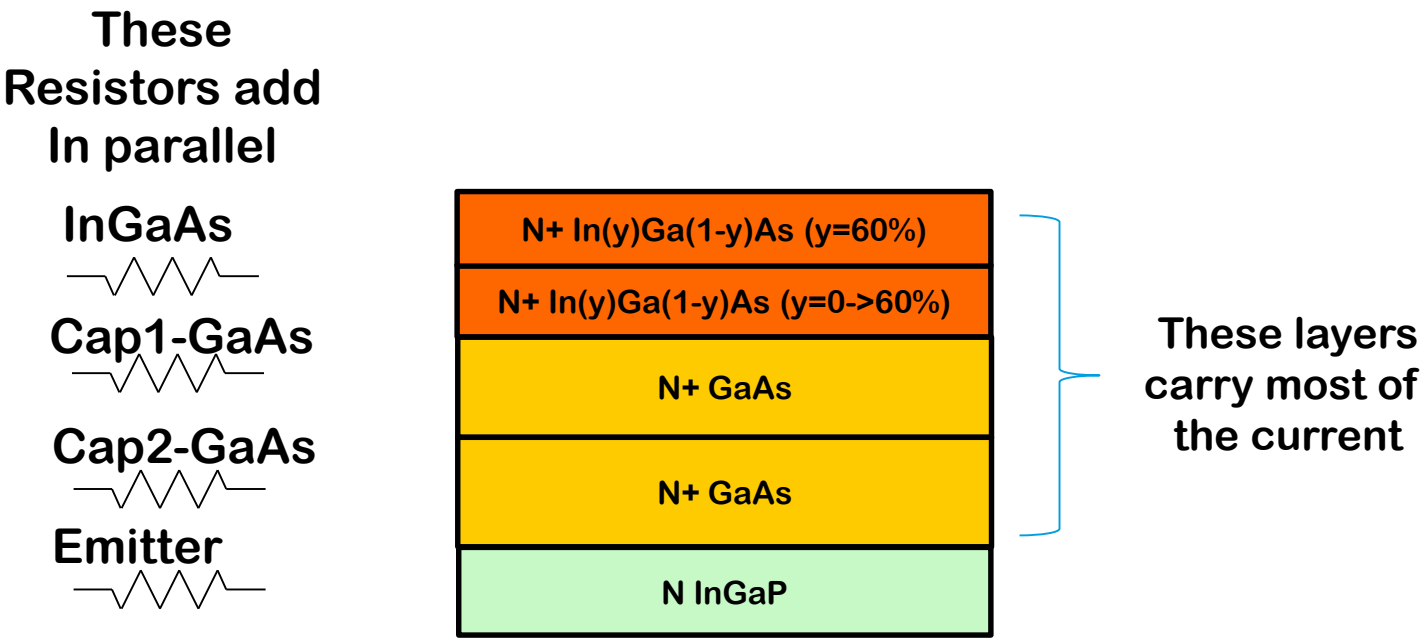
Details of Emitter Sheet Resistance

Useful for monitoring and checking mobilities



This is usually specified to material vendor since both they, and fab, can measure it.

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Example

- Typical Structure
  - In%=50, Thickness=500A/350AGrade, >1e19 cm^{-3}
  - Spec for doping is >1e19, so we estimate 2.5e19 cm^{-3}. Could take value from SIMs data
  - GaAs cap is 0.12um at 4e18 cm^{-3} (mu~1165.3), R_{sh}=115
- Measured sheet resistance=31 Ohm/sq.
  - Using 4000 cm^2/V-s, predicts R_{sh} ~7.2 Ohms.
  - From discussions with material growers, conductivity of heavily strained InGaAs is between 600-850 cm^2/V-s.
  - Using 650 cm^2/V-s, we get R_{sh} =33 Ohm/sq, at least reasonable!

Simple comparisons are useful for uncovering potential issues!

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Base

Base Layer

- For a good device, we want a low base sheet resistance for a given current gain, β
- For HBTs, carbon is de facto standard p-dopant for GaAs (for improved reliability)
  - Carbon doping can behave differently depending on the gallium source during growth - triethylgallium(TEG) or trimethylgallium(TMG)
  - Hydrogen is usually unintentionally incorporated leading to burn-in. InGaAs bases have similar issues with burn-in.
- The ratio of β/R_{bsh} and burn-in are dependent on growth conditions.

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Effect of Base Layer Parameters

Base Sheet Resistance

$$R_{bsh} = \frac{1}{q\mu_p N_A w_b}$$

DC Current Gain (Kroemer)

$$\beta_{\max} = \frac{N_E}{N_B}\frac{v_{nB}}{v_{pE}} e^{\Delta E_v / kT} = \frac{N_E}{N_B}\frac{D_{nB}}{D_{pE}}\frac{w_E}{w_B} e^{\Delta E_v / kT}$$

$$\beta = \frac{v_{nb}}{w_b}\tau(N_b)$$

N_E and N_B = emitter and base dopings, respectively
μ_{NB}, μ_{PE} = minority carrier mobilities in base and emitter, respectively
W_B,W_E = base and emitter thicknesses, respectively
ΔE_v = effective valence-band barrier height.

