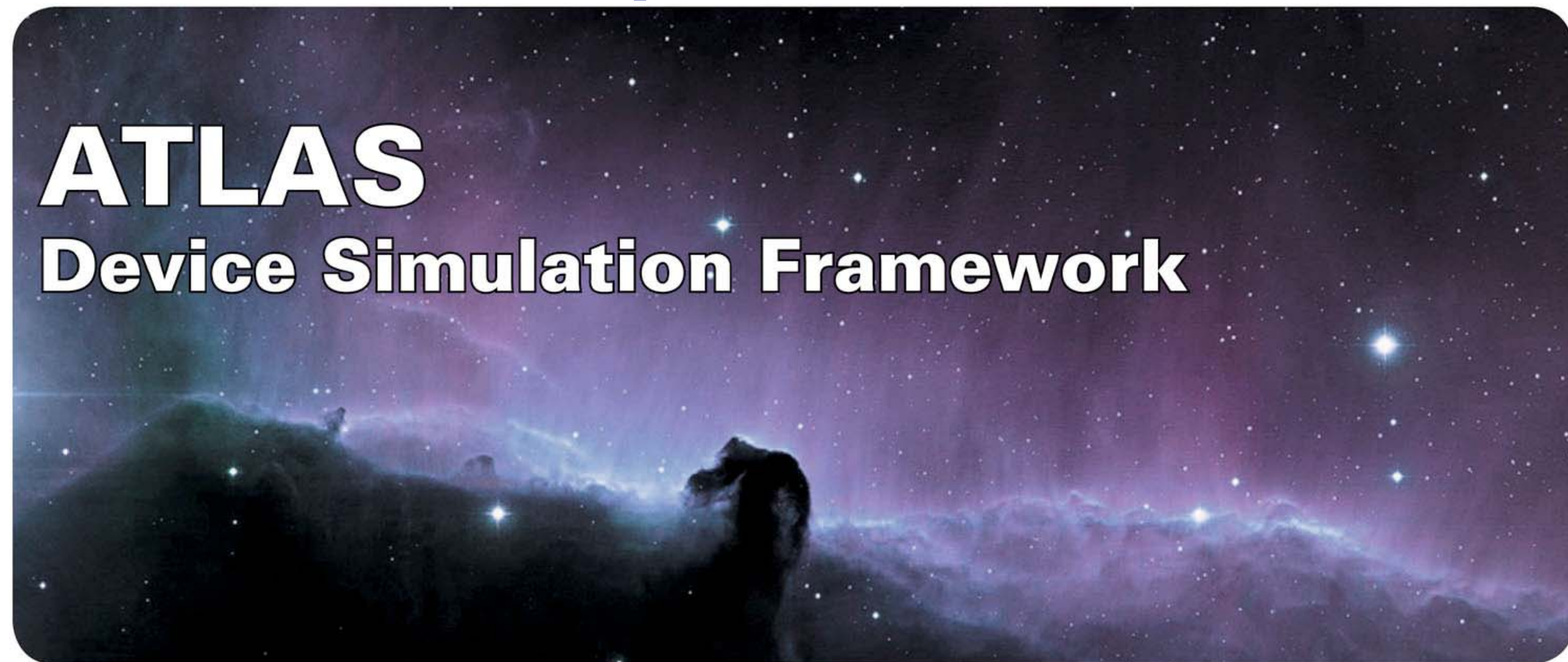
Blaze Workshop



III-V Compound Device Simulation

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Requirements for III-V Device Simulation

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Blaze as Part of a Complete Simulation Toolset

- III-V Device Simulation maturity has conventionally lagged behind silicon leading to many immature standalone tools with a low user base
- Users must ensure that the simulator they evaluate has all the necessary components
- Blaze shares many common components of the ATLAS framework with the mature and heavily used silicon simulator, S-Pisces
- Blaze is able to take advantage of ATLAS improvements in numerics, core functionality and analysis capabilities from Silicon users
- All of the features of ATLAS are available to Blaze users
- Blaze is completely integrated with TonyPlot, DeckBuild and DevEdit. Blaze experiments can be run using Virtual Wafer Fab

The 10 Essential Components of III-V Device Simulation

1 Energy Balance / Hydrodynamic Models
- velocity overshoot effects critical for accurate current prediction
- non-local impact ionization

2 Lattice Heating
- III-V substrates are poor conductors
- significant local heating affects terminal characteristics

3 Fully Coupled Non-Isothermal Energy Balance Model
- Important to treat Energy balance and lattice heating effects together

The 10 Essential Components of III-V Device Simulation (cont.)

4 High Frequency Solutions

- Direct AC solver for arbitrarily high frequencies

5 AC parameter extraction

- extraction of s-, z-, y-, and h-parameters
- Smith chart and polar plot output

6 Interface and Bulk Traps

- effect on terminal characteristics is profound
- must be available in DC, transient and AC

The 10 Essential Components of III-V Device Simulation (cont.)

7 Circuit Performance Simulation (MixedMode)

- for devices with no accurate compact model

8 Optoelectronic Capability (Luminous)

- for devices with optoelectronic applications (e.g. Photodetectors)

9 Speed and Convergence

- flexible and automatic choice of numerical methods

10 C-Interpreter for interactive

- model development
- user defined band parameter equations
- implementing mole fraction dependent material parameters

Material Parameters and Models

- Blaze uses currently available material and model coefficients taken from published data and university partners
- For some materials often very little literature information is available, especially composition dependent parameters for tenrary compounds
- Some parameters (eg. band alignments) are process dependent
- Tuning of material parameters is essential for accurate results

Material Parameters and Models (cont.)

- Blaze provides access to all defaults though the input language and an ASCII default parameter file
- The ability to incorporate user equations into Blaze for mole fraction dependent parameters is an extremely important extra flexibility offered by Blaze
- The C-INTERPRETER allows users to enter material parameters and model equations (or lookup tables) as C language routines. These are interpreted by Blaze at run-time. No compilers are required
- With correct tuning of parameters the results are accurate and predictive

Blaze Applications

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Introduction

- Blaze: One of the simulators in the ATLAS framework simulates general devices based on arbitrary semiconductor materials
  - 2D general purpose heterojunction device simulator
  - All classes of III-V, IV-IV, II-VI semiconductor based devices, and alternative elemental semiconductors
  - HEMTs, MESFETs, HBTs, HIGFETs, etc.
  - Combine with other ATLAS elements for advanced features (eg. Blaze + Giga for lattice heating effects in HEMTs)

Blaze Features

- Built-in material parameter library for common heterojunction compounds including ternary and quaternary materials:
  - GaAs, AlGaAs, InGaAsP, SiGe, SiC, etc.
- Handles abrupt and graded heterojunctions
- Energy Balance modeling for velocity overshoot and non-local impact ionization
- Self-heating effects (with Giga)
- Optoelectronic applications (with Luminous)
- Laser structure simulation including stimulated emission of radiation (with Laser)
- Heterostructure device-circuit simulation (with MixedMode)
- Possible to modify existing and develop new physical models and material parameter correlations (with C-Interpreter)

Simulation of III-V Device with Blaze

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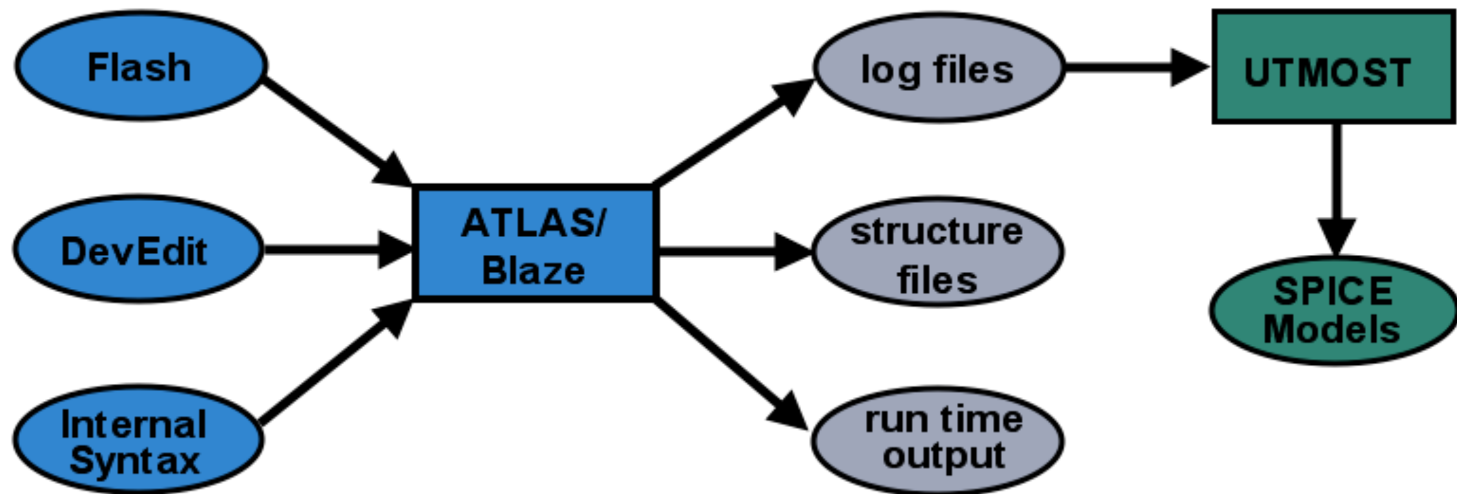
Overview

- As with any ATLAS input deck the following phases are necessary:
  1. Structure definition
  2. Material and model specification
  3. Numerical methods selection
  4. Solution specification
  5. Results Analysis

Information Flow



Applications

- DC Characterization
- Transient Analysis
- Breakdown Calculations
- AC Analysis
- S-Parameter Calculation

Heterostructure Specification

- Heterostructures can be specified by:
  - DevEdit graphical mode
  - DevEdit syntax in DeckBuild
  - ATLAS syntax in DeckBuild
    - (limited to rectangular regions)
- Graded Heterojunctions allowed

Device Specification Using DevEdit

- Add, Modify & Delete Regions
- Deposition of Layers
- Region Numbering
- Electrode Specification
- 2D and 3D Regions
- Circular/Cylindrical Regions

Device Specification Using DevEdit (cont.)

- Region Definition
  - specific (cm^{-3}) Sb, As, B, Ph
  - generic (III-V option)
  - net (cm^{-3})
- Impurity Definition
  - define impurity from list
  - user-specified box
  - x, y roll-off function (Gaussian, ERFC)
  - define 1D profiles from SSuprem3, SSuprem4 and SPDB
  - 1D profiles added to x, y roll-off functions

Note: Mesh must be generated before saving structure.

DevEdit Meshing Features

- Base Mesh Parameters
- Mesh Constraints by region or XY limits
  - min/max triangle size
  - max triangle ratio
  - max angle in a triangle (default=90)
- Refinement on any node based quantity (eg. doping, potential)
- Refinement by XY coordinates.
- Z plane specification for 3D meshing

III-V Material Specification

- Non-Planar Region Specification
  - Recessed Gates
- Generic Region Composition
  - X,Y Mole Fractions
  - Donor/Acceptor Concentrations
  - e.g. $In_{(1-x)}$ $Ga_{(x)}$ $As_{(y)}$ $P_{(1-y)}$
- Graded Region Composition
  - Add Impurity as x, y composition
  - Define x, y Roll-off
  - Draw region
- Doping specification - Standard Generation

Saving Designed Structures

- DevEdit design saved in command line syntax
  - special DevEdit syntax
  - defines geometries and dopings
  - contains generated mesh parameters
  - can be run in DeckBuild
- DevEdit design saved as structure file
  - only for final design
  - Silvaco's master file syntax
  - can be loaded by ATHENA, ATLAS, TonyPlot

Material Specification

- Material Parameter Specifications
  - Explicit Assignments
  - C-Interpreter Assignments
  - Mole Fraction
  - Band Alignment
  - Schottky Barrier Height
  - Checking Parameters (“models print”)

Material Specification

- Accurate Defaults
- Unknown/Disputed Values
- Novel Materials
- University Collaborations
- Recommended References

ATLAS/Blaze References

- S. Adachi "Physical Properties of III-V Semiconductor Compounds InP, InAs, Gats, GaP, InGaAs and InGaAsP," John Wiley, New York, 1992.
- M. Lundstrom and R. Shuelke, "Numerical Analysis of Heterojunction Semiconductor Devices", IEEE Tran, ED 30, 1983.
- M. Klausmeier - Brown, M. Lundstrom and M. Mellach, "The Effects of Heavy Impurity Doping on AlGaAs/GaAs Bipolar Transistors," IEEE Tran. ED 36, 1989.

