ATLAS

ATLAS III-V Advanced Material Device Modeling

ATLAS

Device Simulation Framework

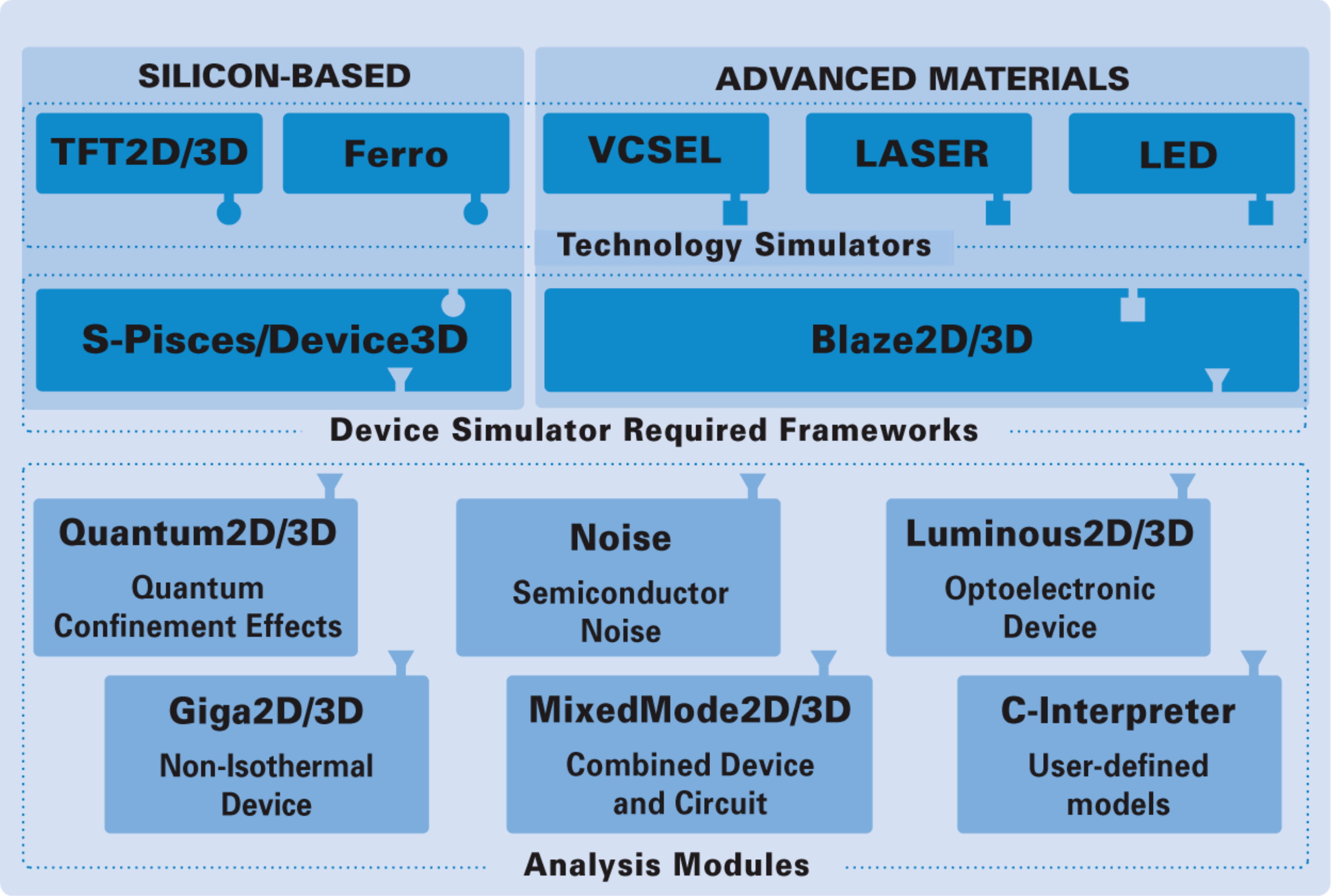
Requirements for III-V Device Simulation

SILVACO

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 the Virtual Wafer Fab

Blaze as Part of the ATLAS Framework



SILICON-BASED

ADVANCED MATERIALS

TFT2D/3D

Ferro

VCSEL

LASER

LED

Technology Simulators

S-Pisces/Device3D

Blaze2D/3D

Device Simulator Required Frameworks

Quantum2D/3D
Quantum Confinement Effects

Noise
Semiconductor Noise

Luminous2D/3D
Optoelectronic Device

Giga2D/3D
Non-Isothermal Device

MixedMode2D/3D
Combined Device and Circuit

C-Interpreter
User-defined models

Analysis Modules

SILVACO

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 Quantum Mechanical Simulation

- Schrodinger solver
- quantum correction models
- Bohm Quantum Potential

5 High Frequency Solutions

- Direct AC solver for arbitrarily high frequencies
- AC parameter extraction
- extraction of s-, z-, y-, and h-parameters
- Smith chart and polar plot output
- FFT for large signal transients

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
- verification of newly developed compact models

8 Optoelectronic Capability (Luminous/Laser)

- ray tracing algorithms
- DC, AC, transient and spectral response for detectors
- Helmholtz solver for edge emitting laser diodes and VCSELs
- LED simulation

9 Speed and Convergence

- flexible and automatic choice of numerical methods

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

10 C-Interpreter for interactive model development

- user defined band parameter equations
- large selection of user defined models
- mole fraction dependent material parameters
- ideal for proprietary model development

Simulation of III-V Device with Blaze

SILVACO

Blaze Applications

- Devices:
    - HEMTs
    - HBTs
    - MESFETs
    - etc
- DC Characterization
- Transient Analysis
- Breakdown Calculations
- AC Analysis
- S-Parameter Calculation

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 ternary compounds
- Some parameters (e.g. 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 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

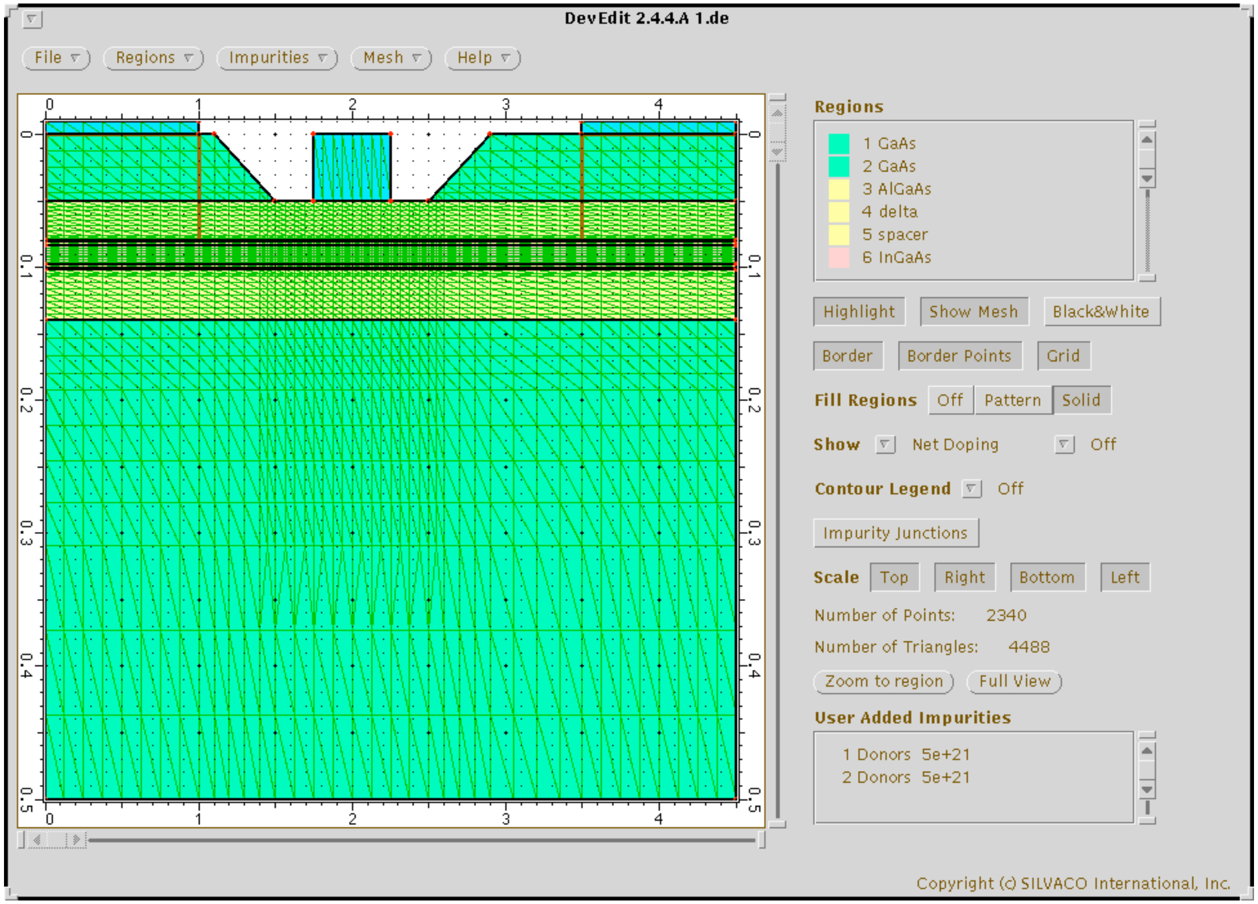
Blaze Simulation Overview

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

Structure Creation

- Three methods exist to create III-V device structures
  - Process simulation (Flash)
  - Internal ATLAS syntax
    - limited to rectangular structures
  - Standalone device editor (DevEdit)
    - GUI to define structure, doping and mesh
    - batch mode for experimentation
    - abrupt and graded mole fraction definition
    - non-rectangular regions supported