$$\frac{\beta}{R_{b,sh}} = qN_E w_E \mu_n e^{\Delta E_v / kT}$$

Beta/Base Sheet Is Figure of Merit For Material Quality

β and R_b track, but slope depends on growth

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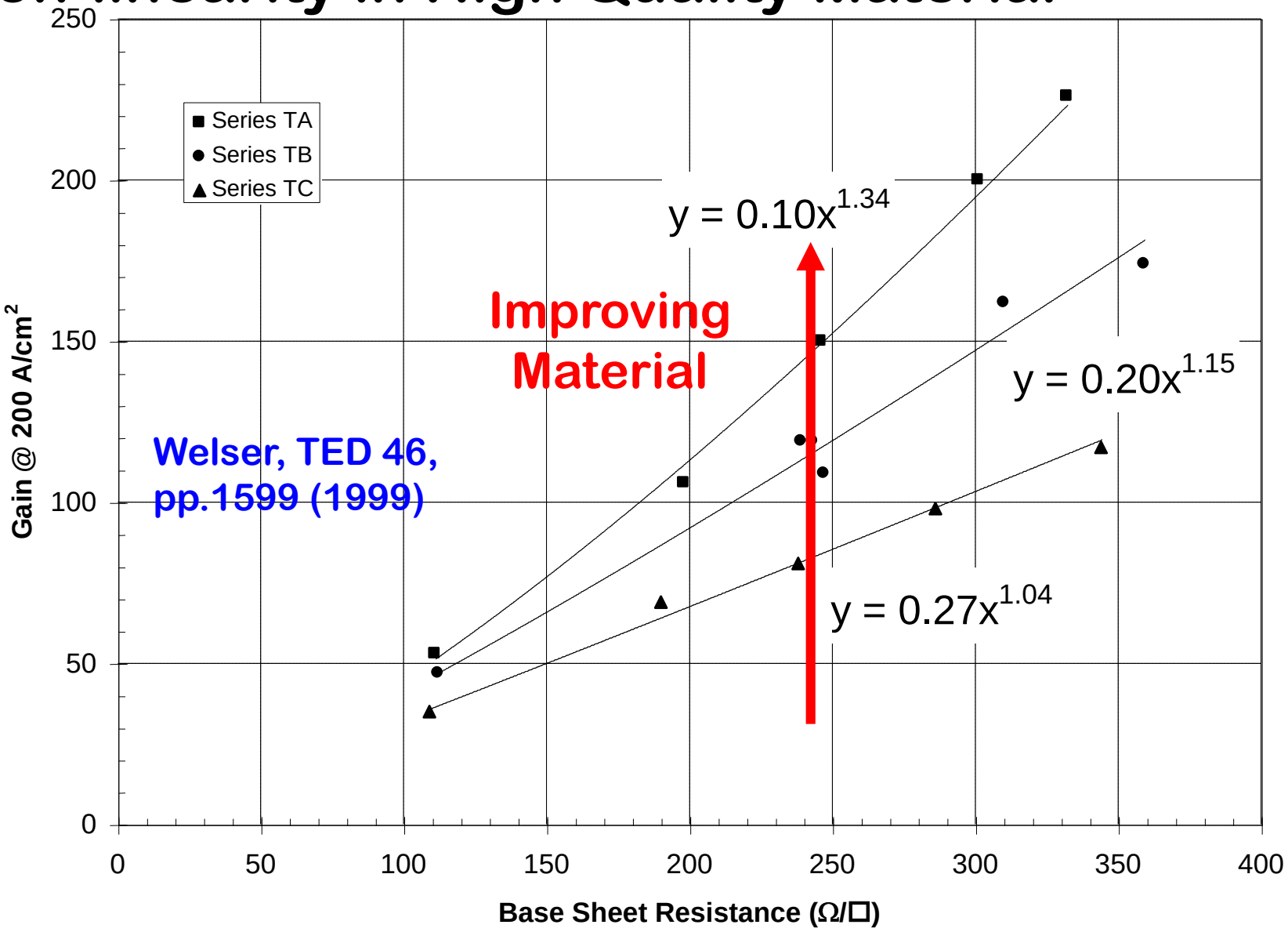
β vs. R_{bsh}: Non-linearity in High Quality Material



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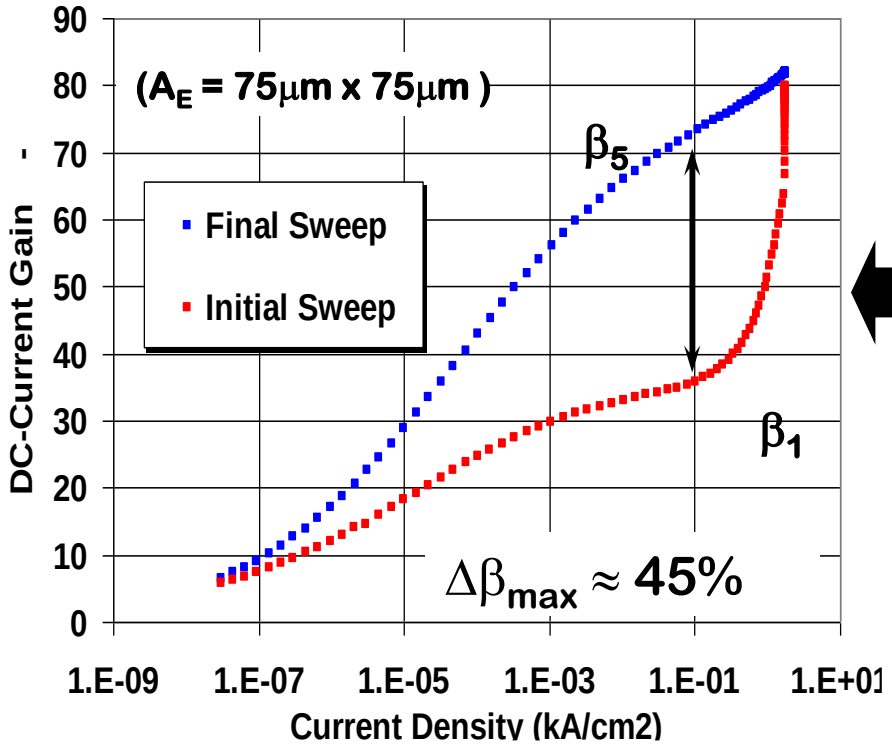
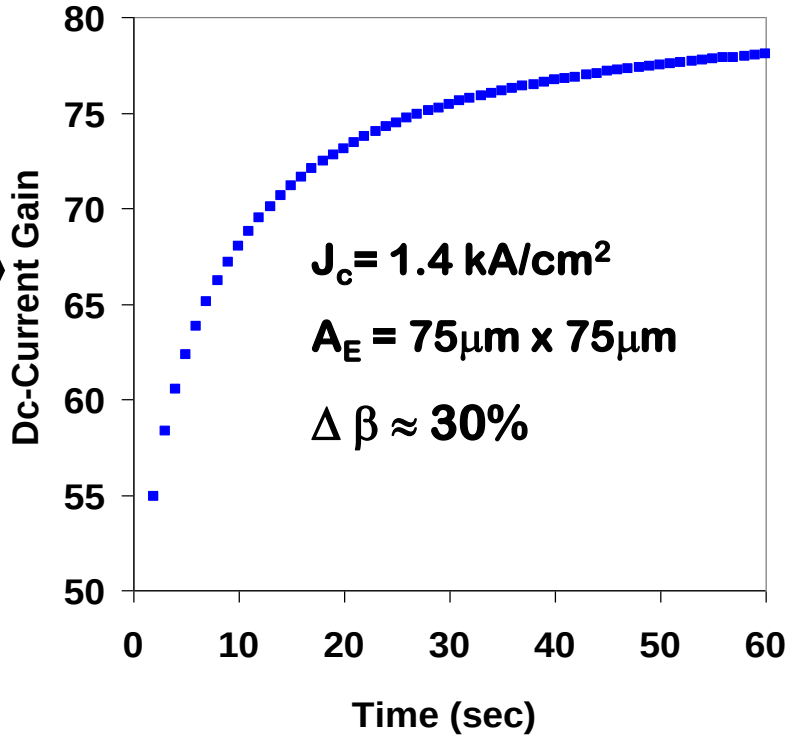
DC β Burn-in: Definition