Material and Model Specification

- Material parameters
  - All important material parameters can be specified in the MATERIAL statement to override the defaults: energy band gap, densities of states in conduction and valence bands, electron affinities, dielectric constants, etc.,

```
MATERIAL MATERIAL=b-SiC EG300=2.2 NC300=6.59E18 NV300=1.68E18   AFFINITY=4.0 \
PERMITTIVITY=9.72 TAUN0=1E-9 TAUP0=1E-9 MUN=100 MUP=100 AUGN=1E-31 AUGP=1E-31

MATERIAL MATERIAL=a-SiC EG300=3.0 PERMITTIVITY=9.66 EGBETA=0.EGALPHA=3.3E-4 \
AUGN=2.8E-31 AUGP=9.9E-32 VSAT=2.0E7 MUN0=330.0 MUP0= 60.0 NSRHN=3.E17 \
NSRHP=3.E17 TAUN0=1.E-7 TAUP0=1.E-7 TMUN=2.25 TMUP=2.25 LT.TAUN=2.3 \
LT.TAUP=2.3
```

  - The C-Interpreter must be used to define more complex relationships (eg. band gap dependence on composition fraction)

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Schottky Contact Specification

- Schottky contacts must always be defined in the CONTACT statement.

```
CONTACT name=gate WORKFUNCTION=4.2
```

- The difference between the contact workfunction and the semiconductor electron affinity approximately determines the potential barrier at the contact

note:

If the ALIGN parameter was used, the default electron affinities may have been changed to ensure specified band alignment. Check on affinities in the material parameter table in the beginning of the ATLAS runtime output (Use MODELS PRINT). Also check that the workfunction specified gives you expected potential barrier

Material Specification

- MESFETs
  - Mobilities
  - Schottky Barrier Height
- HFETs (PHEMTs)
  - Composition Fraction
  - Band Offset
  - Mobilities
  - Schottky Barrier Height
- HBTs
  - Composition Fraction
  - Band Offset
  - Minority Carrier Lifetimes
  - Mobilities

Model Specification

- Carrier Statistics
  - Fermi Dirac / Boltzman
  - Band gap narrowing
- Recombination
  - SRH / Consrh
  - Auger
  - Optical
- Impact Ionization
  - Selberherr / Grants / Crowell-Sze
  - Local / Non-local

Model Specification

- Mobility
  - Standard Low Field Mobility:

$$\mu_n(T) = \mu_{no}\left(\frac{T}{300}\right)^{\alpha_n}$$

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Model Specification

- Standard and Negative Differential Field Dependent Mobility

$$\mu_n(E) = \mu_{no}\left[\frac{1}{1+\left(\frac{\mu_{no}E}{\nu_{satn}}\right)^{\beta_n}}\right]^{\frac{1}{\beta_n}}$$

$$\mu_n(E) = \frac{\mu_{no} + \frac{\nu_{satn}}{E}\left(\frac{E}{E_o}\right)^{\gamma}}{1+\left(\frac{E}{E_o}\right)^{\gamma}}$$

Model Specification

- Models specification
  - Different sets of models can be applied for different regions
  - Specify models on material-by-material basis
  - Concentration dependent mobilities (conmob) can be applied only to the AlGaAs material system
  - It is recommended for AlGaAs and all other materials to specify low-field mobilities in the MATERIAL statement and then apply field dependent mobility in the MODEL statement:

```
MODEL MATERIAL=GaAs   CONMOB FLDMOB SRH OPTR BGN
MODEL MATERIAL=AlGaAs FLDMOB SRH OPTR
MODEL MATERIAL=InGaAs FLDMOB SRH
```

  - Use MODELS PRINT to check model and material parameters in the run-time output
  - Use IMPACT SELB for impact ionization. The default parameters are for GaAs only

Model Specification

- Thermionic emission model
  - This can be used to describe transport through abrupt heterojunction instead of the classical model (drift-diffusion)
  - It is the only physical model NOT activated using the MODEL statement
    - for structures specified using ATLAS syntax use the REGION or INTERFACE statement
    - for structures specified using DevEdit use the INTERFACE statement only

Advanced Models

- Energy Balance / Simplified Hydrodynamic
  - Higher order approximation than Boltzmann Transport
  - Two extra equations representing electron and hole “temperatures”
  - Key parameter - Energy relaxation time

$$\nabla \overline{S}_n = \overline{J}_n \nabla \psi - W_B - \frac{3}{2} k \frac{\partial}{\partial t} (\lambda_n^* n T_n^*)$$

- Adds two coupled equations to the drift diffusion equation set

Advanced Models

- Lattice Heating
  - No longer assume lattice temperature is constant
  - Establish thermal boundary conditions

$$C\frac{\partial T_L}{\partial T} = \nabla(k\nabla T_L) + H$$

  - H includes generation/recombination, Thomson and Peltier
  - Adds an extra coupled equation to the drift diffusion equation set

Solution Techniques

- The Mesh
  - Critical for accurate and robust simulations
- Solution Methods
  - Newton (3 - 6 equations)
  - Gummel
  - Block
- Number of Carriers
  - 0 / 1 / 2
- Solution Type
  - DC
  - Transient
  - AC
- Curve Tracer
- External Effects

Solution Techniques

- Small-signal Parameter Calculation
  - ATLAS/BLAZE calculates capacitance/conductance
  - Y-Parameter conversion
  - S-Parameter conversion
  - Z-Parameters
  - H-Parmeters
  - ABCD-Parameters
  - Power Gains (GU_{max}, GT_{max}, G_{ma}, G_{ms})

Case Study - HBT

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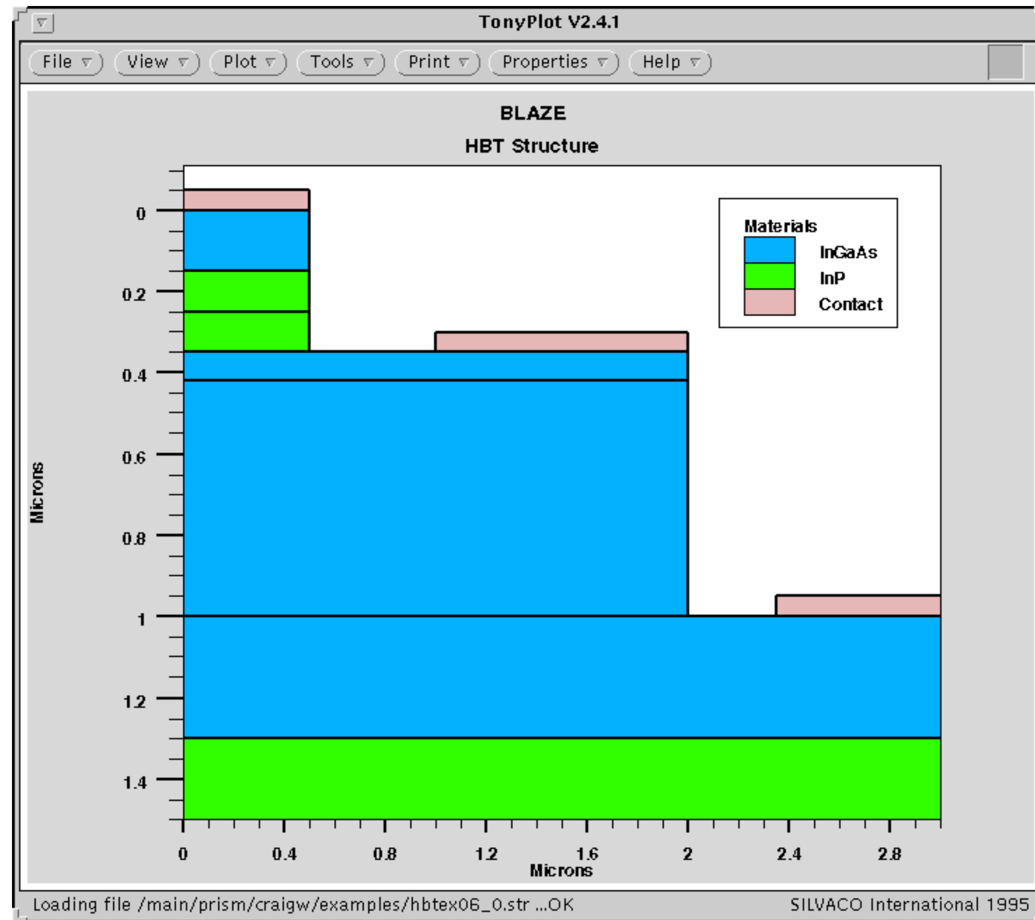
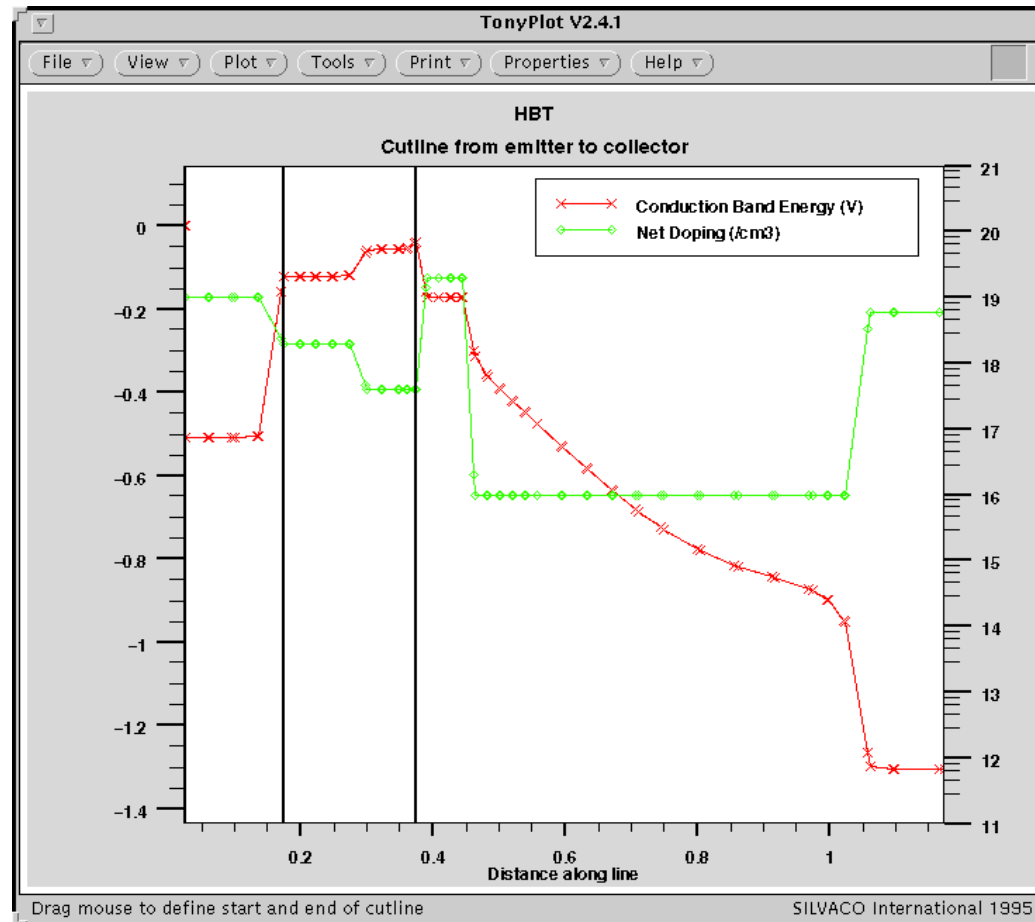
Case Study – HBT

- HBT
  - Structure generated and meshed in DevEdit
  - Non-planar surfaces possible
  - Alignment and minority carrier lifetimes key to success
  - DC, AC solutions
  - TonyPlot functions can be used for gain etc.