Structure Creation Using DevEdit



Regions

- 🟩 1 GaAs
- 🟩 2 GaAs
- 🟨 3 AlGaAs
- 🟨 4 delta
- 🟨 5 spacer
- 🟥 6 InGaAs

Fill Regions Off Pattern [✓ Solid]

Show Net Doping Off

Contour Legend Off

Number of Points: 2340

Number of Triangles: 4488

User Added Impurities

1 Donors 5e+21
2 Donors 5e+21

SILVACO

Material Specification for Typical Devices

- 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

- 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

Model Specification (cont.)

- 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 (cont.)

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

Model Specification (cont.)

- Mobility
  - Low Field Mobility:

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

  - Field Dependent Mobility:

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

Model Specification (cont.)

- Differential Field Dependent Mobility

$$\mu_n(E) = \frac{\mu_{no} + \dfrac{v_{satn}}{E}\left(\dfrac{E}{E_0}\right)^{\gamma}}{1 + \left(\dfrac{E}{E_0}\right)^{\gamma}}$$

Models Specification (cont.)

- Advanced Models
  - Thermionic emission model
    - This can be used to describe transport through abrupt heterojunctions instead of the classical drift-diffusion model
    - 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
  - Traps
    - Bulk and Interface traps may be defined in the materials
    - Additional rate equation solved for each trap

Model Specification (cont.)

- Energy Balance / Simplified Hydrodynamic
  - Higher order approximation than Boltzmann Transport
  - Two extra equations representing electron and hole “temperatures”
  - Key parameter - Energy relaxation time
  - Adds two coupled equations to the drift diffusion equation set:

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

$$\nabla \vec{S}_p = -\vec{J}_p \nabla \psi - W_p - \frac{3k}{2}\frac{\partial(\lambda_p^* p T_p^*)}{\partial t}$$

Model Specification (cont.)

- Lattice Heating
  - No longer assume lattice temperature is constant
  - Establish thermal boundary conditions
  - H includes generation/recombination, Thomson and Peltier
  - Adds an extra coupled equation to the drift diffusion equation set:

$$C\frac{\partial T_L}{\partial t} = \nabla\left(\kappa\nabla T_L\right) + H$$

Model Specification (cont.)

- Quantum Mechanics
  - Solution of the Schrodinger equation
  - Quantum correction model provides self-consistent solution
  - Bohm Quantum Potential

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

Solution Techniques (cont.)

- S-Parameter Calculation
  - ATLAS/Blaze calculates capacitance/conductance
  - Y-Parameter conversion
  - S-Parameter conversion

$$Y_{11} = -\left[g_{11} \times Z_0 \times W, (\varpi \times C_{11} \times Z_0 \times W)i\right]$$

$$S_{11} = \frac{(1 - Y_{11})(1 + Y_{22}) + Y_{12}Y_{21}}{(1 + Y_{11})(1 + Y_{22}) - Y_{12}Y_{21}}$$

$$S_{12} = \frac{-2Y_{12}}{(1 + Y_{11})\ 1 + Y_{22}\ - Y_{12}Y_{21}}$$

Solution Techniques (cont.)

- Fast Fourier Transform
  - Log file data generated by Blaze can be transformed from the time domain to the frequency domain by using the FFT statement
  - The frequency domain data can be displayed using TonyPlot
- Circuit Simulation
  - Using the MixedMode module, up to 10 ATLAS devices can be embedded in a circuit simulation

Conclusions: Blaze

- Blaze meets all requirements for III-V compound device simulator
- Offers flexible range of materials, models and solutions techniques
- C-Interpreter can be used to specify custom models
- 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 the Virtual Wafer Fab

Simulation of III-V Device with Blaze and SiC

Simulation of III-V Device with Blaze and SiC

SILVACO

SiC as Part of the ATLAS Framework

- Simulation of Silicon Carbide devices using anisotropic mobility models is implemented as part of the ATLAS device simulation framework
  - ATLAS provides framework integration
  - Blaze provides III-V device simulation
  - SiC provides anisotropic mobility models

Overview of SiC

- SiC works within the framework of ATLAS and Blaze. ATLAS provides the framework integration. Blaze provide electrical simulation of heterostructure devices and material models for common III-V semiconductors
- Hall mobilities in Silicon Carbide are different depending on the crystalline axis where conduction takes place
- This “anisotropic” mobility could dramatically affect device simulation results, particularly in power devices where current flow may be fully two-dimensional

Features of SiC

- Automatically accounts for the change in mobility as the current vector moves through 360 degrees
- User just specifies the mobility parameters in the two crystallographic planes
- Works with all of the existing mobility models in ATLAS and Blaze

Syntax

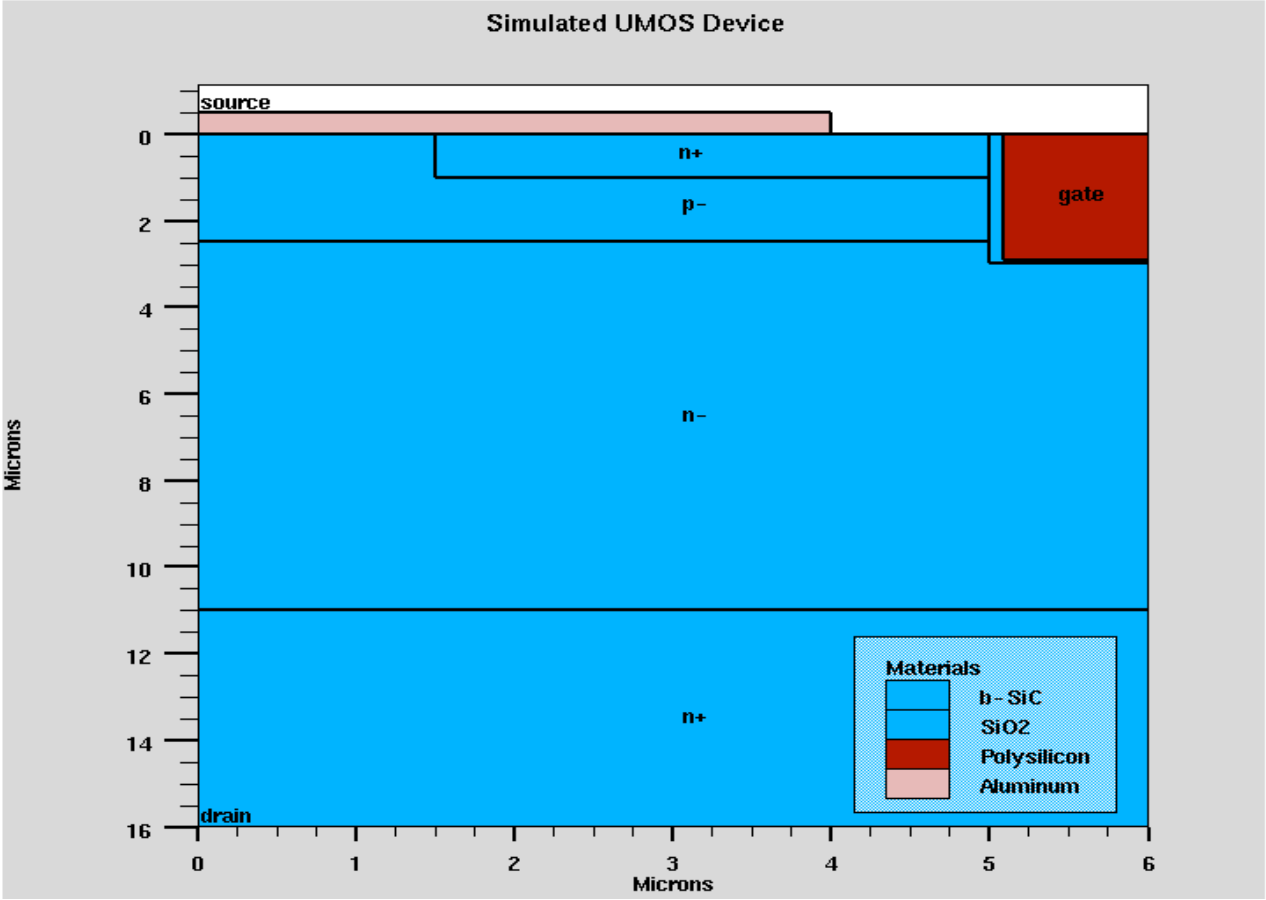
- Anisotropic mobility model syntax
  - First define mobility in plane <1100>

```
MOBILITY MATERIAL=b-SiC VSATN=2e7 VSATP=2e7 BETAN=2 \
    BETAP=2 MU1N.CAUG=10  MU2N.CAUG=410 \
    NCRITN.CAUG=13e17 DELTAN.CAUG=0.6 \
    GAMMAN.CAUG=0 ALPHAN.CAUG=-3 BETAN.CAUG=-3 \
    MU1P.CAUG=20 MU2P.CAUG=95 NCRITP.CAUG=1E19 \
    DELTAP.CAUG=0.5 GAMMAP.CAUG=0 \
    ALPHA[.CAUG=-3 BETAP.CAUG=-3
```