Burn – In: Initial Transient in β





- Increase in β between first and fifth IV trace

  $\Delta\beta_{max}$ (J_c=100 A/cm²) = (β_5 - β_1)/ β_5

- Short-term increase in β with time (bias, temperature dependencies)

III-V HBTs usually require "burn-in" to stabilize β before measurement

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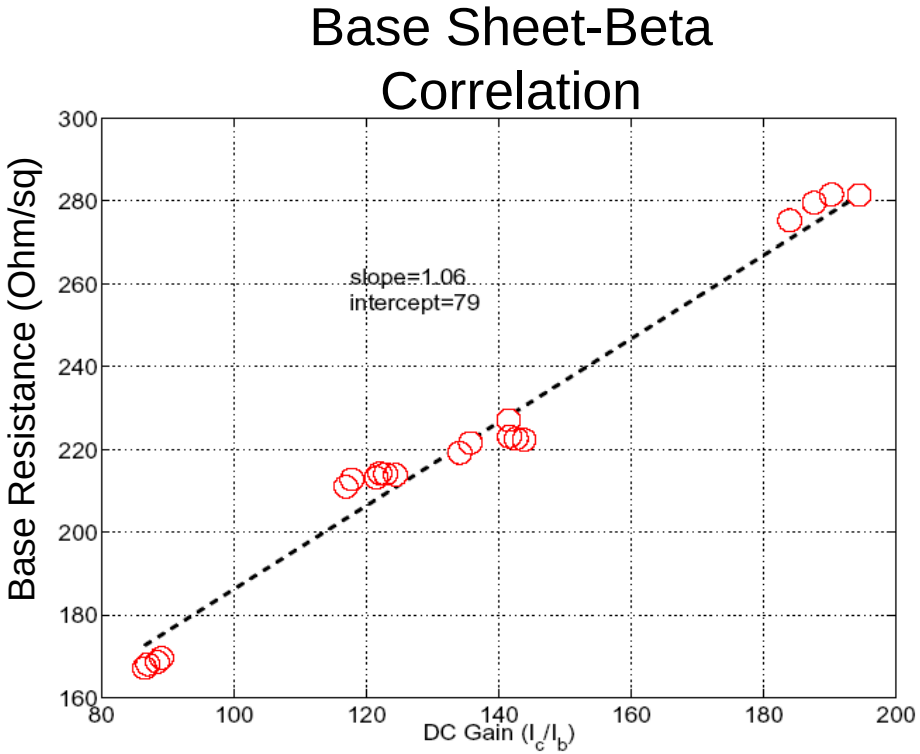
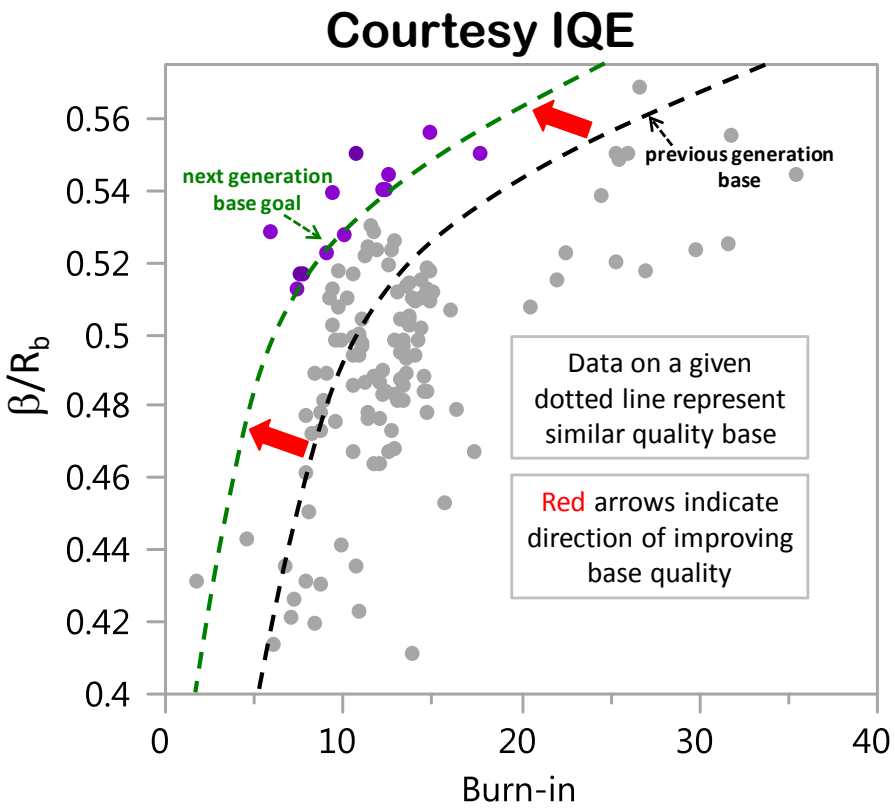
Knowing the Doping and Thickness of Base is Not Sufficient for III-V



Zampardi, Mantech 2004



β/R_{bsh} and burn-in can vary a LOT from vendor to vendor for the same spec!

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Material Models

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Base Parameters

Using Sheet Resistances

- The base sheet resistance is measured using transmission line method (TLM) or Van der Pauw (VDP). The sheet resistance is inverse to the product of the doping, thickness, and mobility. $R_{bsh}=1/(q\mu N_{aB}t_b)$

- This is a good place to compare the material spec (doping and thickness) vs. the electrical data (sheet resistance). Even better if you have multiple material structures or wafers from a base doping and thickness design-of-experiment.

- If the values are very different, then something is wrong.