HBT Created in DevEdit



HBT Cutline From Emitter to Collector



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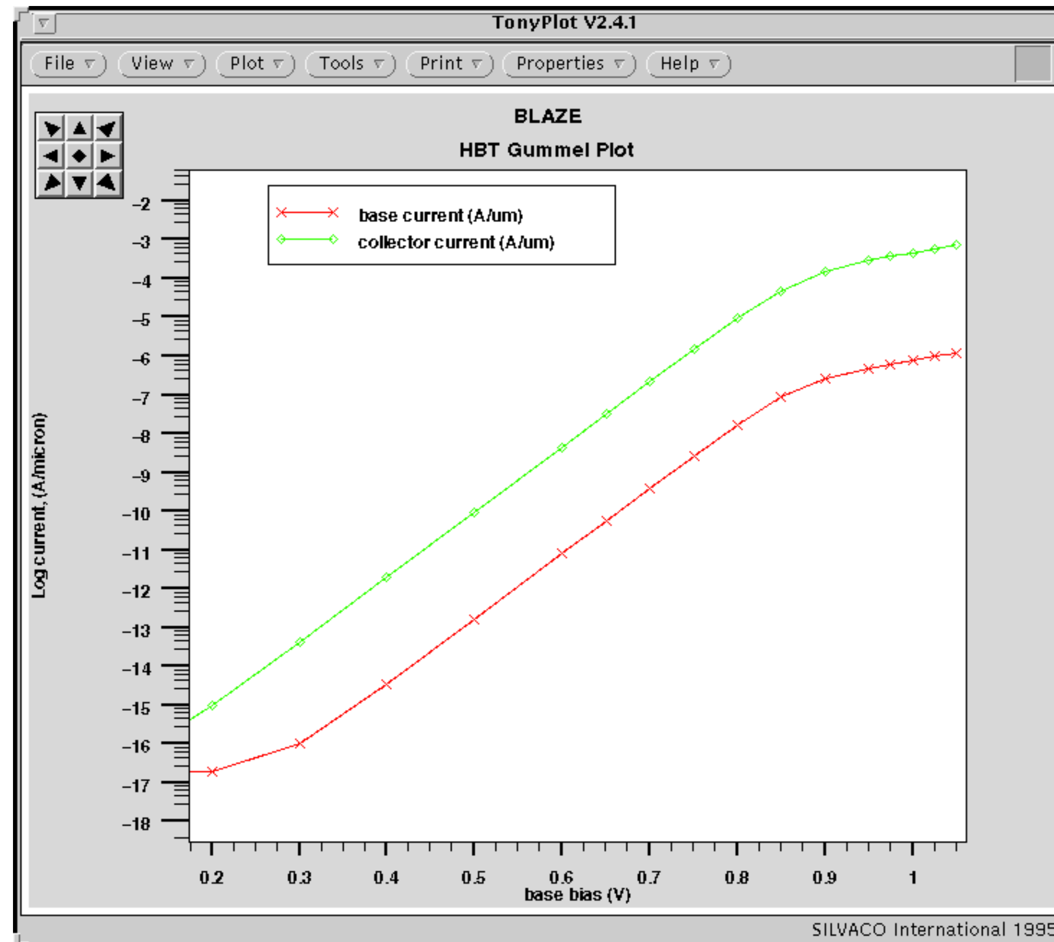
HBT Gummel Plot



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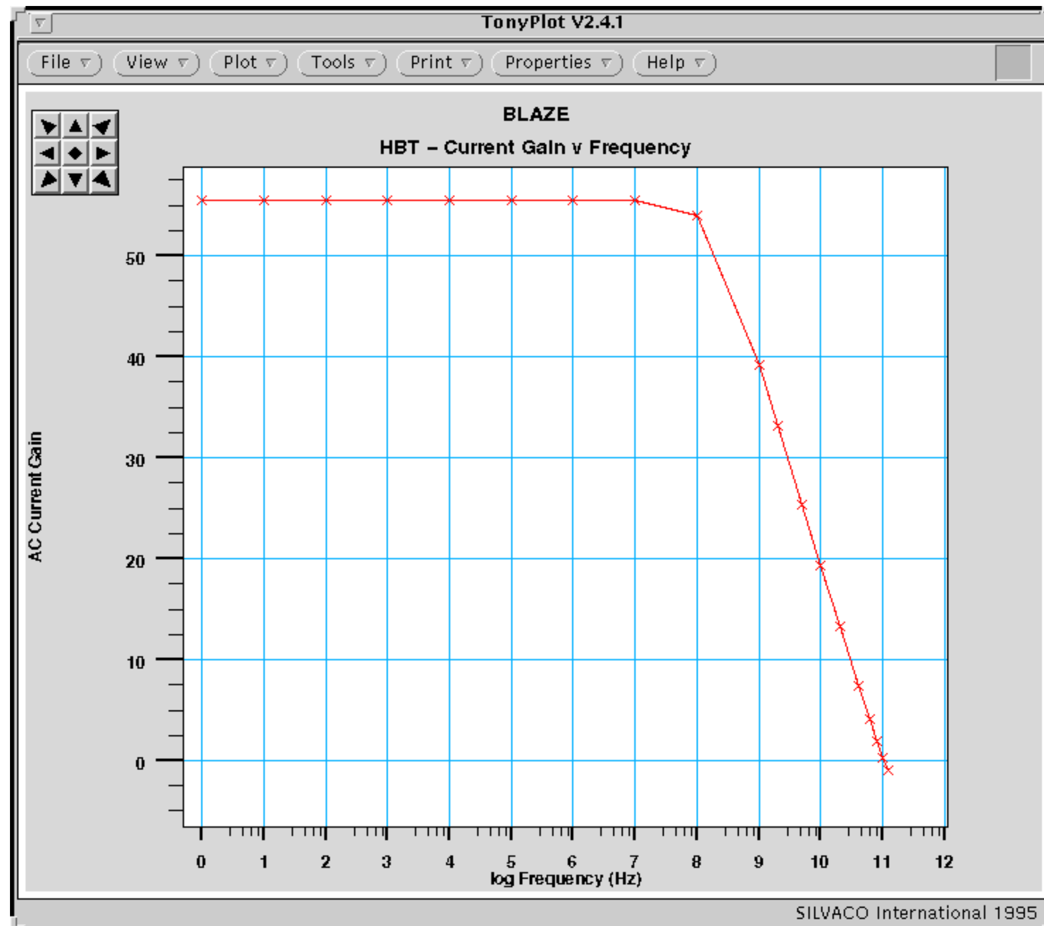
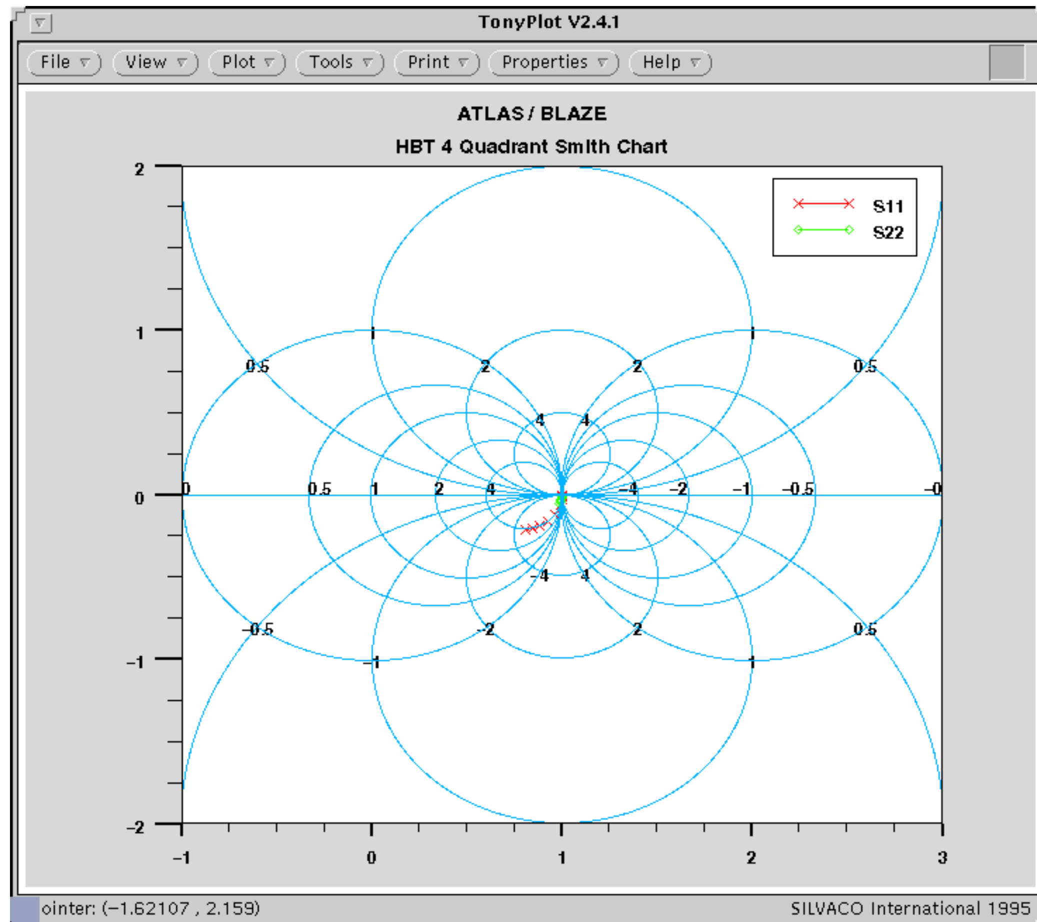
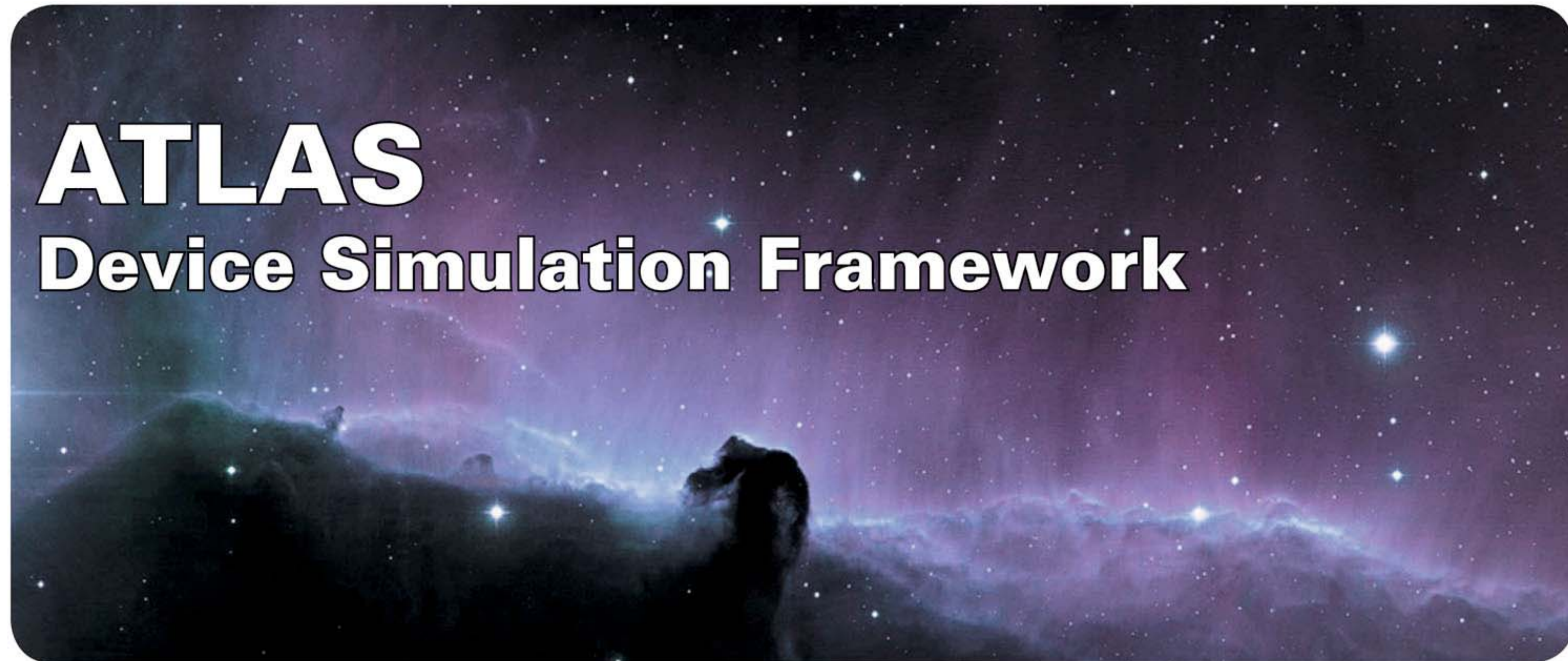
HBT Cut-off Frequency