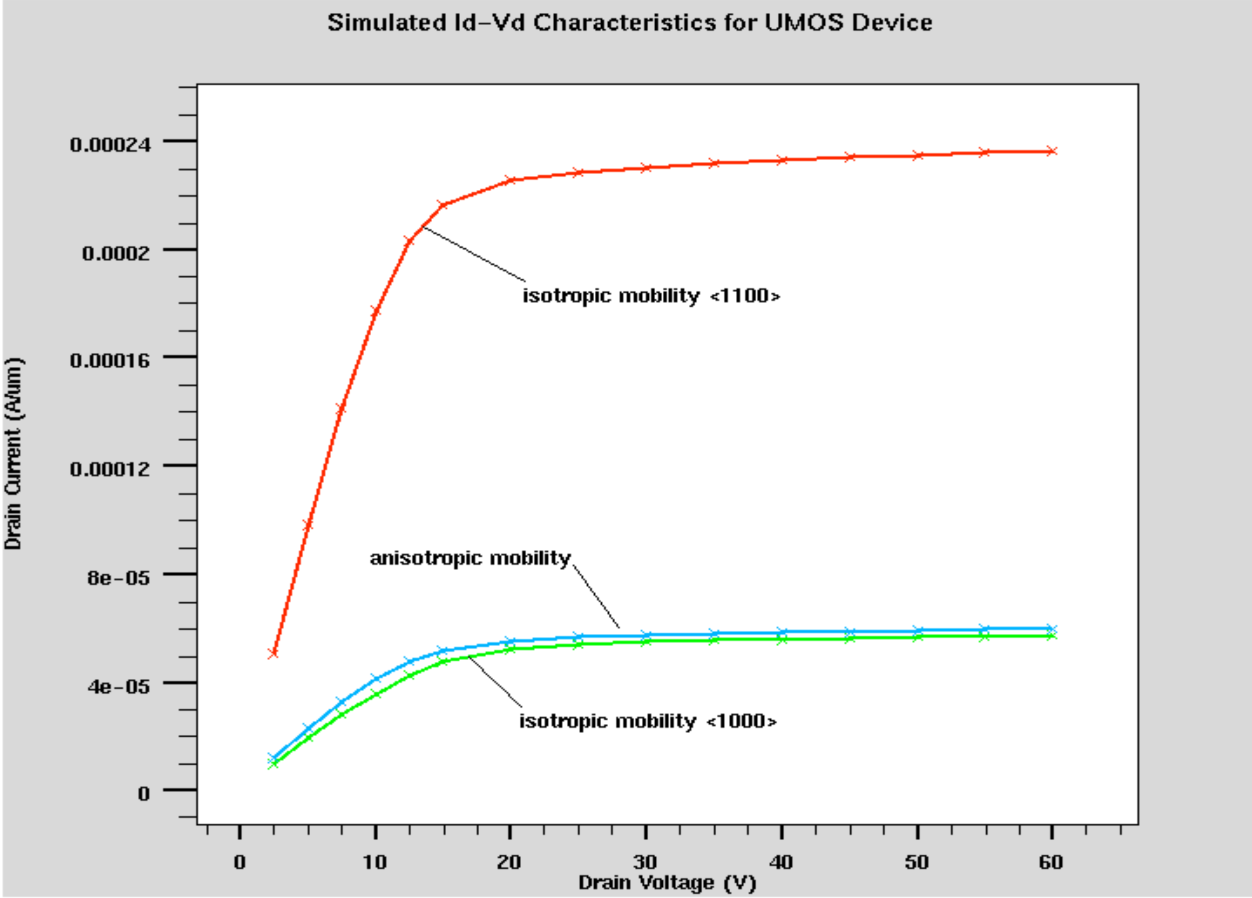
  - Now define mobility in plane <1000>

```
MOBILITY MATERIAL=b-SiC N.ANGLE=90.0 VSATN=2E7 \
        VSATP=2e7 BETAN=2 BETAP=2 MU1N.CAUG=5 \
                MU2N.CAUG=80 NCRITN.CAUG=13e17 \
                        DELTAN.CAUG=0.6 GAMMAN.CAUG=0
    \                   ALPHAN.CAUG=-3 BETAN.CAUG=-3
    MU1P.CAUG=2.5 \     MU2P.CAUG=20 NCRITP.CAUG=1e19
    DELTAP.CAUG=0.5 \   GAMMAP.CAUG=0.0 ALPHAP.CAUG=-3
    BETAP.CAUG=-3
```