Best to use a DOE or get vendor data
Instead of relying on old papers or text-books

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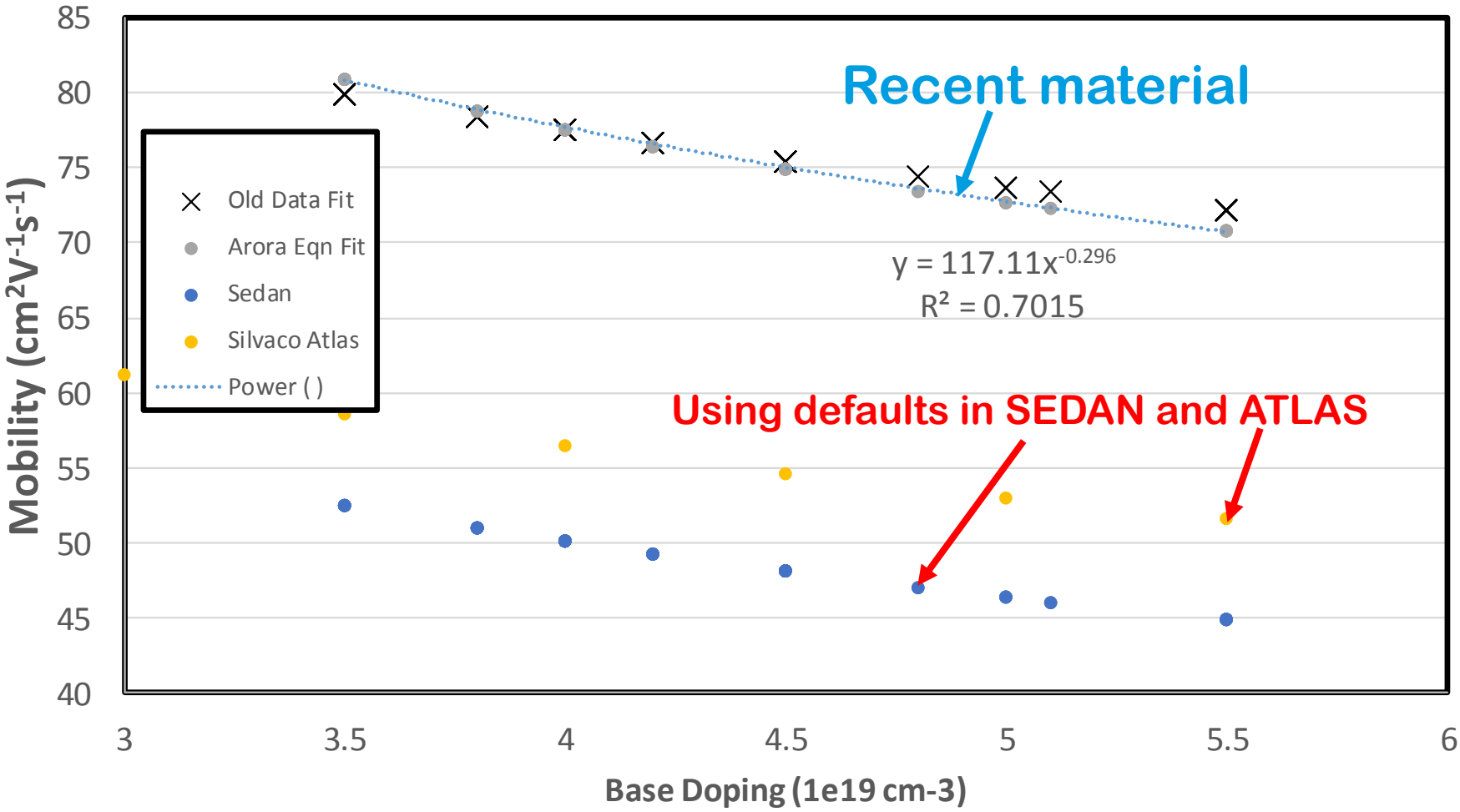
Example of Mobility vs. Doping

Material has IMPROVED. Better to use your own data.



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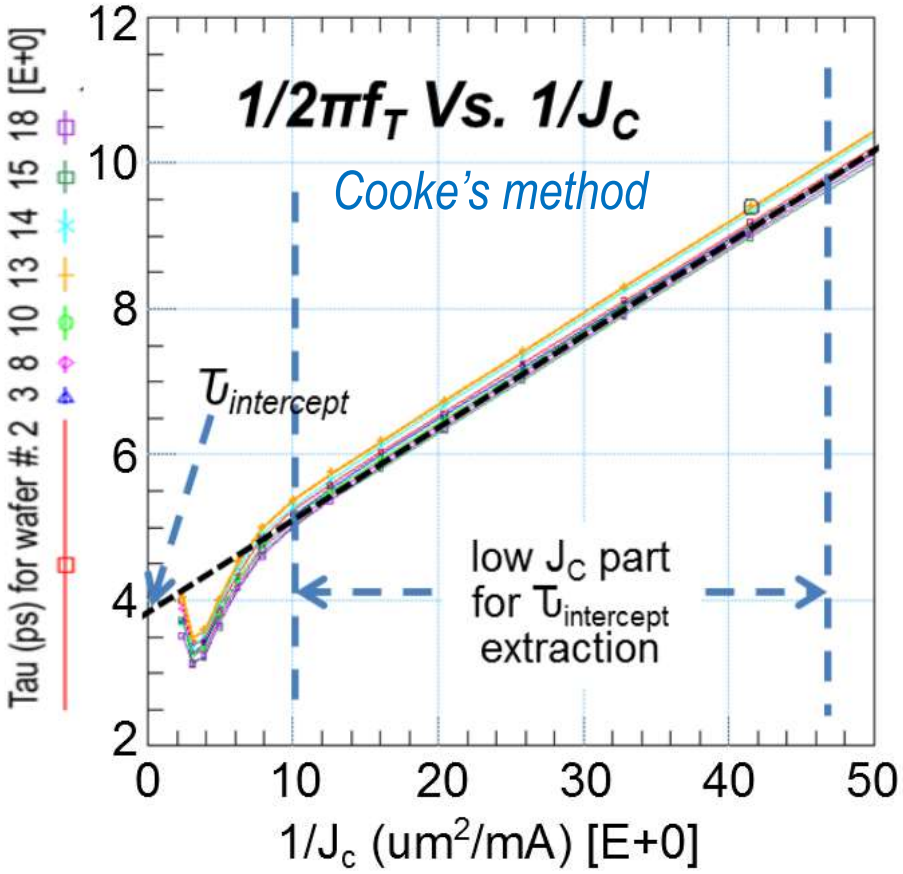
Extracting Minority Carrier Diffusion