HBT 4 Quadrant Smith Chart



Case Study – PHEMT



Case Study – PHEMT

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Case Study - PHEMT

- Definition of the Problem
  - InGaAs material parameters
  - Accurate simulation of gate leakage
  - Accurate simulation of transconductance
  - Effects of temperature on the device performance

Case Study - PHEMT

- Device Definition
  - Mesh
  - Regions (Note - Composition Fraction)
  - Electrodes
  - Doping

Case Study - PHEMT

- Material Parameter Specification
  - Band alignment offset
  - Baseline mobilities
  - Saturation velocities
  - Effective Richardson Constant
  - Minority carrier lifetimes

Case Study - PHEMT

- Contact Definition
  - Work Function
  - Lumped resistance
  - Slave contacts
  - Images force lowering
  - Thermal contacts

Case Study - PHEMT

- Models Definition
  - Print statement
  - Temperature
  - Recombination models
  - Mobility models
  - Energy balance models

Case Study - PHEMT

- Non-isothermal Models
- User defined models (C-interpreter)
- Mobility statement
- Impact ionization

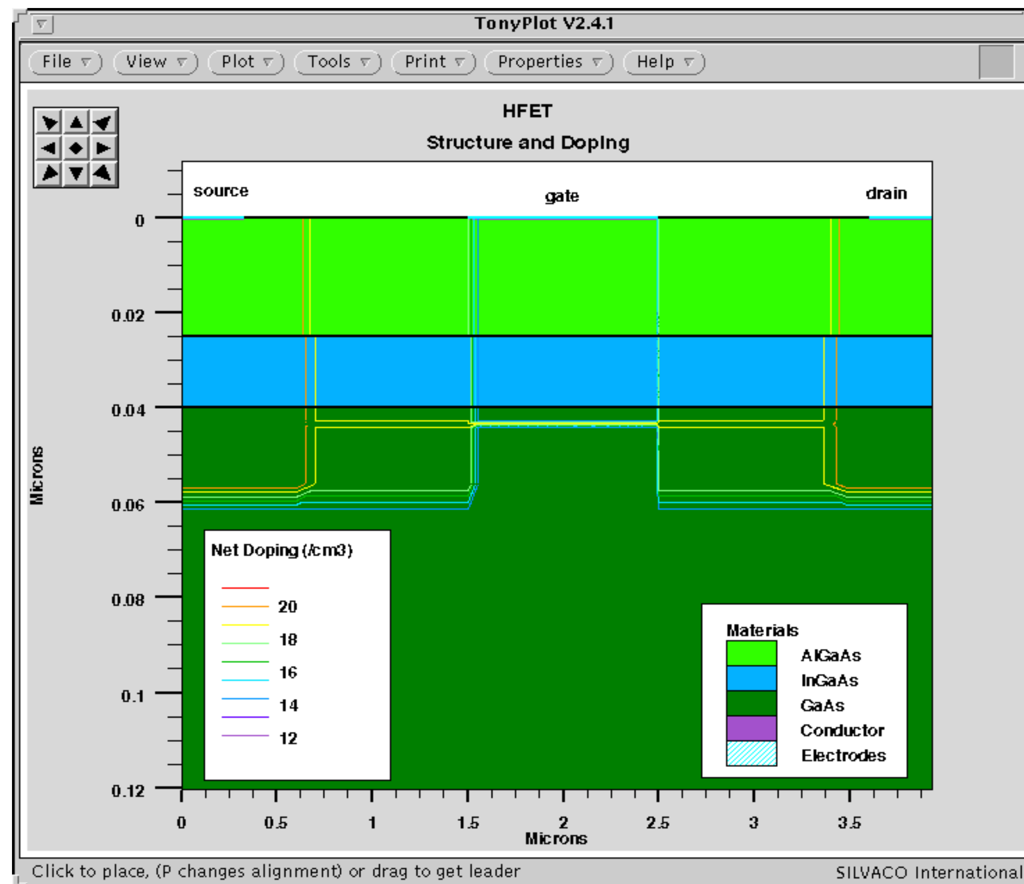
Case Study - PHEMT

- Solution Techniques
  - Method
  - Output
  - Solve
  - Log and Save
  - Extract

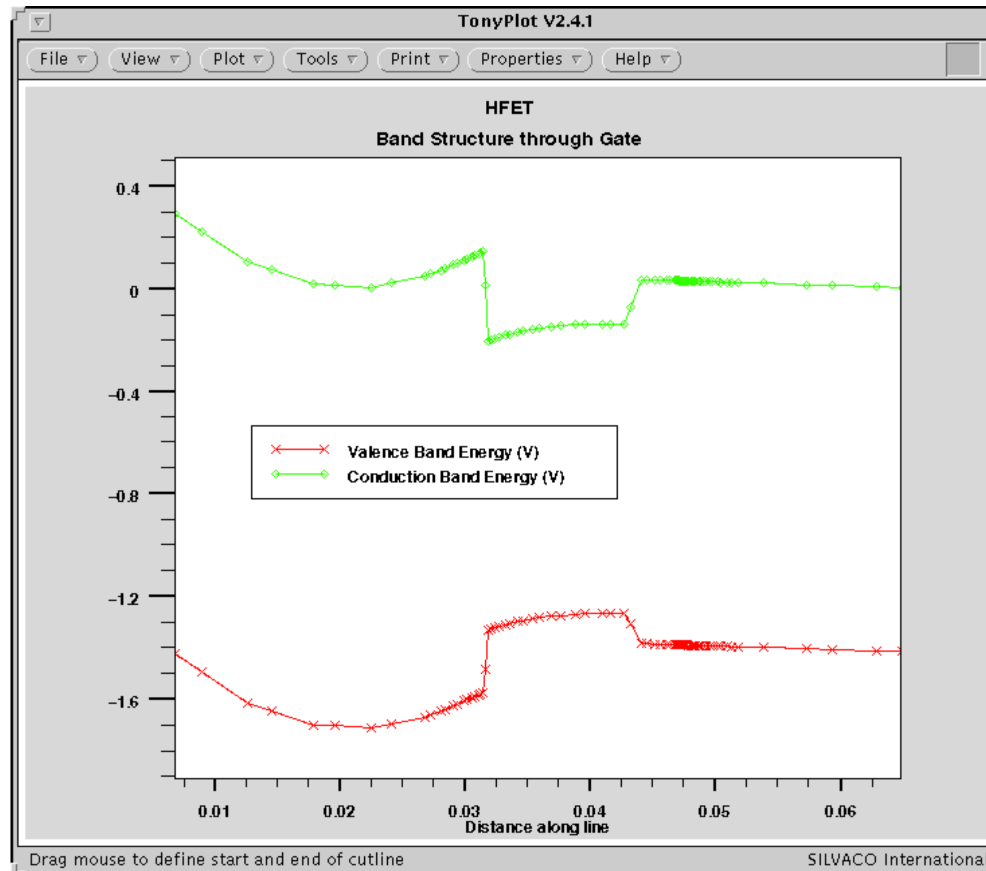
Case Study - PHEMT

- Summary of Input Deck Features
  - Other Options
    - DevEdit
    - Flash
  - Solution Times
  - Use of Tools (DeckBuild, TonyPlot)

Structure and Doping Profile



Band Structure Through Gate



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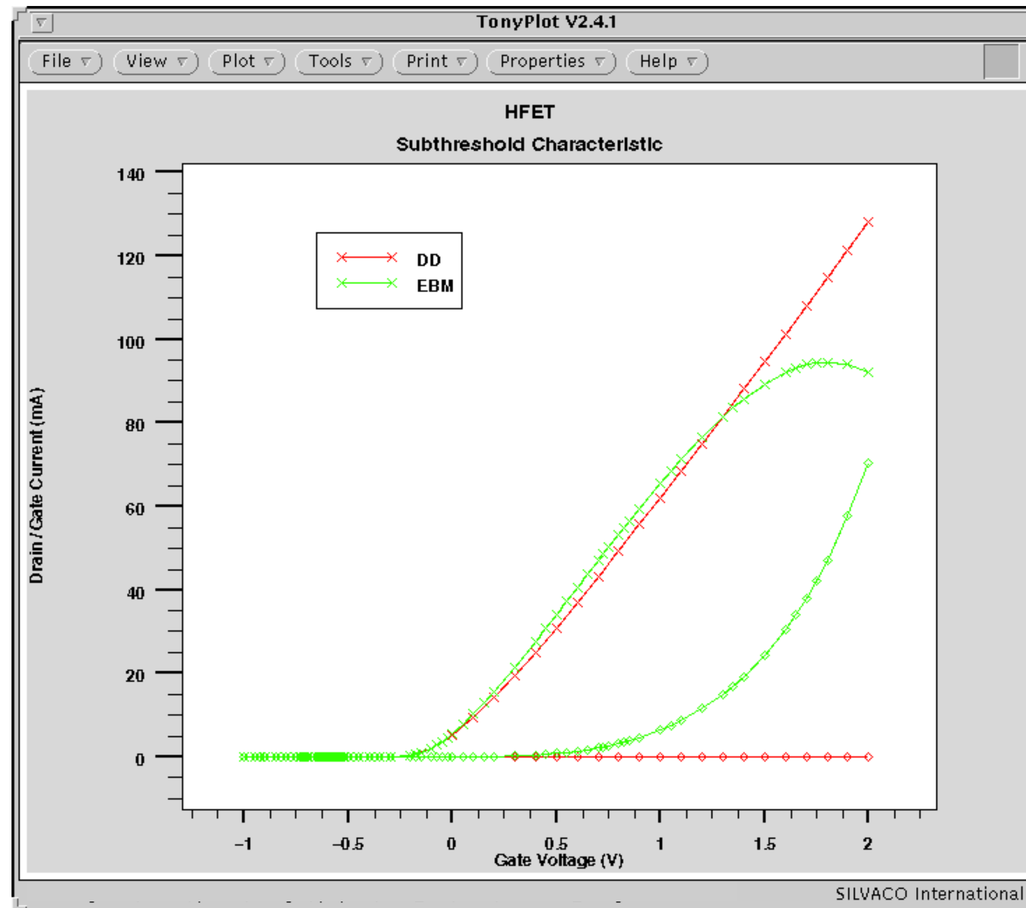
Case Study - PHEMT

- DC Characteristics
  - Id/Vg
  - Id/Vd
  - Comparison with experiment
- AC Characteristics
- Tuning