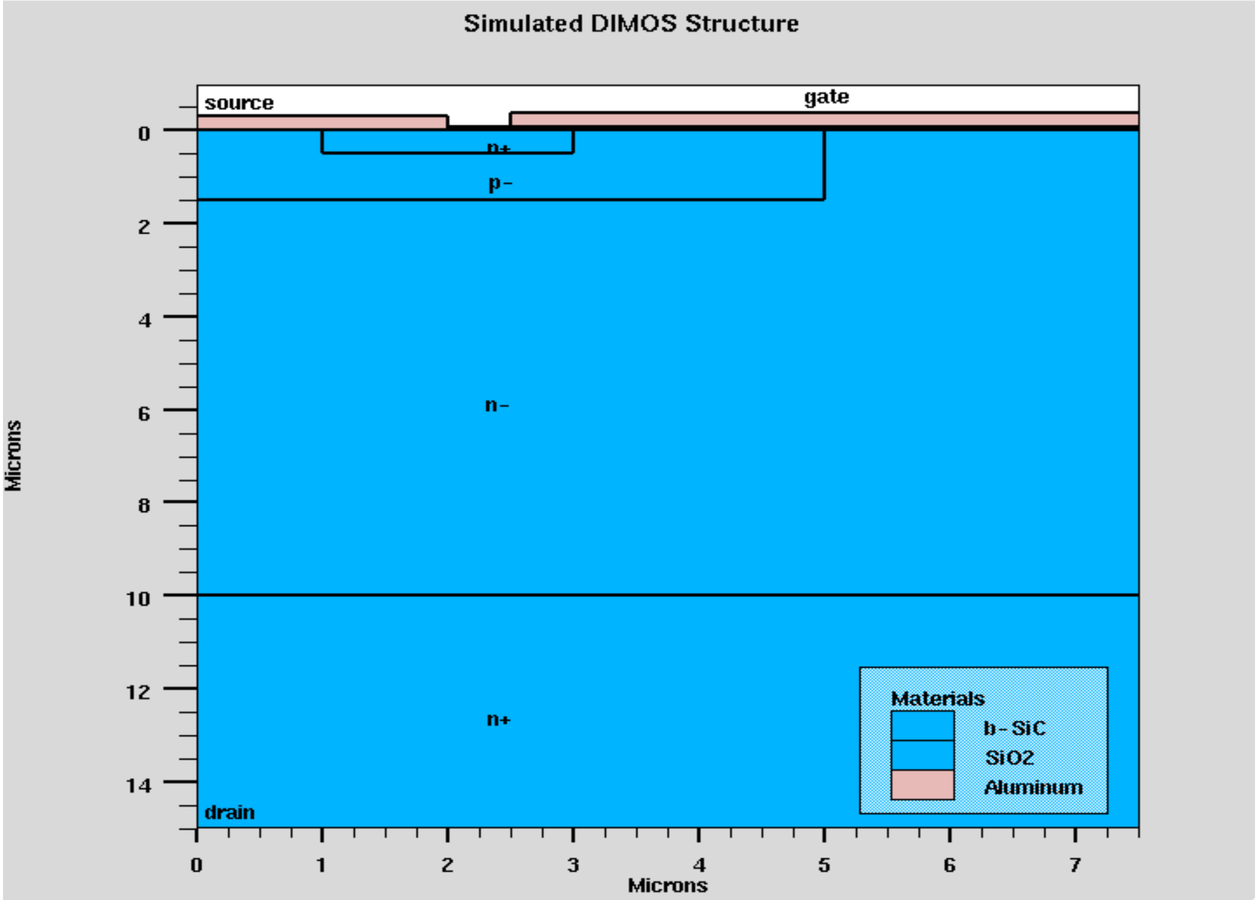
Trench-gated MOS (UMOS) Device



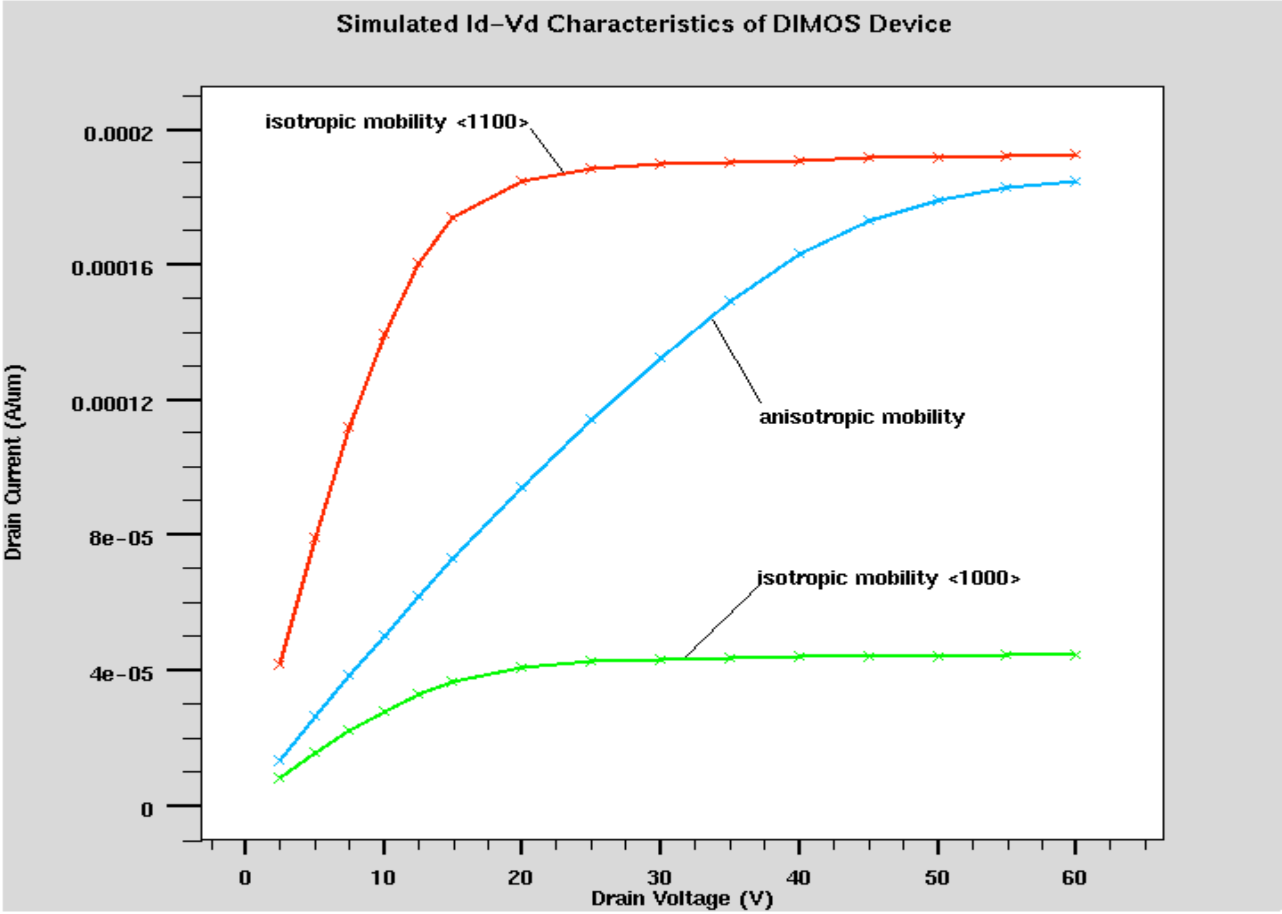
Id-Vd Characteristics for UMOS Device



Double Implanted MOS (DIMOS) Device



Id-Vd Characteristics for DIMOS Device



Conclusions: SiC

- Hall mobilities in SiC are different depending on the crystalline axis
- User just needs to specify mobility parameters in the crystallographic planes
- Change in mobility due to current flow vector automatically calculated
- Works with all ATLAS and Blaze mobility models

Simulation of III-V Device with Blaze and Laser

SILVACO

Laser as Part of the ATLAS Framework

- Laser simulation is implemented as part of the ATLAS device simulation framework
  - ATLAS provides framework integration
  - Blaze provides III-V device simulation
  - Laser provides optical emission capabilities

Overview of Laser

- Laser works within the framework of ATLAS and Blaze. ATLAS provides the framework integration. Blaze provide electrical simulation of heterostructure devices and material models for common III-V semiconductors
- Self-consistently solves the Helmholtz equation to calculate optical field and photon densities
- Accounts for carrier recombination due to stimulated emission
- Calculates optical gain which depends on photon energy and quasi-Fermi levels
- Predicts laser light output power and light intensity profiles corresponding to the fundamental transverse mode
- Calculates the light output and modal gain spectra for multiple longitudinal modes
- For Quantum wells optical gain accounts for bound state energies

Features of Laser

- Arbitrary stripe geometries
- Devices with multiple insulators and electrodes
- Allows any material as the active layer
- Delta doped layers
- Standard Blaze III-V, II-VI and GaN materials supported
- DC and transient modes of operation
- Near field and far field patterns, spectra and I-V curves

Laser Solution Methodology

- Blaze is used to obtain the initial dc starting condition by solving
  - Poisson’s equation
  - Electron continuity equation
  - Hole continuity equation
- Laser solves the 2D Helmholtz equation to find the transverse optical field profile E(x,y)
  - E(x,y) is found for the fundamental transverse mode
  - The Helmholtz equation may be solved for either
    - a single longitudinal mode of greatest optical power
    - multiple longitudinal modes
  - Multiple transverse modes can also be simulated

Laser Solution Methodology (cont.)

- The central model in laser simulation is the optical gain model which is the ability of the semiconductor media to amplify light. Laser contains three gain models
  - Empirically based model. This has no frequency dependence and is only a function of carrier concentrations
  - Physically based model. This takes into account frequency dependence and may be used for spectral analysis when simulating multiple longitudinal modes
  - Quantum well model. This accounts for optical gain within quantum wells including effects of bound state energies

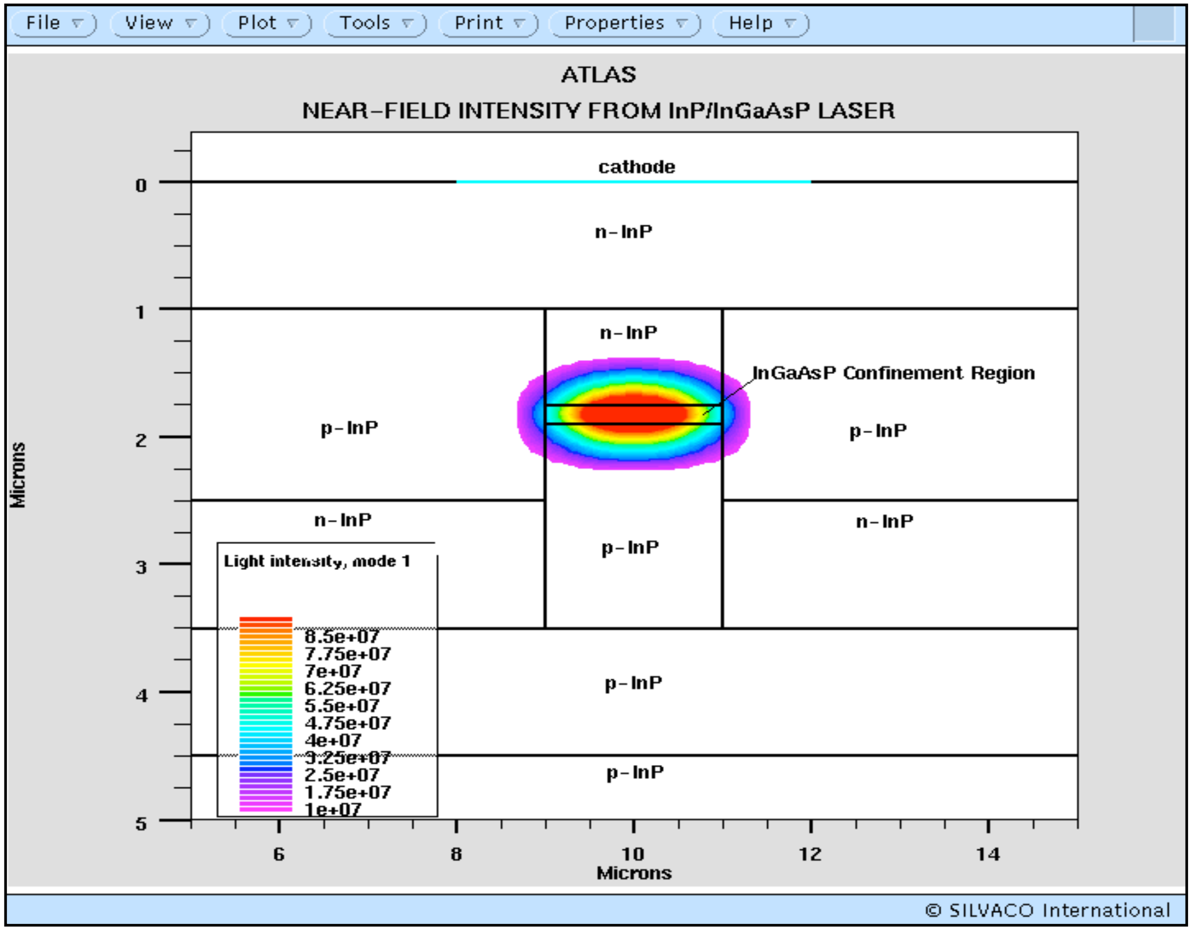
Laser Solution Methodology (cont.)