$\tau_{intercept}$ Extraction @Low J_C

$$\tau_{EC} = \frac{kT}{qI_C}(C_{BEj} + C_{BCj}) + \left[\frac{W_E}{2n_E D_n} N_B W_B + \frac{W_B^2}{2D_n} + \tau_{SCR} + (R_E + R_C) C_{BCj}\right]$$

$\tau_{intercept}$



	DOE Factors			$\tau_{intercept}$
Wafer #	W_B (Å)	N_B (cm^{-3}) x10^{19}	W_C (μm)	(ps)
2	930	4.2	0.90	***3.99***
3	930	4.2	0.75	***3.92***
8	850	4.2	0.90	***3.84***
10	900	4.0	0.80	***3.88***
13	1000	3.5	0.90	***4.09***
14	1000	3.5	0.75	***4.01***
15	800	4.5	0.90	***3.77***
16	800	4.5	0.75	***3.69***
18	850	4.2	0.75	***3.76***

Yang 2015 CSICS

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Extracting Minority Carrier Diffusion, Cont'd

$$\tau_{Intercept} = \frac{W_E}{2n_E D_n} N_B W_B + \frac{W_B^2}{2D_n} + \tau_{SCR} + (R_E + R_C) C_{BCj}$$

$$\tau_{Intercept} = a_1 W_B^2 + a_1 \frac{W_E}{n_E} (N_B W_B) + a_3 W_C + a_4$$

where $a_1 = \frac{1}{2D_n}$ $a_3 = c_1 C_{BCj}$ $a_4 = \tau_{SRC} + R_E C_{BCj} + c_0 C_{BCj}$

a_1 is ps/A²

	Term	Estimate
a4	Intercept	**2.31**
a3	W_C	**0.47**
a1	W_B^2	**9.17e-7**

We assume W_e/n_e are known for this calculation.

$$D_n = \frac{10^{-4}}{2a_1}$$

From a_1, D_n=43.21 to 54.25 cm²/s vs. 26 cm²/s in old work.

We can find the D_n (minority carrier diffusion in the base) for the transit-time fit.

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Collector

Collector Resisance

Resistance Components

- Collector resistance consists of several parts:
  - A vertical component (when HBT is near knee, some of collector is no longer depleted),
  - Spreading resistance (from vertical flow to horizontal flow)
  - Lateral resistance – including contact.
- Collector sheet resistance is directly measurable using TLM or VDP. The sheet resistance is inversely to the product of the doping, thickness, and mobility.
  $R_{csh}=1/(q\mu_{nSubC}N_{nCSub}tC_{sub})$

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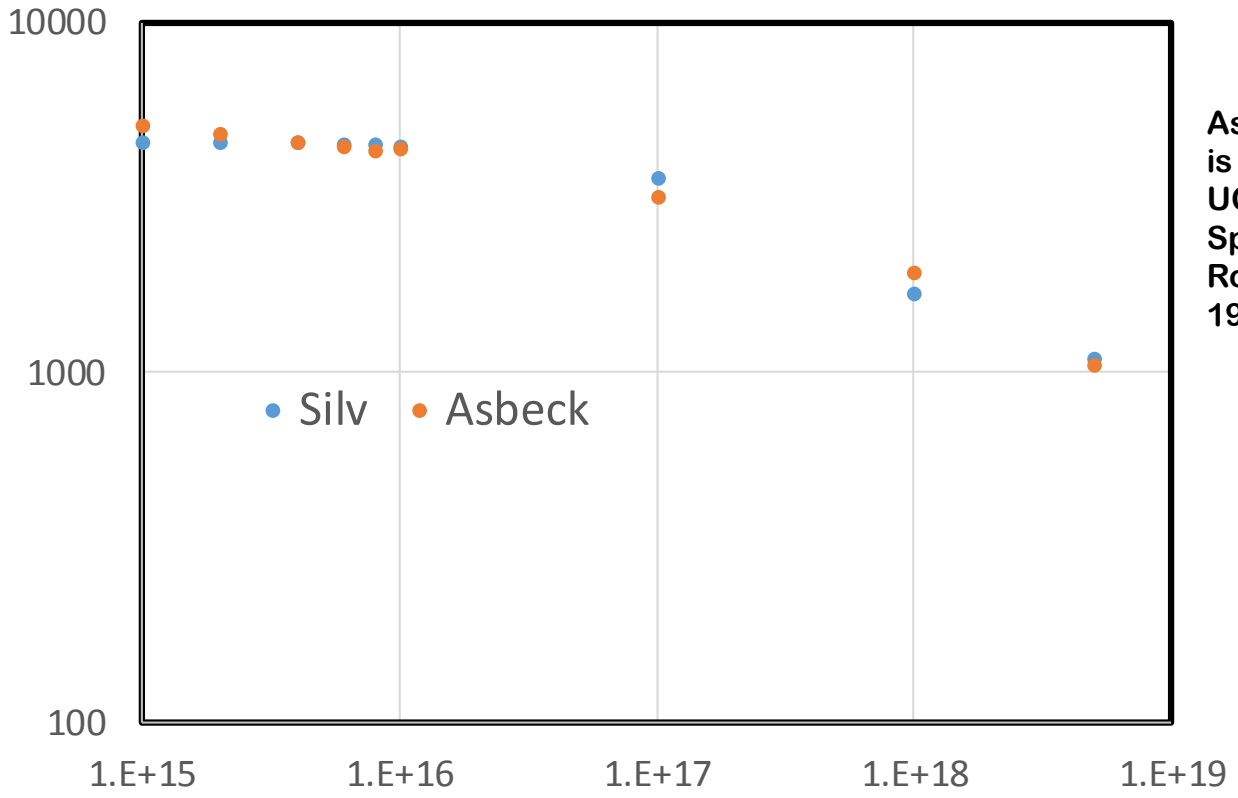
Collector Resistance – Mobility Fit

Adjust Mobility Model Parameters to Fit Old Data



Asbeck data is from UCSD HBTEST Spreadsheet, Robb Johnson 1994

$$\mu_n = mu1_n\left(\frac{T_L}{300k}\right)^{Alphan.caug} + \frac{mu2_n\left(\frac{T_L}{300k}\right)^{Betan.caug} - mu1_n\left(\frac{T_L}{300k}\right)^{Alphan.caug}}{1+\left(\frac{T_L}{300k}\right)^{Gamman.caug}\left(\frac{N}{N_{critN}}\right)^{Deltan.caug}}$$

mu1n	mu2n	Ncrit
908.647	4552.772	2.64E+17

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Junction Capacitances

Base-Collector Capacitance

Good for checking some parameters

- Built-in potential calculated using the base doping, the doping of the first collector, and the bandgaps of the materials. The doping dependence of the collector bandgap was included.
- Capacitance calculated using doping, built-in potential, and dielectric constant
- Used two-layer capacitance formulation since doping values mean that the depletion edge extends into 2nd collector
- Value for Cjc(0) agreed well with spec'd value. 0.257 (calc) vs. 0.259 (spec)

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Base-Emitter Capacitance

This is an example of how unknowns show up!