Energy Balance Shows Accurate Gate Current



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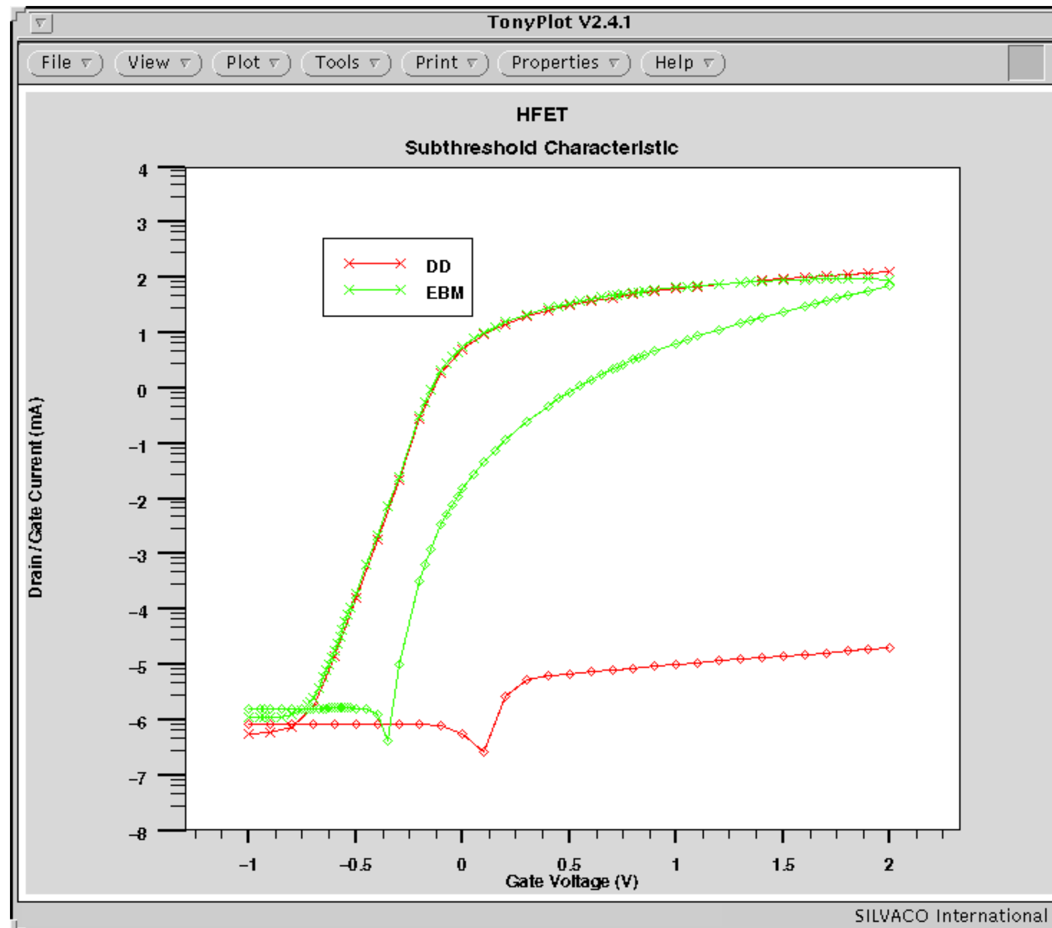
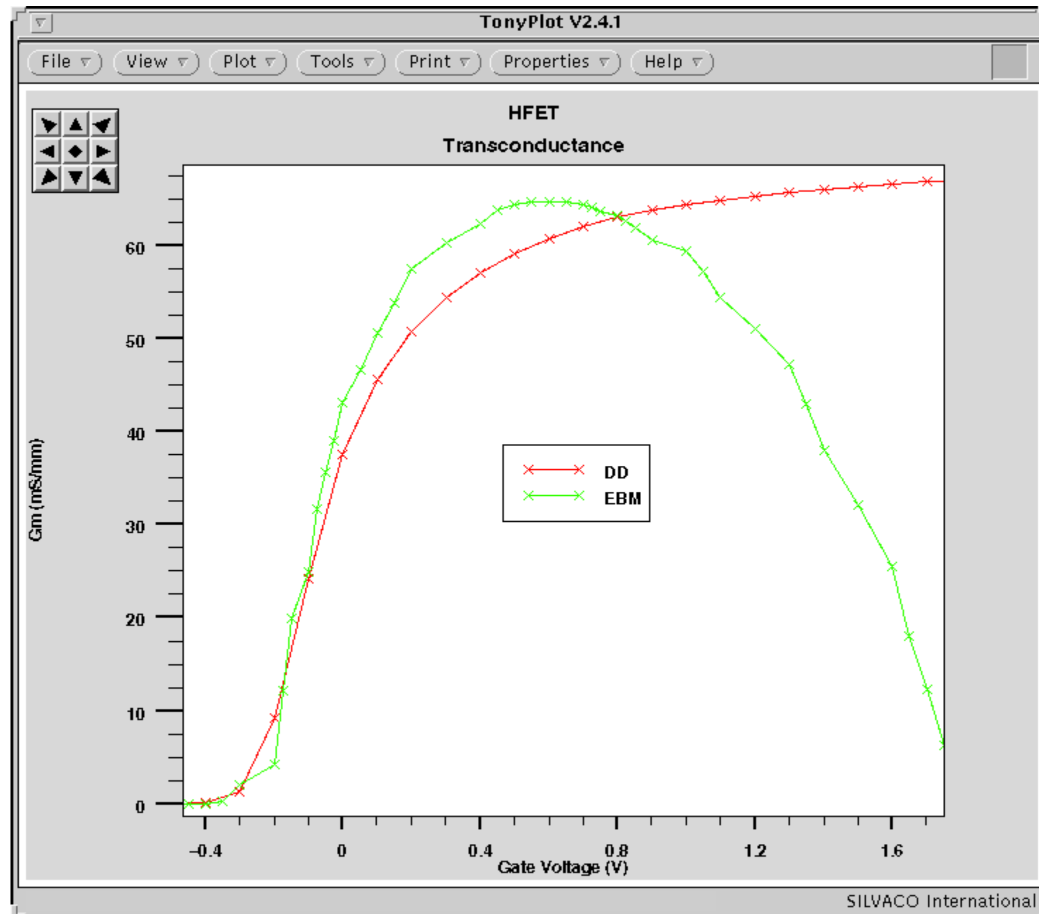
HFET Subthreshold Characteristic



HFET Transconductance



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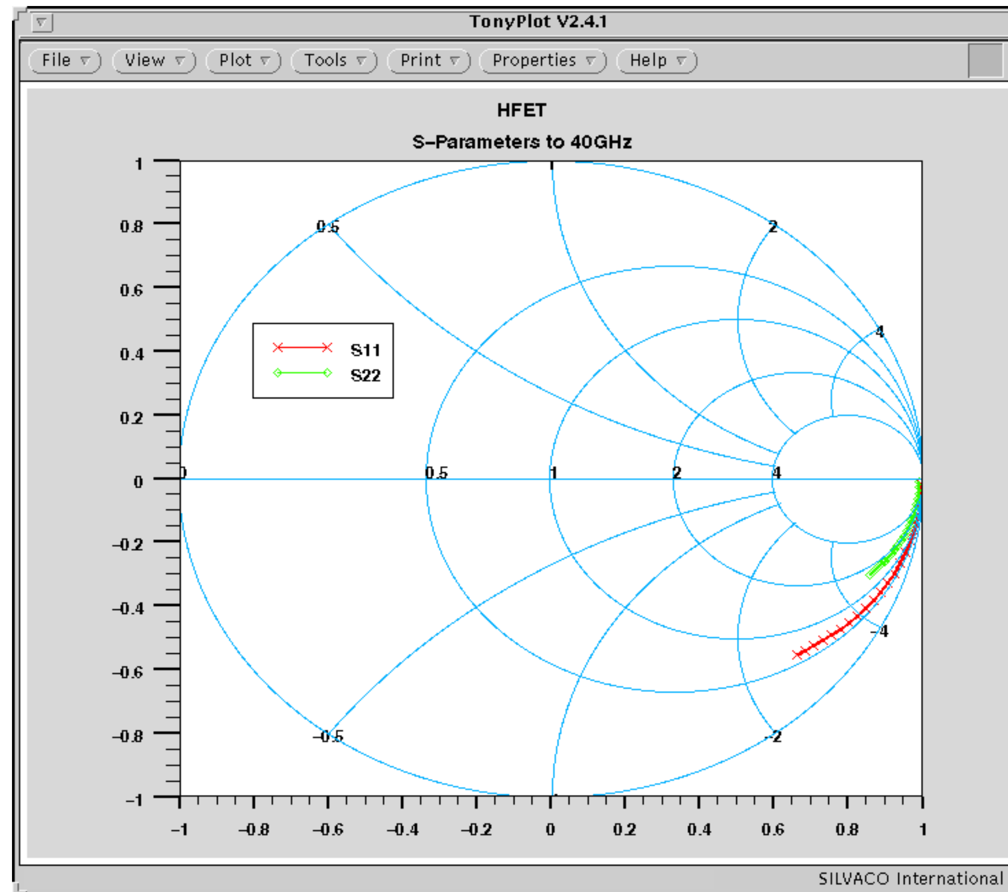
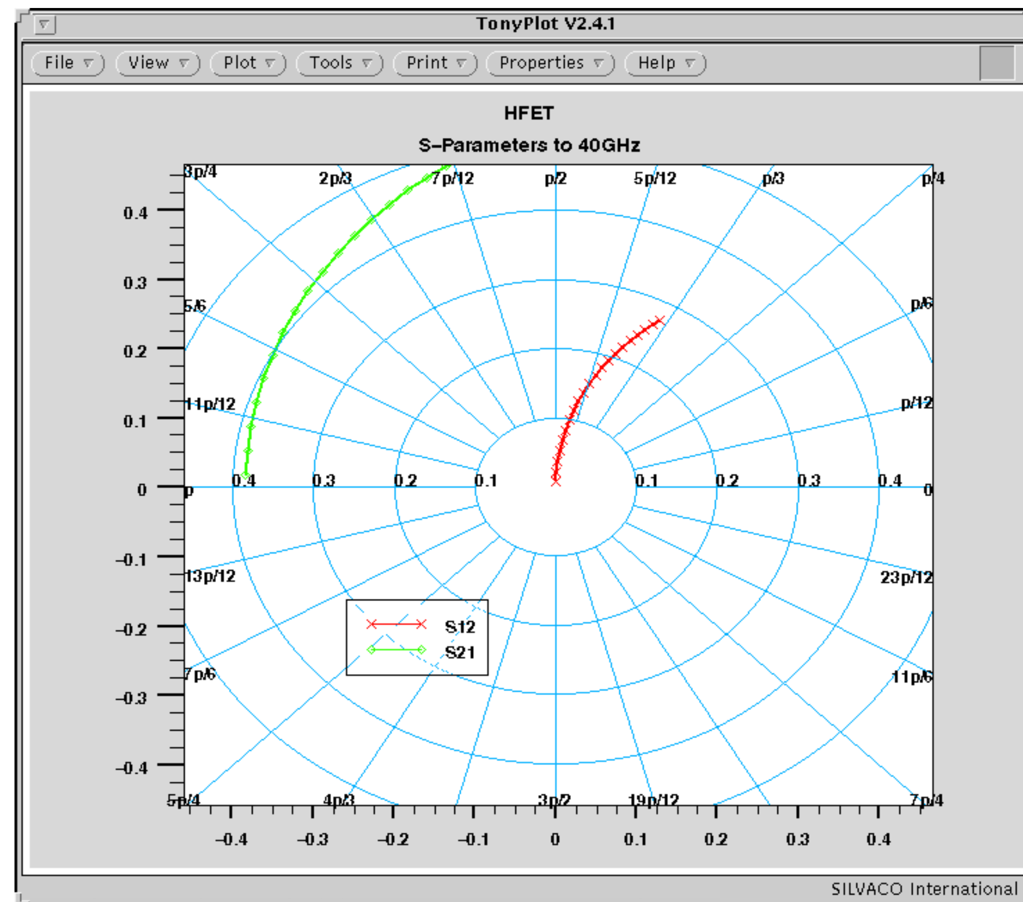
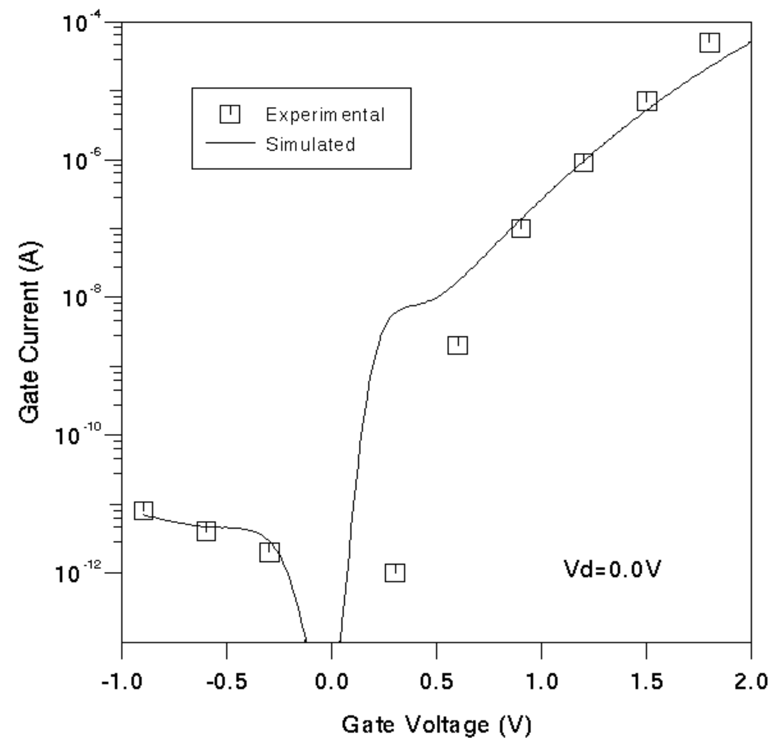
S-Parameter Smith Chart