- Laser uses E(x,y) and g(x,y) to solve the photon rate equation, to calculate the total photon density for each longitudinal mode
- Blaze and Laser simulations are coupled in three areas
  - the optical gain g(x,y) is a function of the quasi-Fermi levels
  - the dielectric permittivity is a function of the optical gain g(x,y)
  - an additional optical recombination term is added to the RHS of the continuity equations and is a function of g(x,y), E(x,y) and the photon density

Output from Laser

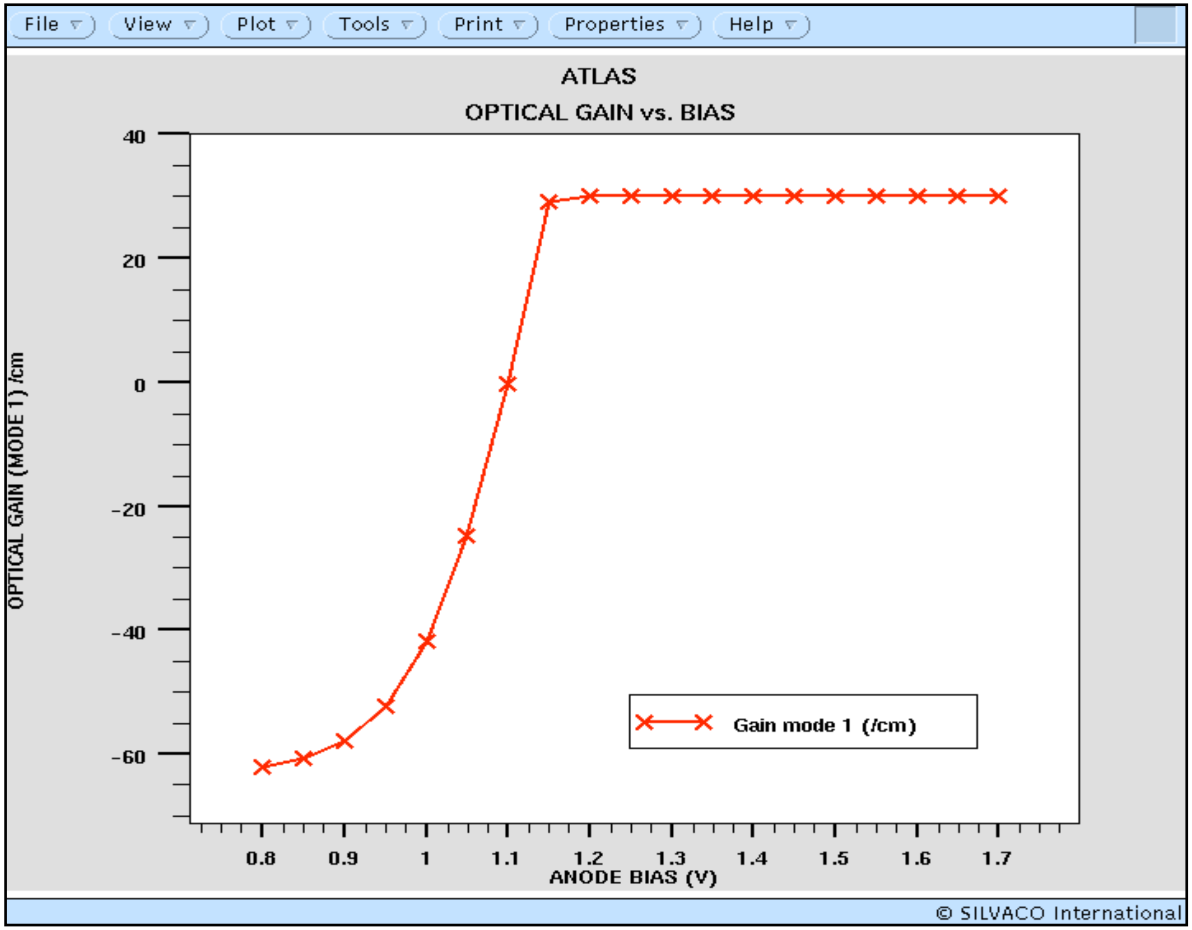
- Single mode operation
  - optical intensity profile E(x,y)
  - laser gain g(x,y)
  - photon density
  - optical power
  - total optical gain
- Multiple mode operation
  - all single mode output but summed over all modes
  - laser spectra file for each dc bias or transient solutions

Near Field Light Intensity in the Fundamental Transverse Mode for an InP/InGaAsP Laser Diode