- Built-in potential calculated using the base doping, the doping of the active emitter, and the bandgaps of the materials. An example of how unknown ordering and Eg comes into play
- Dielectric constant is composition dependent – use equation from ioffe website. This could use some correction.
- Assuming no sheet charge due to dEc or ordering at InGaP/GaAs interface, we use two region cap model to get zero bias depletion width
- Value from calculation is a little off. Spec is 2.33 fF/μm^2, calculation is 2.47 fF/μm^2. This is sensitive to the InGaP layer. Under normal operating conditions, this value is not too important because the diffusion capacitance dominates in forward bias but is useful for validation of material parameters and models

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First Principles Calculations

Simple Calculations Give Clues to Where Things Can Be Wrong

EMITTER						Emitter Material Constants		
Emitter spec. cont. resist.; Resc	2.00E-06	ohms-cm^2	B-E Built-in voltage;VbiBE	1.57	V	Bandgap; EgE	1.89	eV
InGaP doping; NdE	2.30E+17	cm^-3	Total emitter resistance; Re	1.28	ohms	Effective density of states; NcE	6.50E+17	cm^-3
InGaP thickness; te	0.04	µm	Emitter depletion width (0 V); WdE	0.0421	µm	(n) mobility; munE	2689	cm^2/V-s
Ga composition; Ga_comp	0.51		Emitter C/A (0 V)	2.4797	fF/µm^2	Dielectric constant; DCE	11.786	
InGaP spec. cont. resist.; Rasc	4.04E-08	ohms-cm^2	CJE0 (Cbe tot @ 0 V)	396.75	fF			

BASE						Base Material Constants		
Base doping; NaB	2.80E+19	cm^-3	Int. base sheet resistance; Rbshi	274.64	ohms/sq	Bandgap; EgB	1.42	eV
Base thickness; tb	0.0825	µm	Ext. base sheet resistance; Rbshe	274.64	ohms/sq	Effective density of states; NvB	7.00E+18	cm^-3
Front/Back doping ratio	1		Base resistance modulation (1=Yes)	0		(p+) mobility; mupB	98	cm^2/V-s
Front/Back In comp. difference	0	%	Base resistance modulation factor	0		Electron diffusivity; DnB	26	cm^2/sec
Base spec. cont. resistance; Rbsc	1.00E-08	ohm-cm^2						

COLLECTOR						Collector Material Constants		
(n1-) collector doping; NdC1	7.50E+15	cm^-3	BC Vbi	1.39	V	Bandgap; EgC	1.41	eV
(n1-) collector thickness; tc1	0.45	µm				Effective density of states; NcC	4.70E+17	cm^-3
(n1-) coll depletion width; WdC1	0.4500	µm	Collector characteristic length; LcC	7.0072	µm	(n1-) mobility; munC1	6471	cm^2/V-s
(n1-) coll neutral width	0.0000	µm	Collector contact resistance	0.0821	ohm-mm	(n1-) mobility; munC2	5557	cm^2/V-s
(n1-) coll spec. cont. resist.; Rc_1sc	0.00E+00	ohm-cm^2	Rc contact; Rc_cont	1.83	ohms	(n+) mobility; munC3	2919	cm^2/V-s
(n1-) coll area eff; Ac_1	4.51E-07	cm^2	Rc lateral; Rc_lat	2.08	ohms	Dielectric constant; DCC	12.9	
(n1-) coll resistance; Rc_1	0.00	ohms	Sub-coll R ext tot; Rsc_tot	3.91	ohms	Electron diffusivity; DnC	167.60	cm^2/sec

From HBTEST, 1994

Built-in potential calculations (only used for CV formulation)
Bandgaps not adjusted for bandgap narrowing (base)
The VbiBE is also influenced by partitioning of Eg – this is function of ordering of InGaP and Eg (In composition).

Calculation
Assumes 0.208*(EgE-EgC) ~0.1, assuming disordered InGaP. The value can be different for ordered or partially ordered. It would be lower bringing the two values for potential closer together.

VJE(Model Card)=1.428 vs. 1.57 calculated, VJC(Model Card)=1.0795 vs. 1.39 calculated.

Converting CV to N vs. X may help determine if this is thickness or doping that is off. Very typically used in III-V

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Heterojunctions

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Emitter

Resistance Components and Heterojunction

- **Vertical Resistance**
  - Calculate the bulk vertical resistance in the emitter the same as we calculated the collector intrinsic. Here we keep the emitter (InGaP) in the stack since it is higher doped and the mobility is worse than GaAs. We use the default model #'s for InGaP because it is all that is available (epi vendors more focused on capacitance than mobility)
  - Summing these two values for vertical resistance, we notice we do not come close to the emitter specific resistance (resistance*Area). This is because there are two heterojunctions (InGaAs/GaAs and GaAs/InGaP) that look like resistors
  - What the calculations do tell us is how much we are changing the R_e with the contact or bulk layers
- **Sheet Resistance**
  - We discussed this earlier

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Emitter Resistance

Vertical Resistance

- From previous page, we note that there are several iso-Heterojunctions in the emitter. Each of this MAY contribute something that looks like emitter resistance.

- Some observations:
  - Observed resistance increases with increasing Al concentration (Zampardi, CMRF 2004)
  - Observed emitter resistance increases if InGaP or AlAs layers are added in the emitter stack (Zampardi, CMRF 2007)
  - Emitter resistance decreases with temperature

All of these observations support the heterojunction theory. Means that knowing the InGaP ordering and composition matters!