HFET S-Parameters to 40GHz

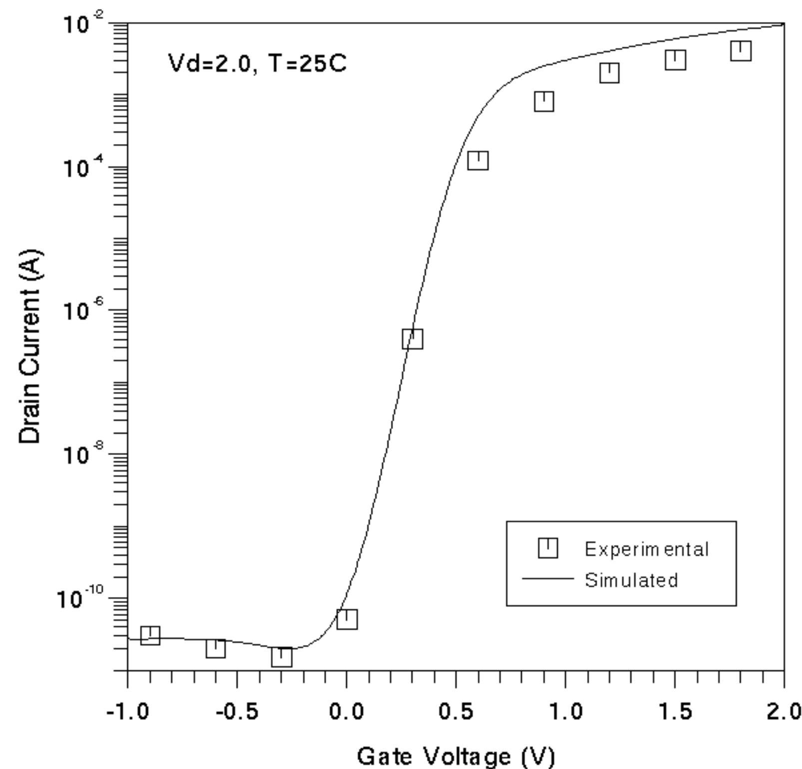


Experimental and Simulated Gate Current of a 0.7 micron HEMT



The experimental and modeled n-channel CHFET subthreshold characteristic at 25°C. The results confirm a strong correlation between the device simulator and experimental results at this temperature. [Dr. C. Wilson, PhD Thesis]

Experimental and Simulated Drain Current of a 0.7 micron HEMT

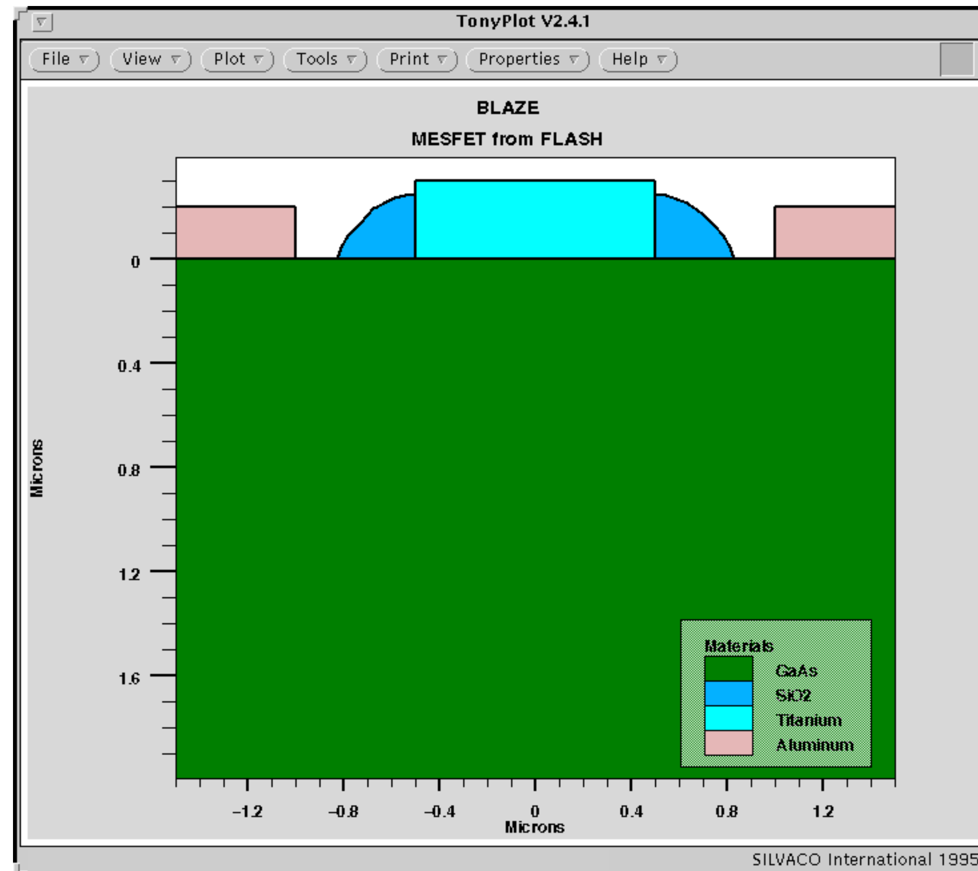


The experimental and modeled n-type CHFET gate characteristic at 25°C. The plots show good agreement over the voltage range, and particularly in the leakage condition, which is important for high temperature performance evaluation. [Dr. C. Wilson, PhD Thesis]

Case Study Examples

- MESFET
  - Structure generated in ATHENA/Flash
  - Implanted channel doping and source/drain contact regions
  - Gate Schottky barrier specification
  - Energy balance vs. drift diffusion
  - AC analysis
  - Transient analysis

MESFET Created in Flash (Process Simulation)



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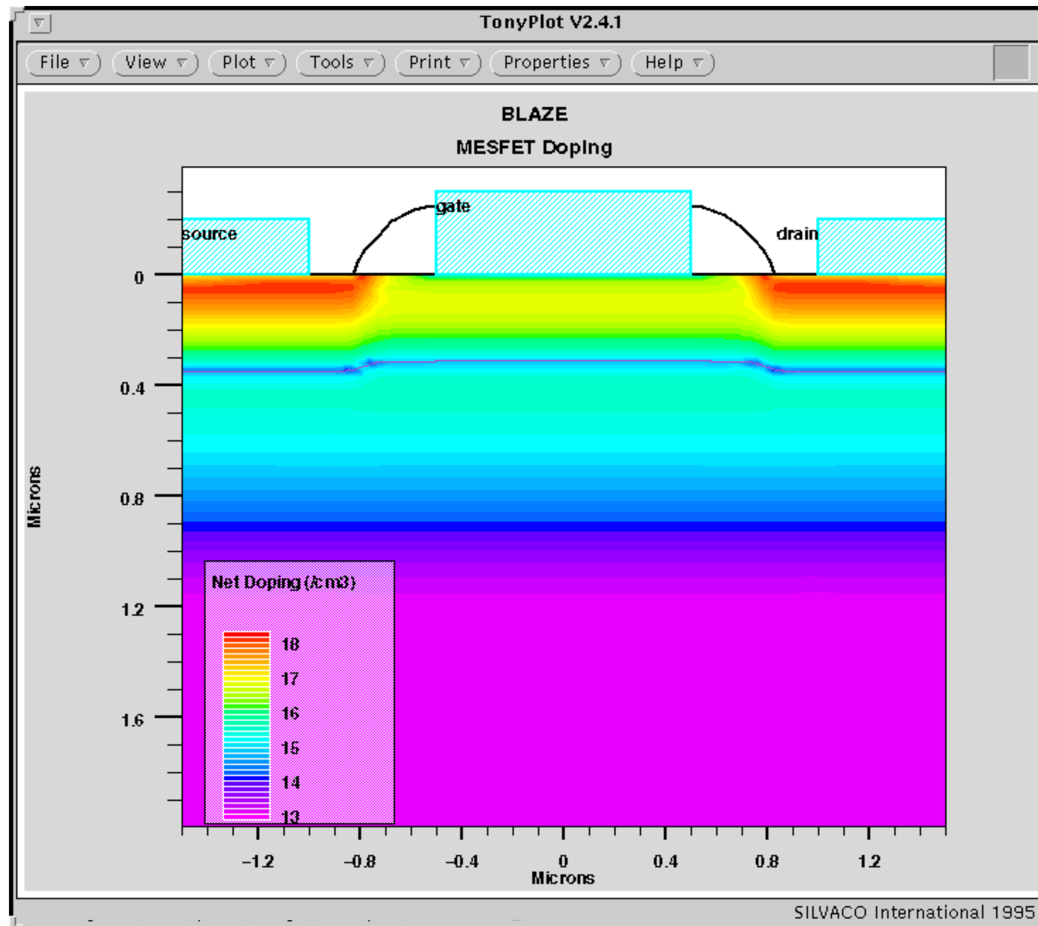
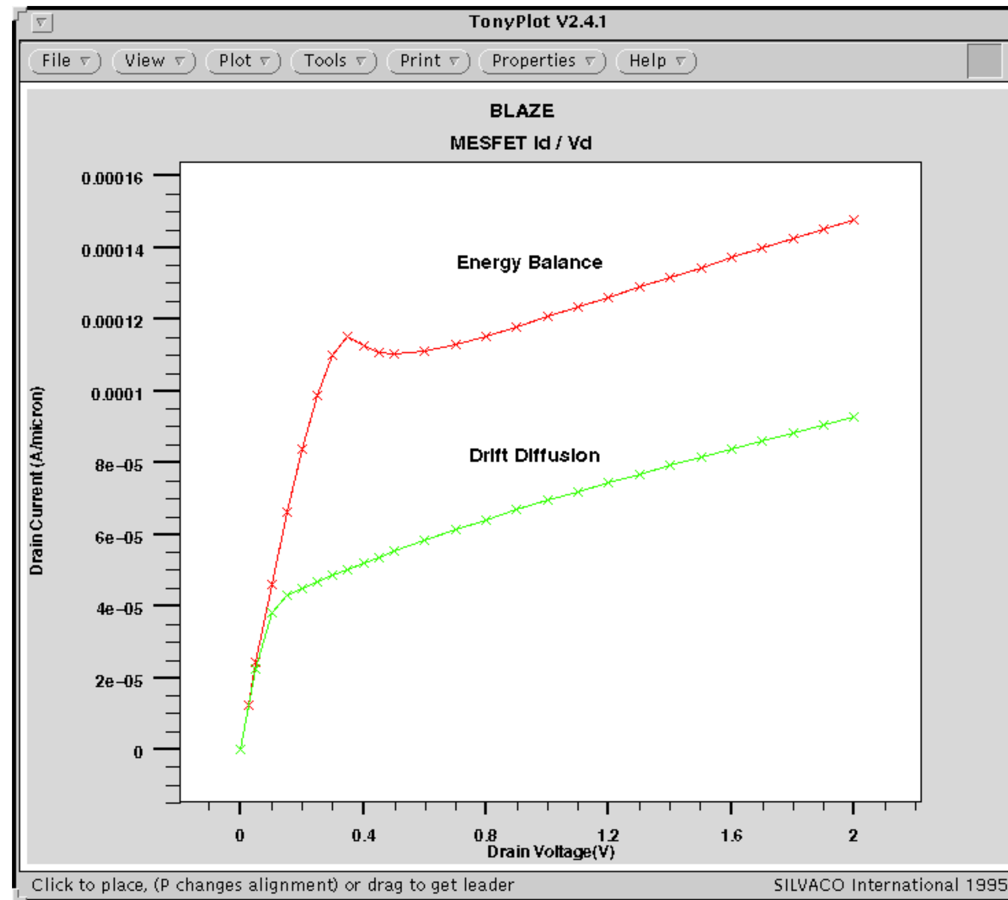
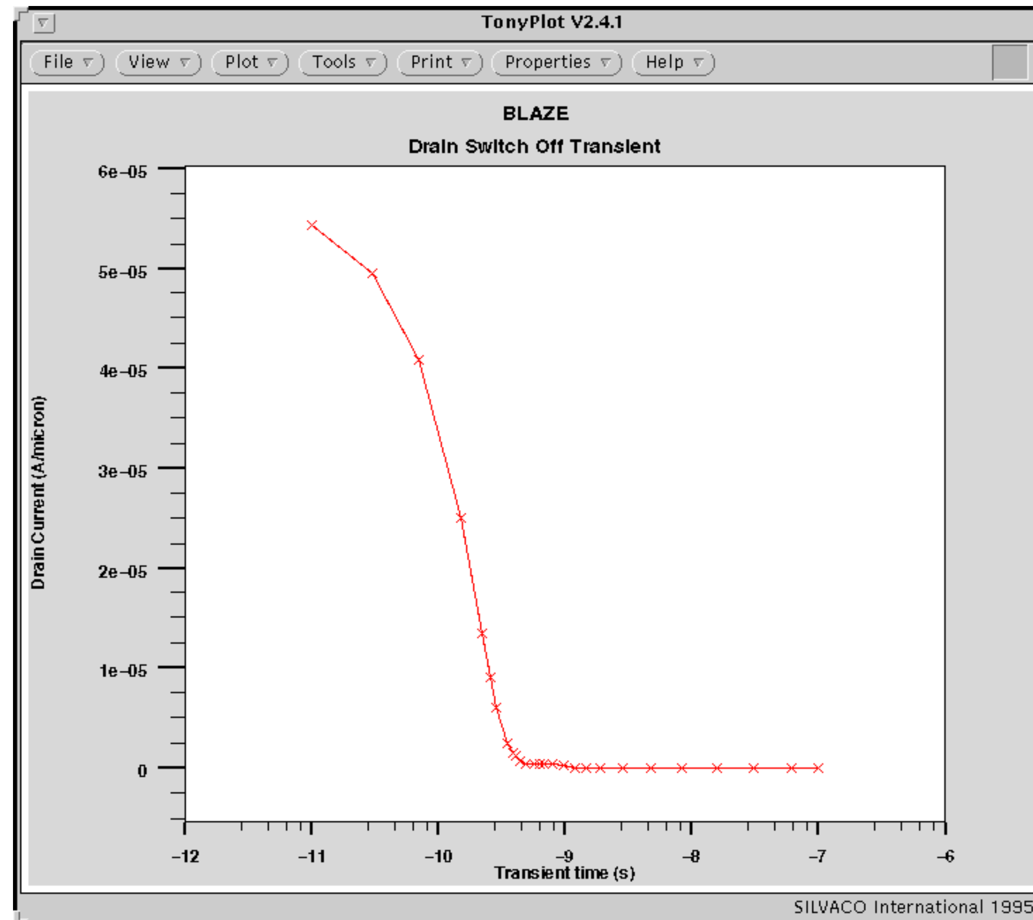
Accurate Doping Profiles Produced by Flash