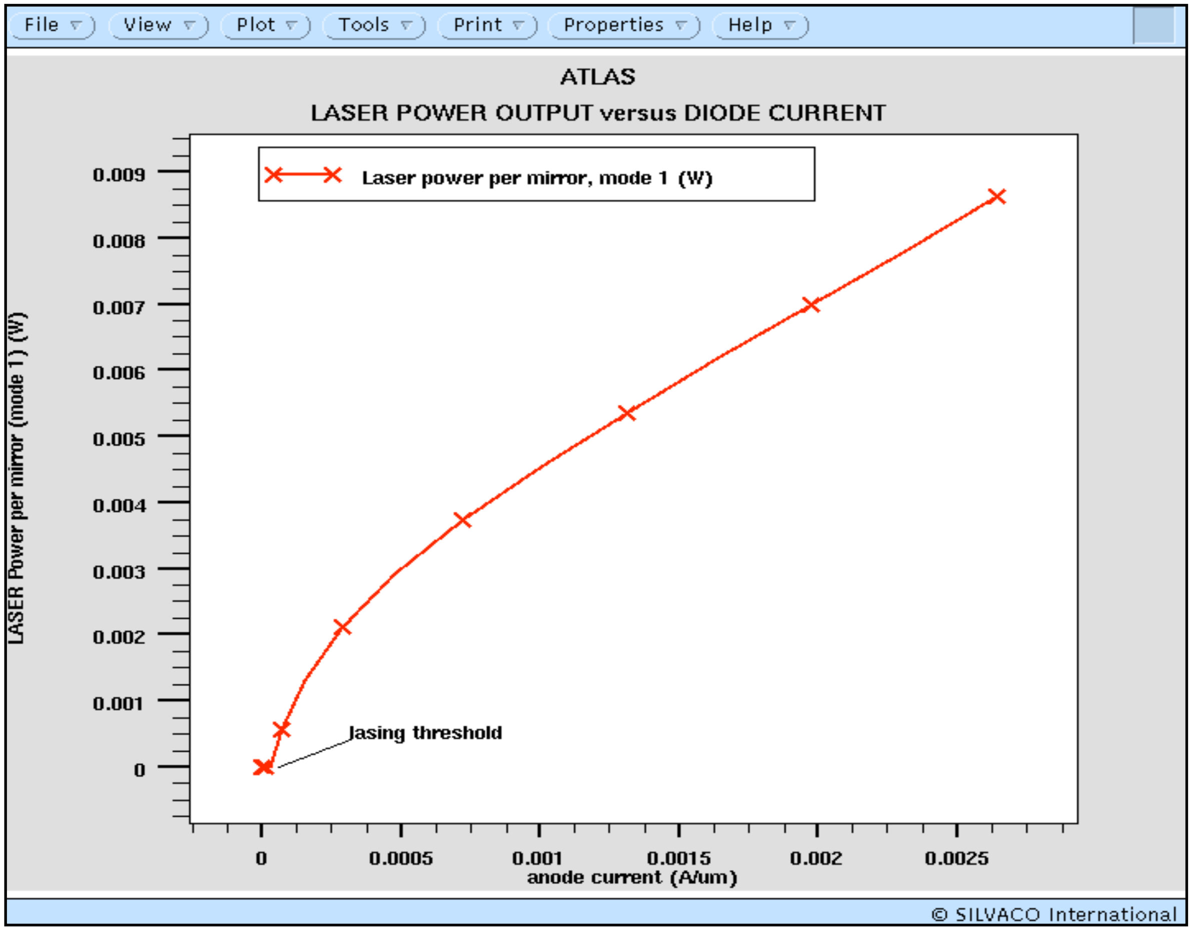


SILVACO

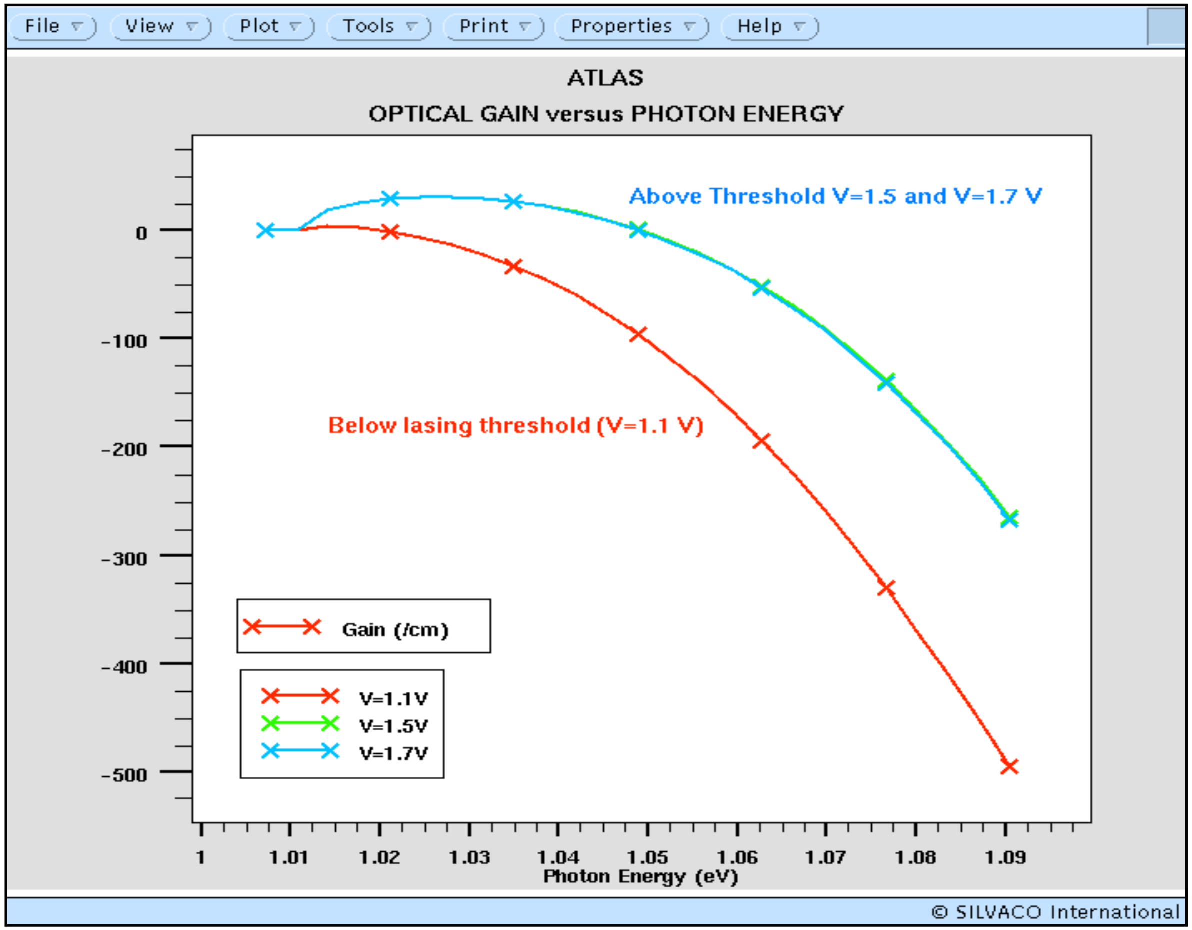
Optical Gain as a Function of Bias



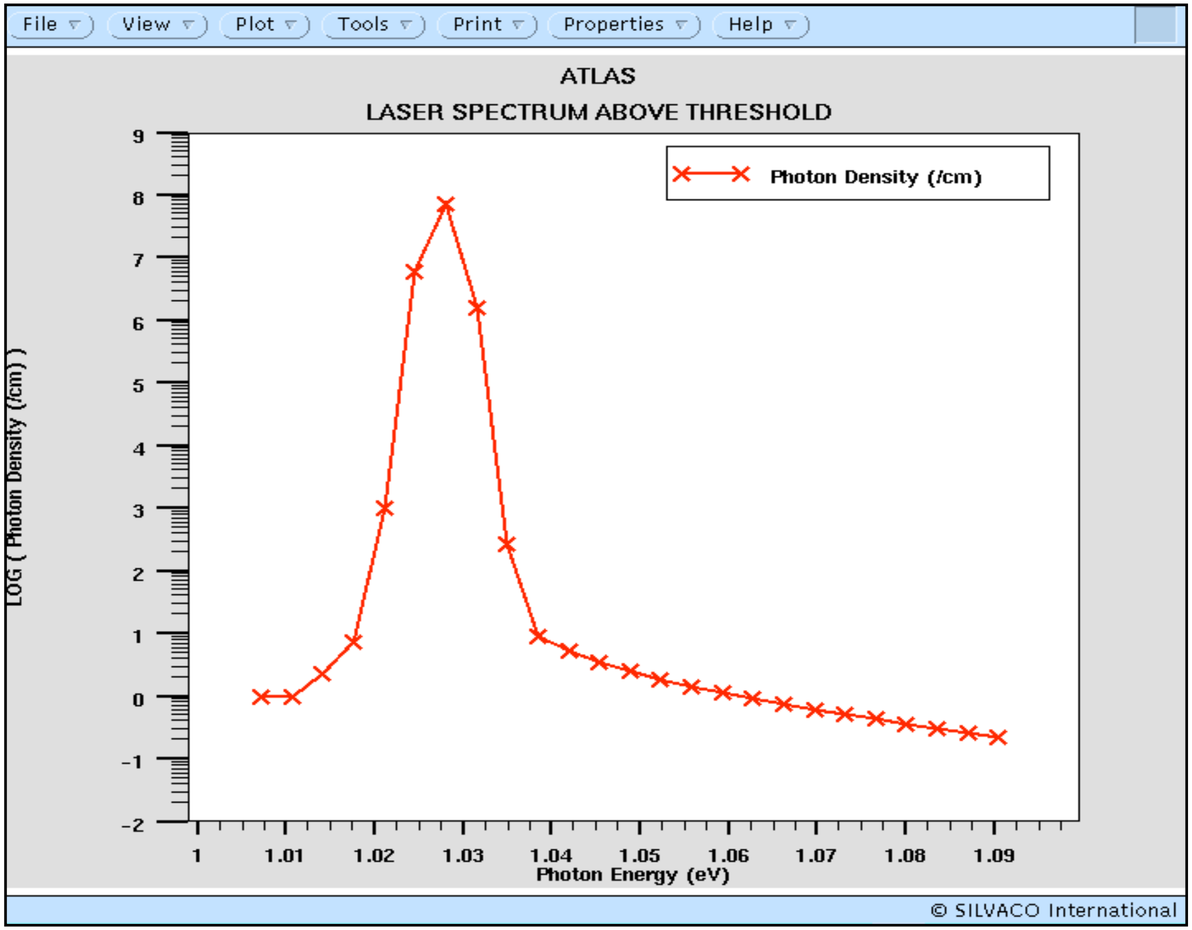
Optical Output Power as a Function of Anode Current