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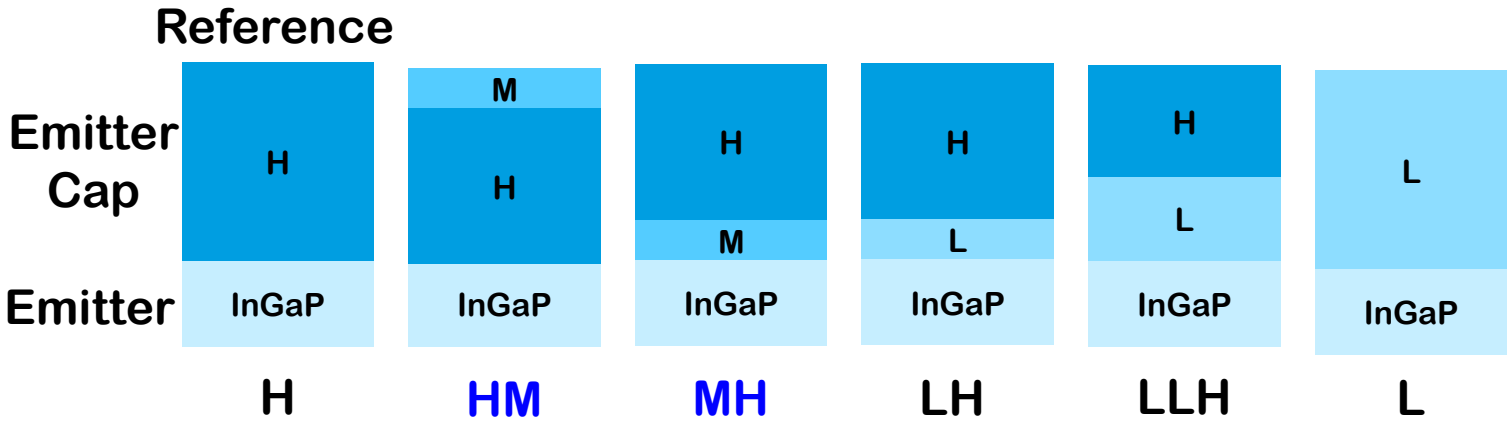
Heterojunction Impact Example

R_e contains heterojunction (GaAs/InGaP)



Structure	% Re Change Measured	% Re Change Calculated
H	0	0
HM	12	2
MH	76	2
LH	68	10
LLH	52	36
L	100	42

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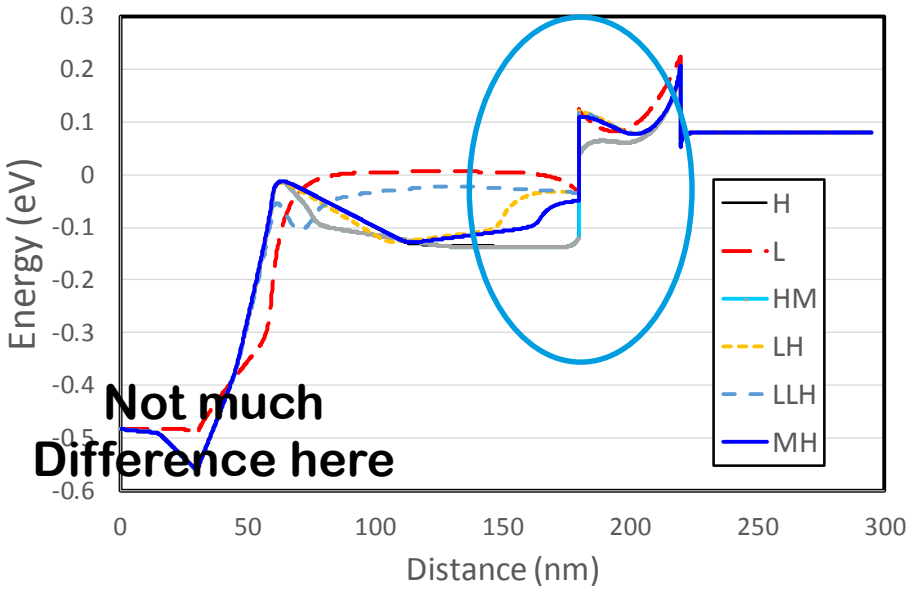
Bandprof Simulations

Demonstrates/validates Importance of dE_c



Emitter ground, base 1.4 Volts. Each potential step will act like a "resistor" and thermionic emission over the barrier will make it looks like resistance goes down with temperature.

Calculate Re by hand and identify dEg contribution

Structure	% Re Change Measured	% Re Change Calculated
H	0	0
HM	12	2
MH	76	2
LH	68	10
LLH	52	36
L	100	42

From bulk HM and MH, expect the same Re. Heterojunction looks like emitter resistance.

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Velocity vs. Field

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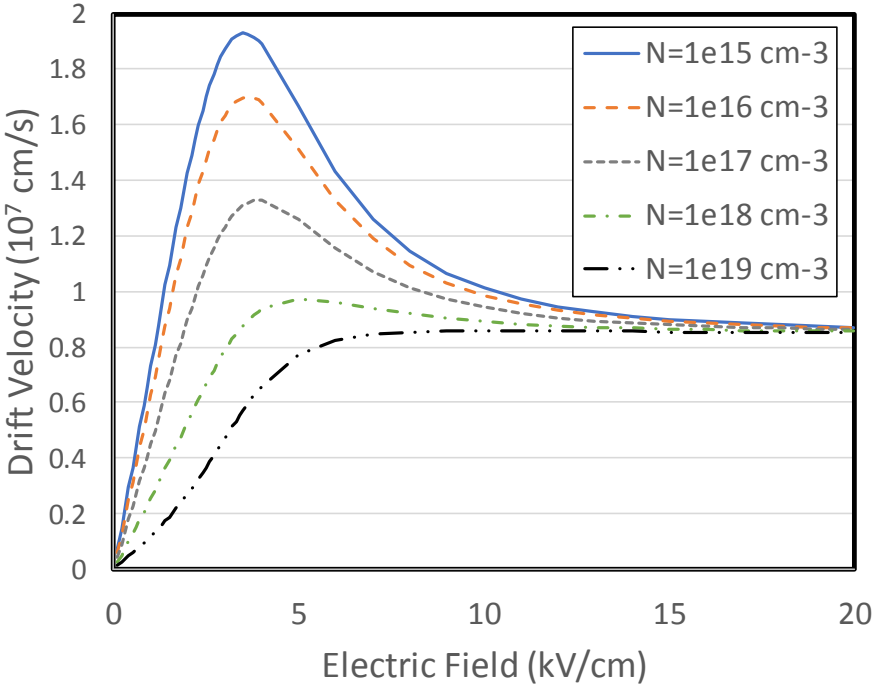
Velocity vs. Field