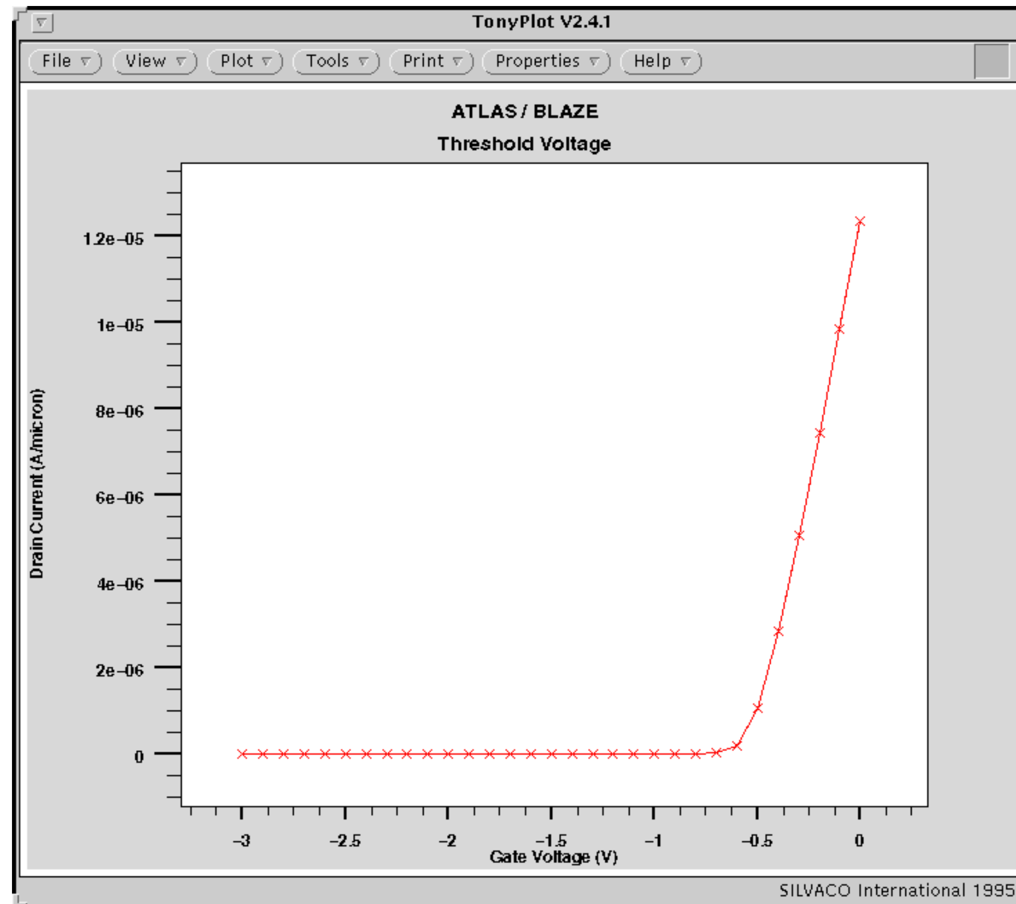
Energy Balance Produces a More Accurate Calculation



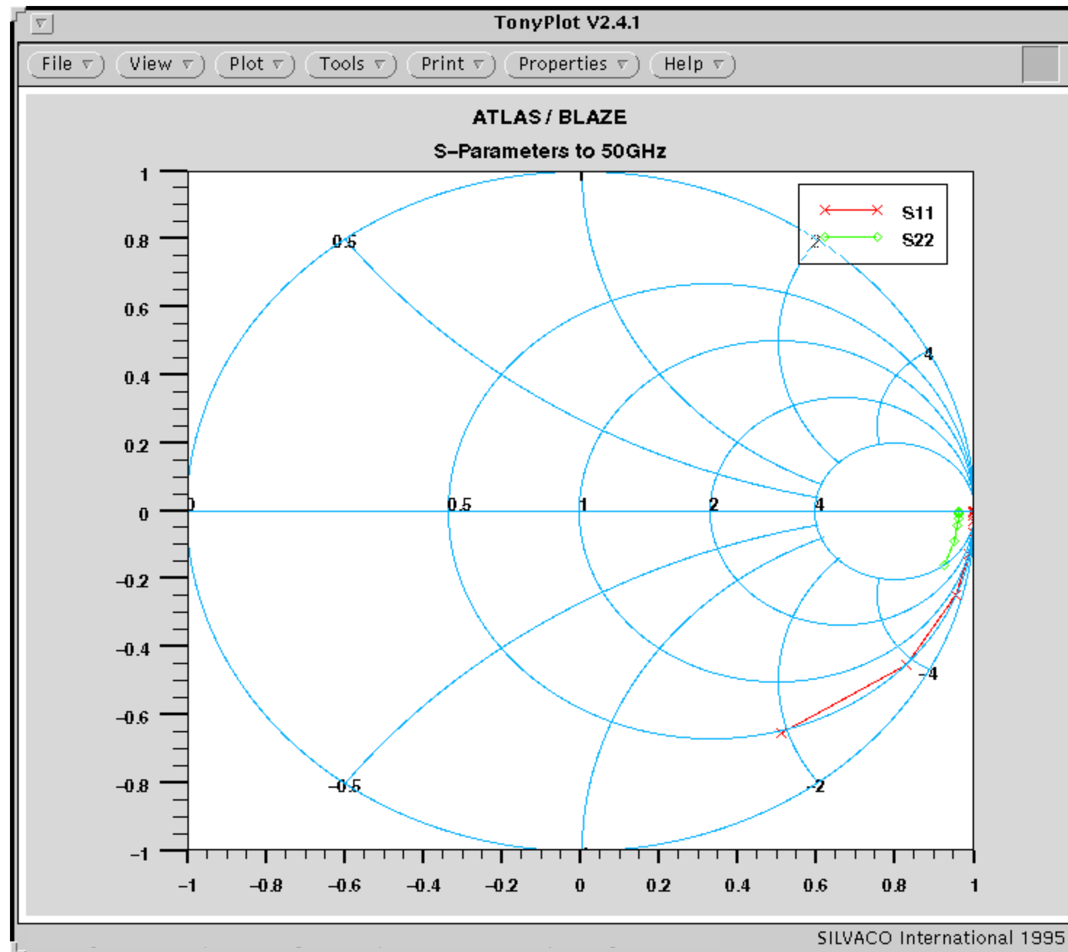
Traps are Important for Accurate Transient Simulation