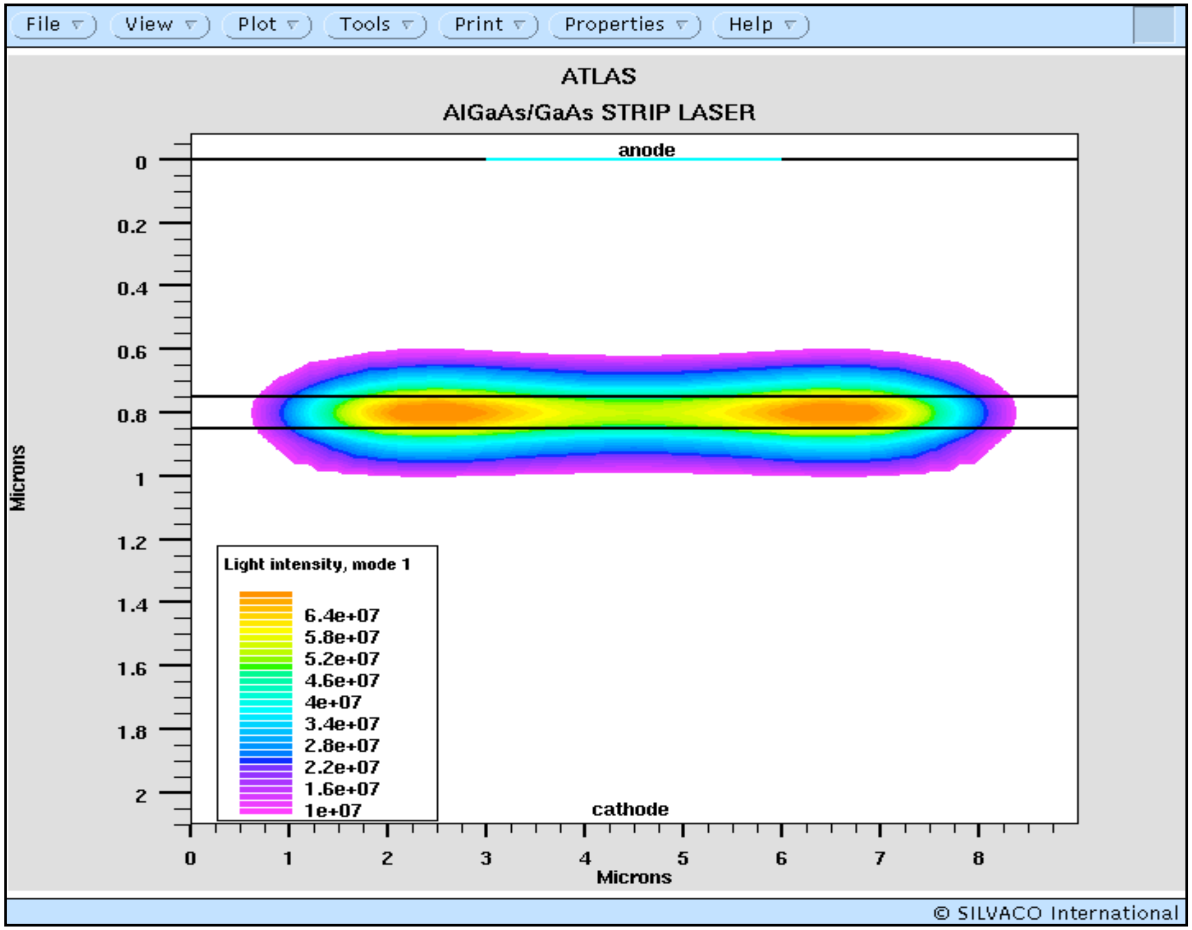
Gain Spectra Below and Above Lasing Threshold