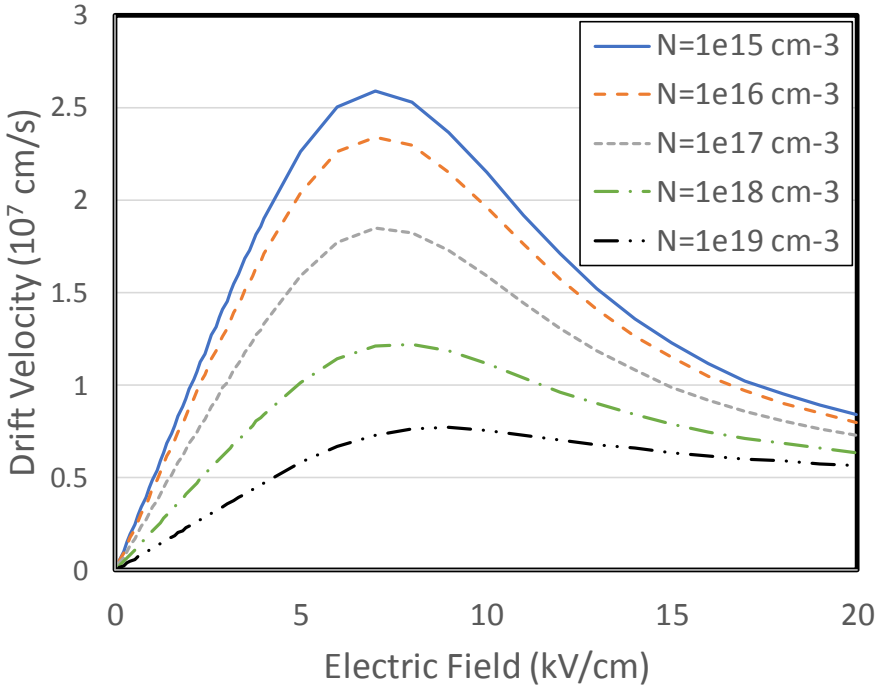
Steady-State Velocity vs. Field

GaAs



After Wen Liu, Ph.D. Dissertation, UCLA
And SEDAN III Manual

InP



After Sootadeh & J.C. Li

For high-speed devices, collector is higher doped, current density high
For power amplifier, collector is low doped, current density low

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Problems with NDM

Reported by Wedel, Nardmann, and Schroter

Problems in Hydrodynamic and Drift-Diffusion Simulators using v(E) formulation.

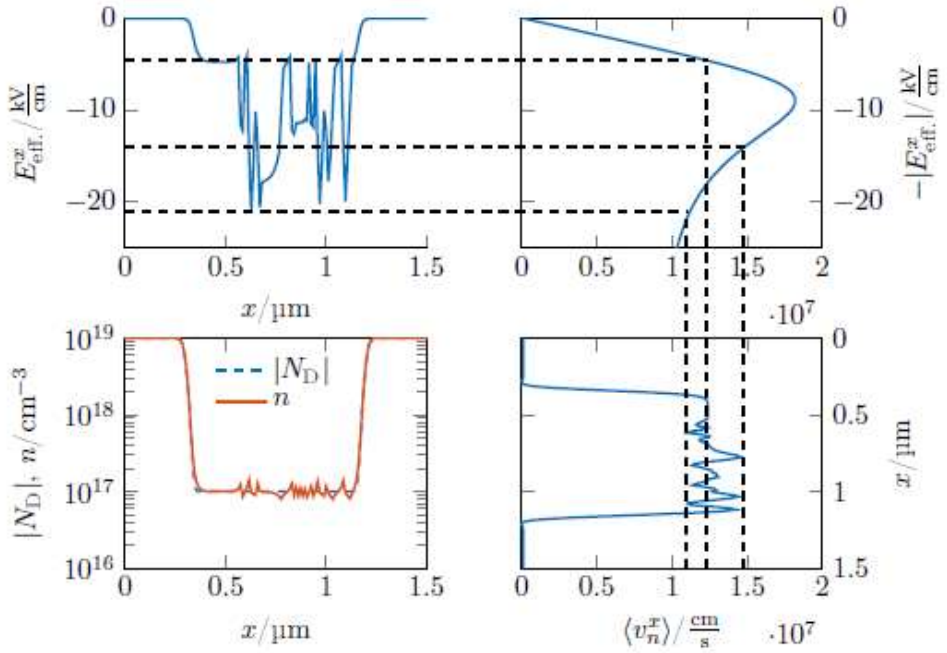

Figure 1: Effective DD field, NDM-model, electron density and electron velocities of the n^+nn^+ structure for V_{RL}=0.8 V obtained by the in-house simulator.

Oscillations from NDM. Not Gunn (collector design is not in right region)

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Work-Around?

Why Isn't This Discussed More?

- For high-speed devices, the doping is high enough to mask some of the peaking of the field.
- For most PA related designs (GaAs), the usable current density is well below where the NDM kicks in. GaAs may be a little more benign, but required use of transferred electron model.
- Li showed two improvements to allow "good" f_T simulations
  - Re-fitting the energy band formulation to be more representative, this allowed convergence past peak ft for InP devices.
  - Using the transferred electron model and using driving force, instead of field to improve convergence
  - This required very detailed analysis of all the transport models and making them self-consistent.
  - The more advanced the transistor, the harder it is to get a result that converges

For InP, Some Fundamental Issues May Exist for TCAD of High Performance Devices – An Opportunity!

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Summary

III-V Devices Have More Subtleties Than Si!

- Material Design and Specification
  - Many TCAD issues are the result of not knowing what the material properties of the received wafer are
- Material Models
  - Model parameters can be extracted from device measurements and then fit to proper equations
- Heterojunctions
  - SIMS is not so useful for III-V because of heterojunction complications. Many of these can be understood from growing a series of materials and using proper characterization
- Velocity vs. Field
  - Care must be taken in how devices with strong NDM are simulated to avoid oscillations. If the oscillations can't be avoided, this is a show stopper for proper TCAD use in III-V

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Other Useful References

III-V Epi-growth - Wayne Johnson, Mantech 2013 Tutorial, “I have a PA spec… Now what? Or HBT Growth by MOCVD)

Ordering – Gomyo, et al, Journal of Crystal Growth, vol. 77, 1986, pp. 367-373

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Non-uniform base (spacer) - E.M. Rehder, Digest of the Compound Semiconductor IC Symposium, Monterey, California, pp. 75-78, 2004

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