Threshold Voltage



Smith Chart – S-Parameter to 50 GHz



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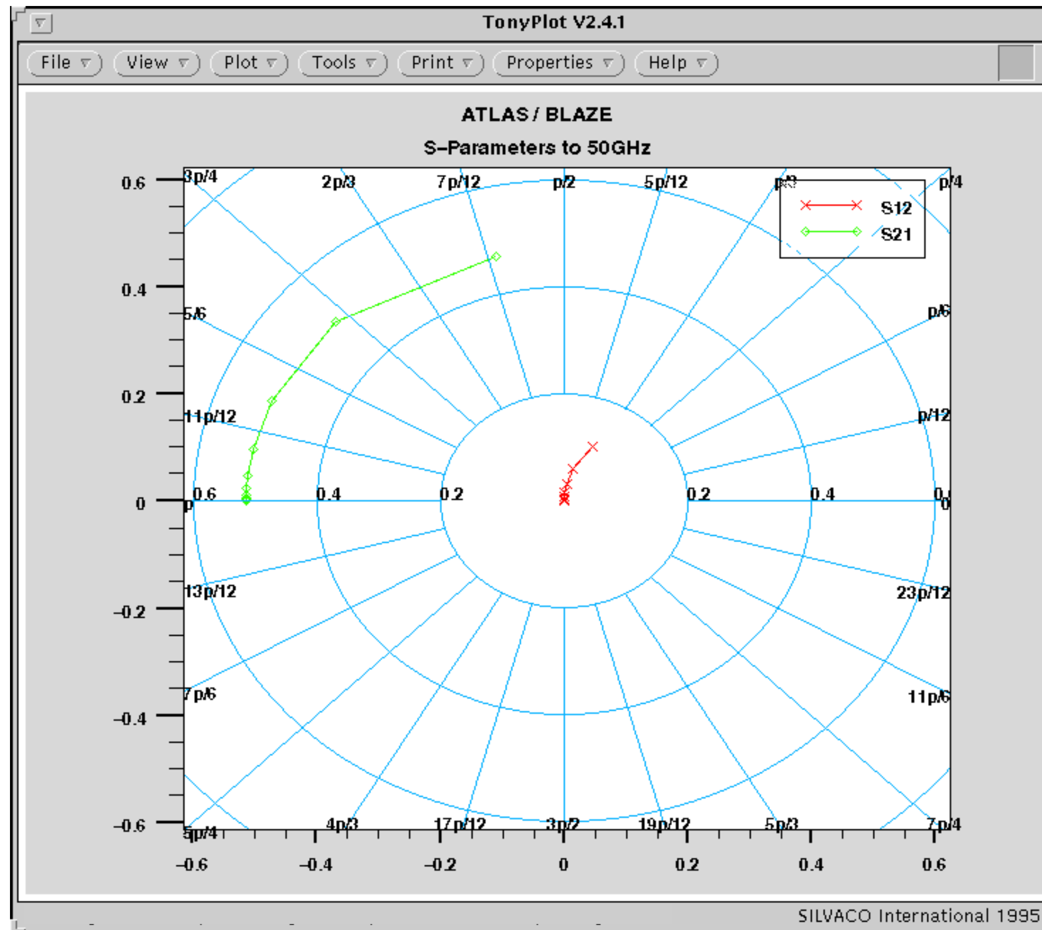
Polar Plot – S-Parameters to 50GHz



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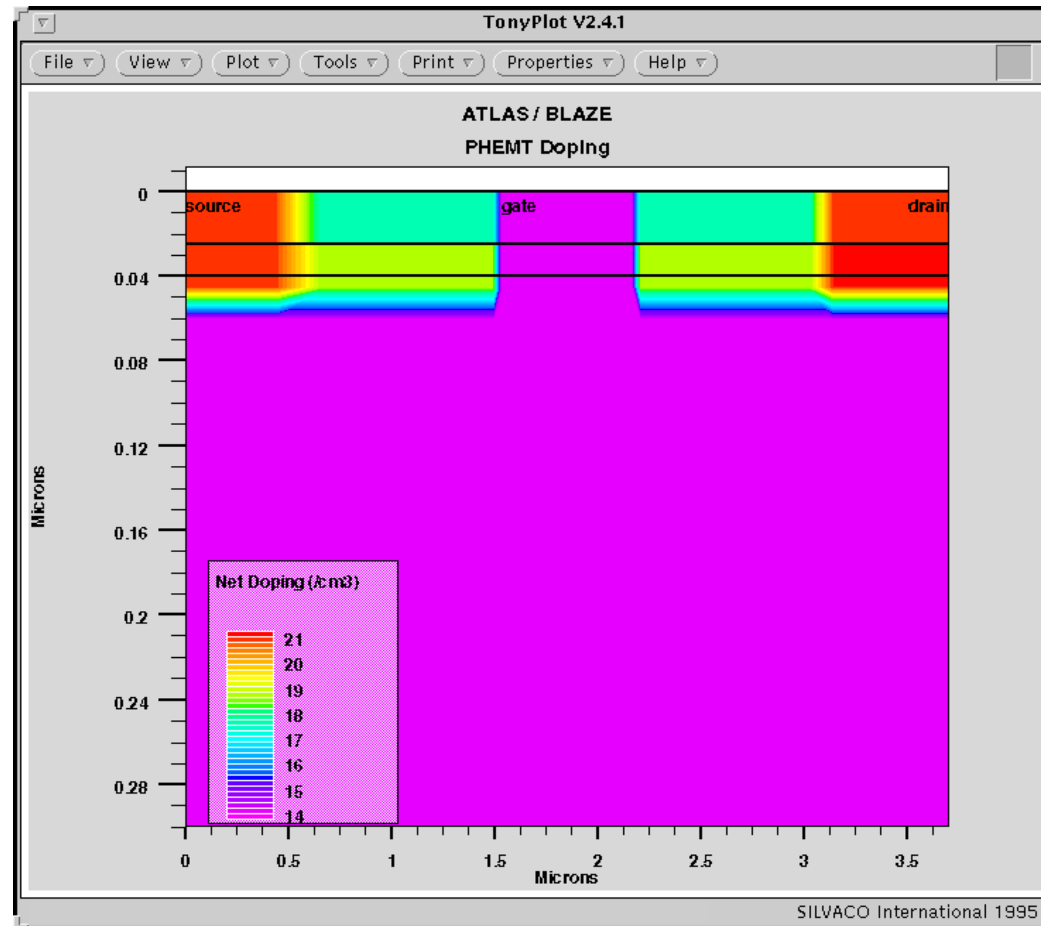
Case Study Examples

- Pseudomorphic HEMT
  - Structure generated by ATLAS internal syntax
  - Ohmic contacts require special attention
  - Band offsets, Schottky barrier height and material parameters
  - Energy balance vs. drift diffusion
  - DC and AC solutions

PHEMT Structure Created with Internal Syntax



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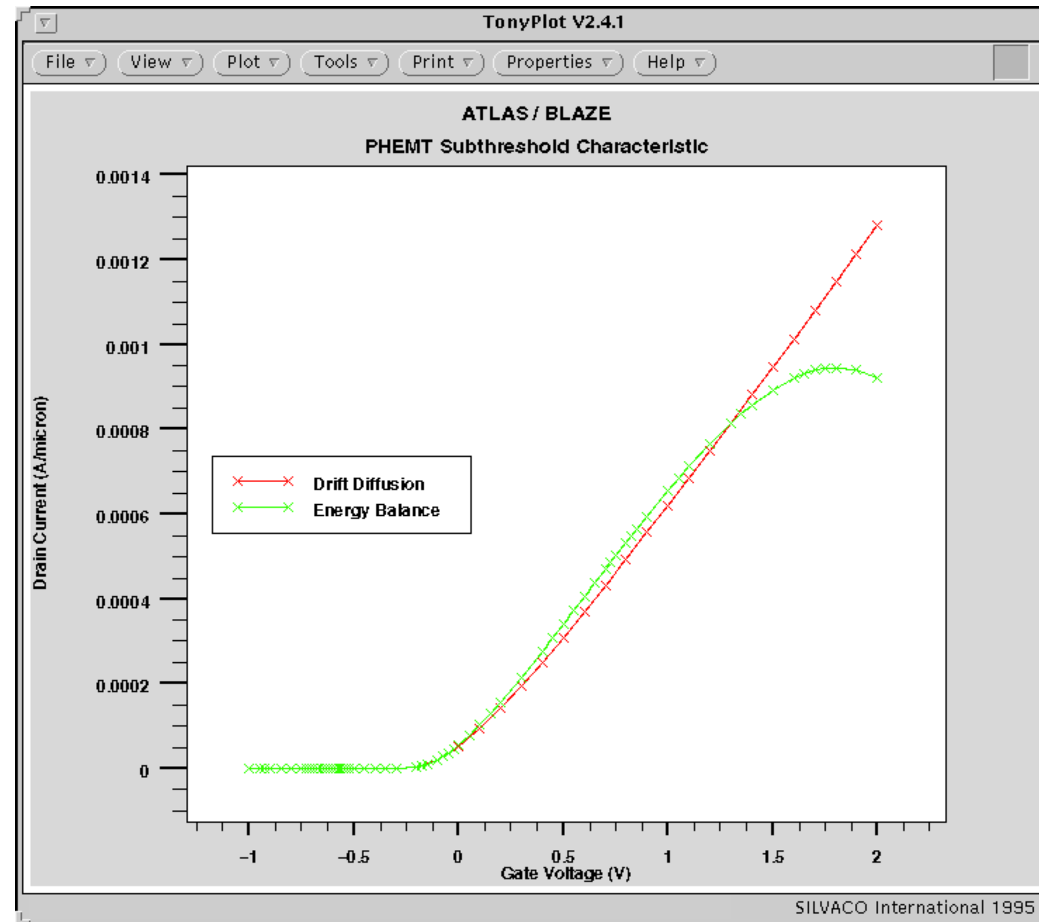
Energy Balance Shows Correct Drain Current Downturn



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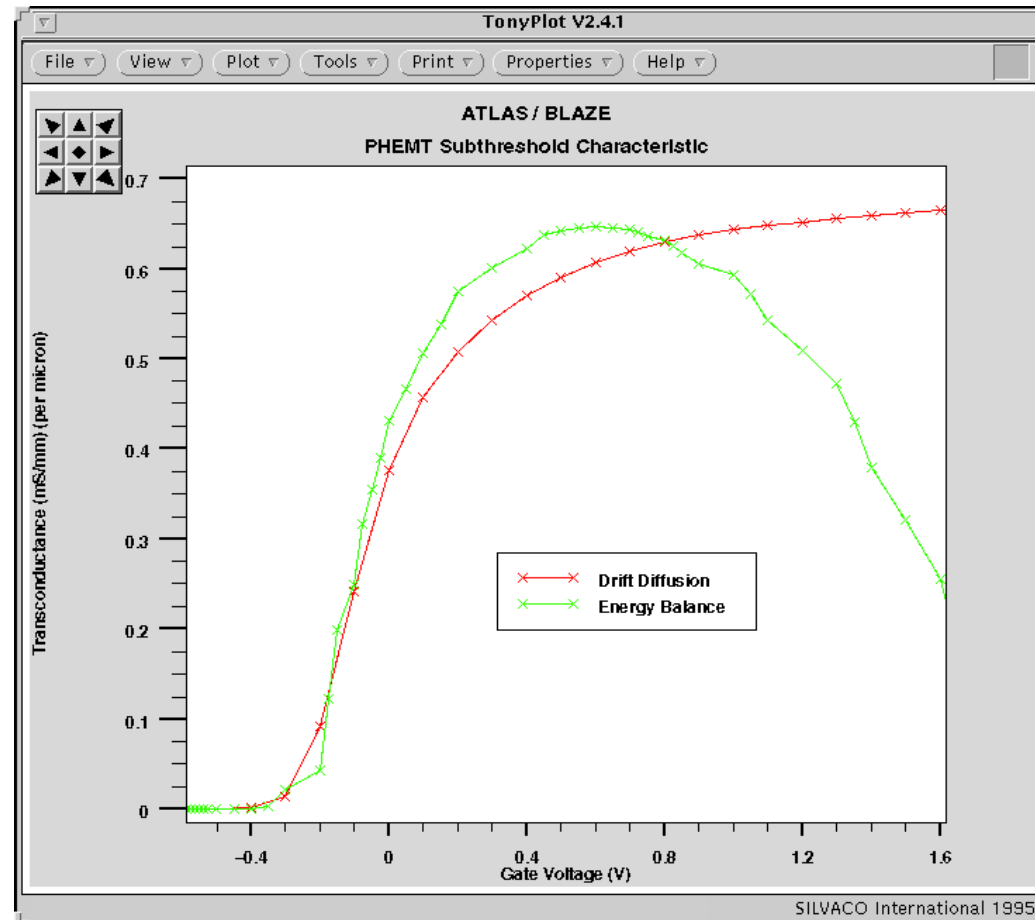
Energy Balance Gives Accurate Transconductance



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Conclusion to III-V Device Study

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2 Lattice Heating
3 Fully Coupled Non-Isothermal Energy Balance Model
4 High Frequency Solutions
5 AC parameter extraction
6 Interface and Bulk Traps
7 Circuit Performance Simulation (MixedMode)
8 Optoelectronic Capability (Luminous)
9 Speed and Convergence
10 C-Interpreter

Blaze is a Fully Integrated part of the Silvaco Tool Set

- Maturity of Silvaco tool suite significantly enhances Blaze
- Blaze is able to take advantage of ATLAS improvements in numerics, core functionality and analysis capabilities from Silicon users
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