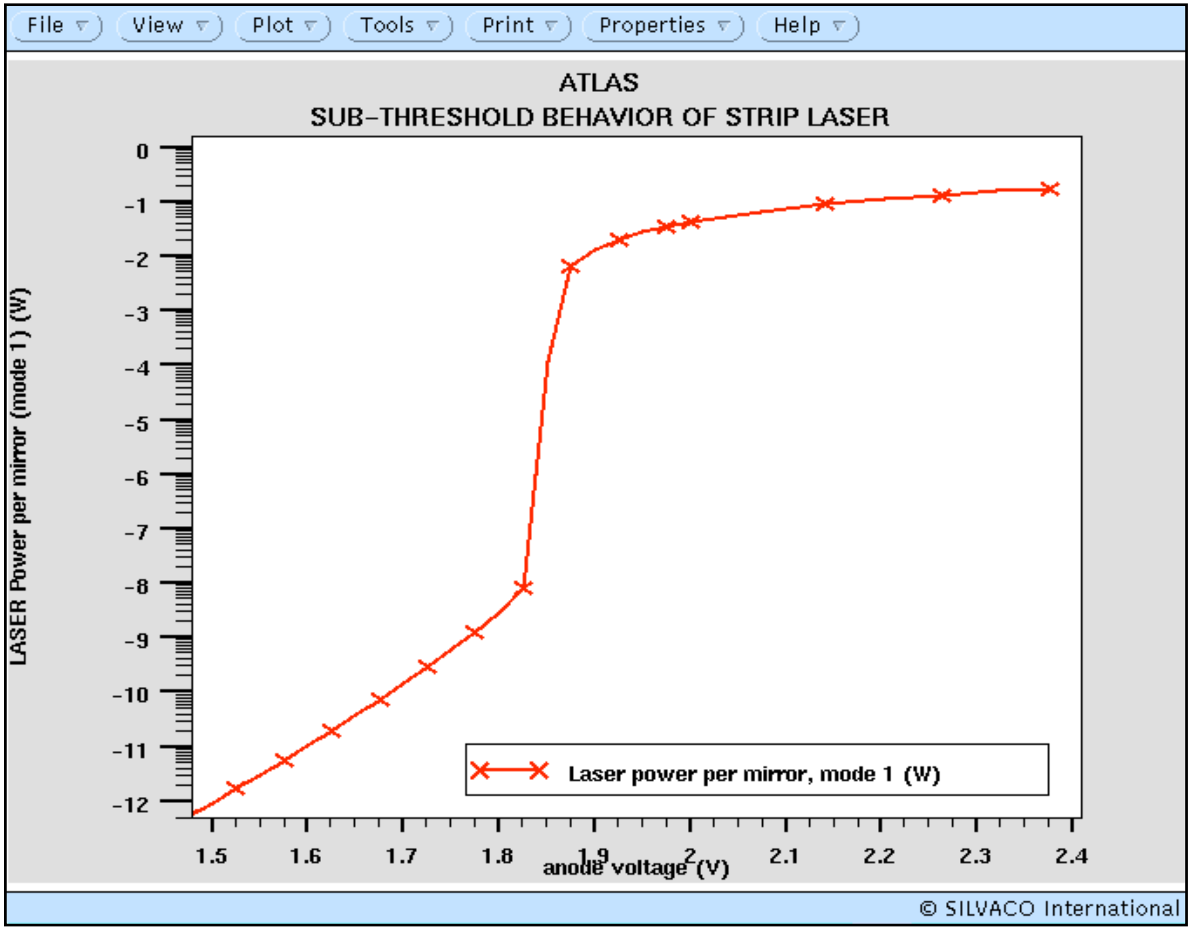
Laser Spectrum Above Threshold



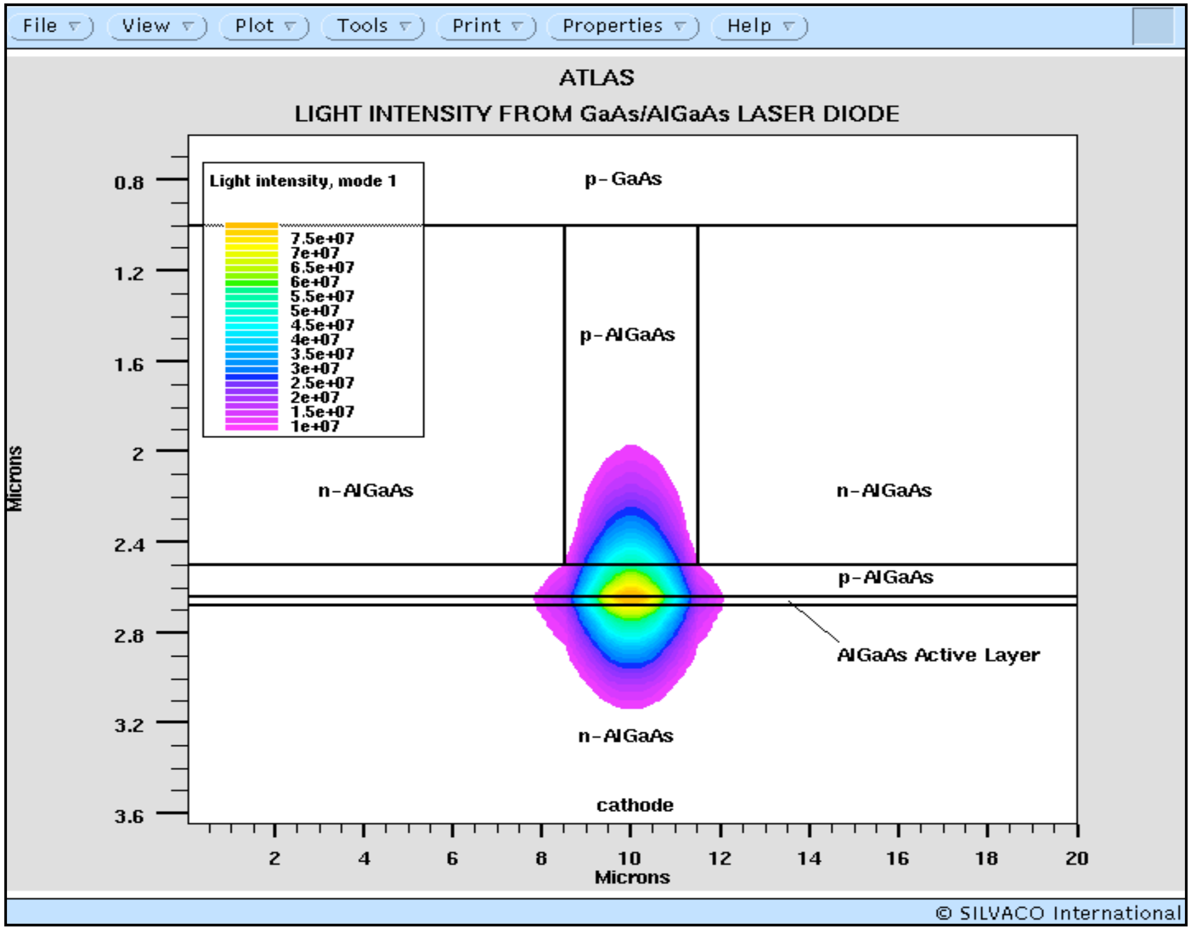
Near Field Pattern for a Strip Laser



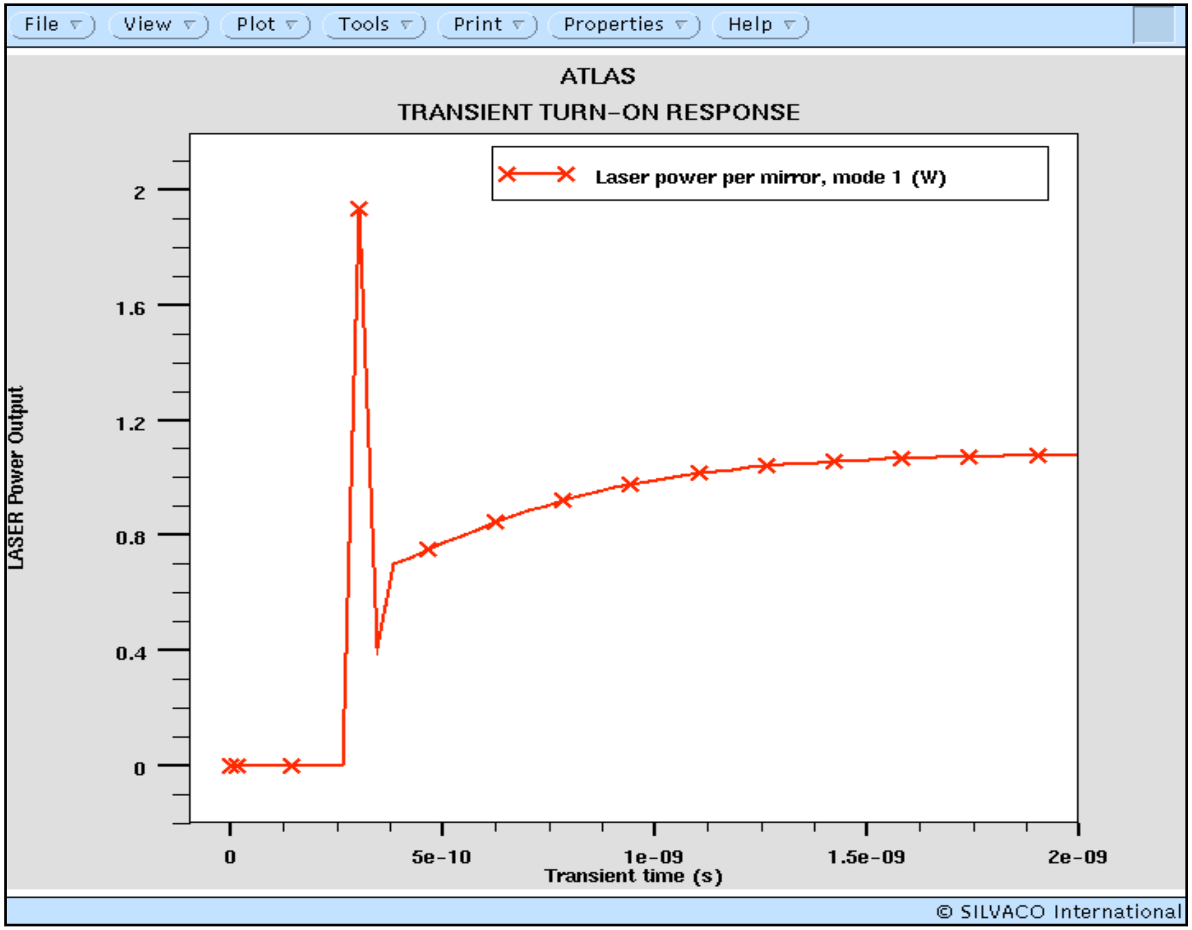
Threshold and Sub-Threshold Characteristics for a Strip Laser



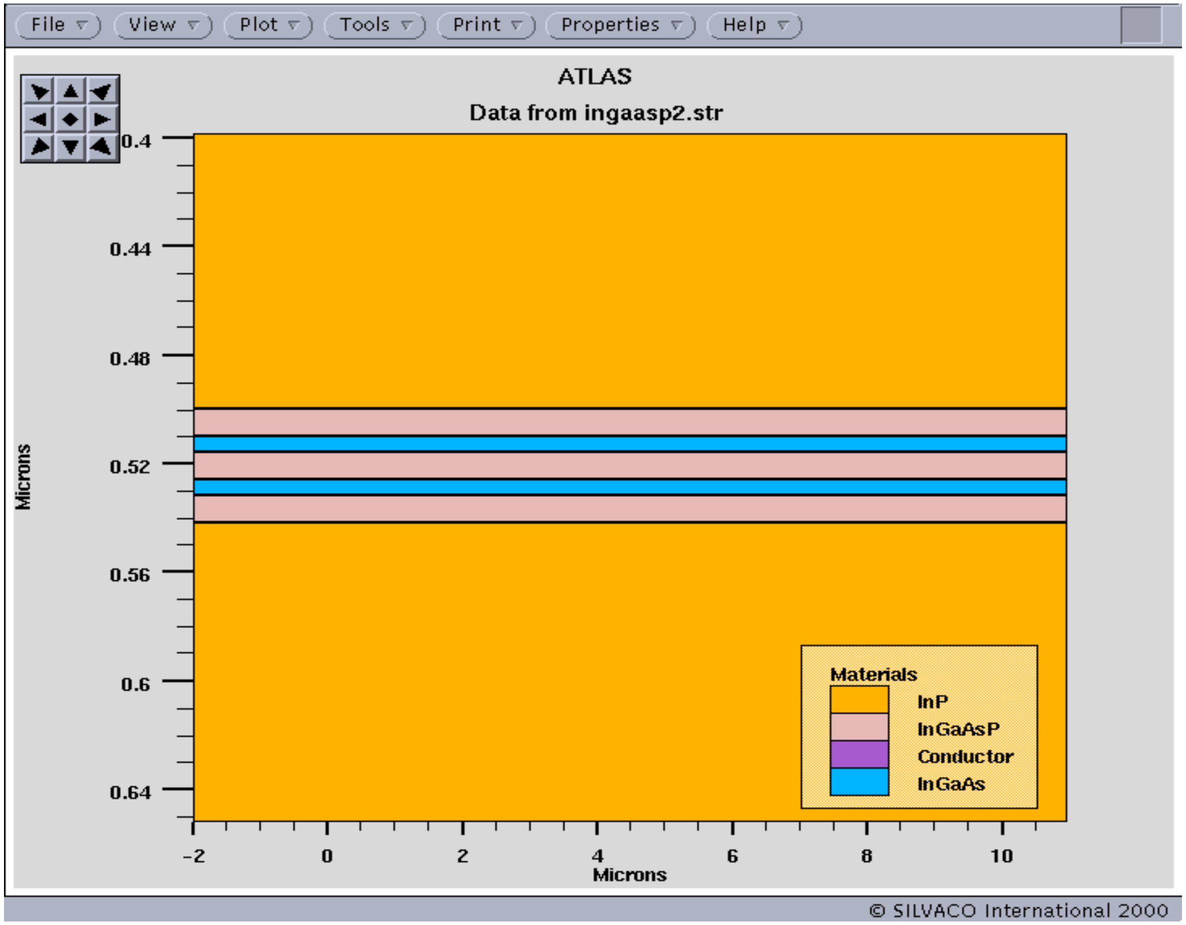
Fundamental Transverse Mode Near Field Light Intensity



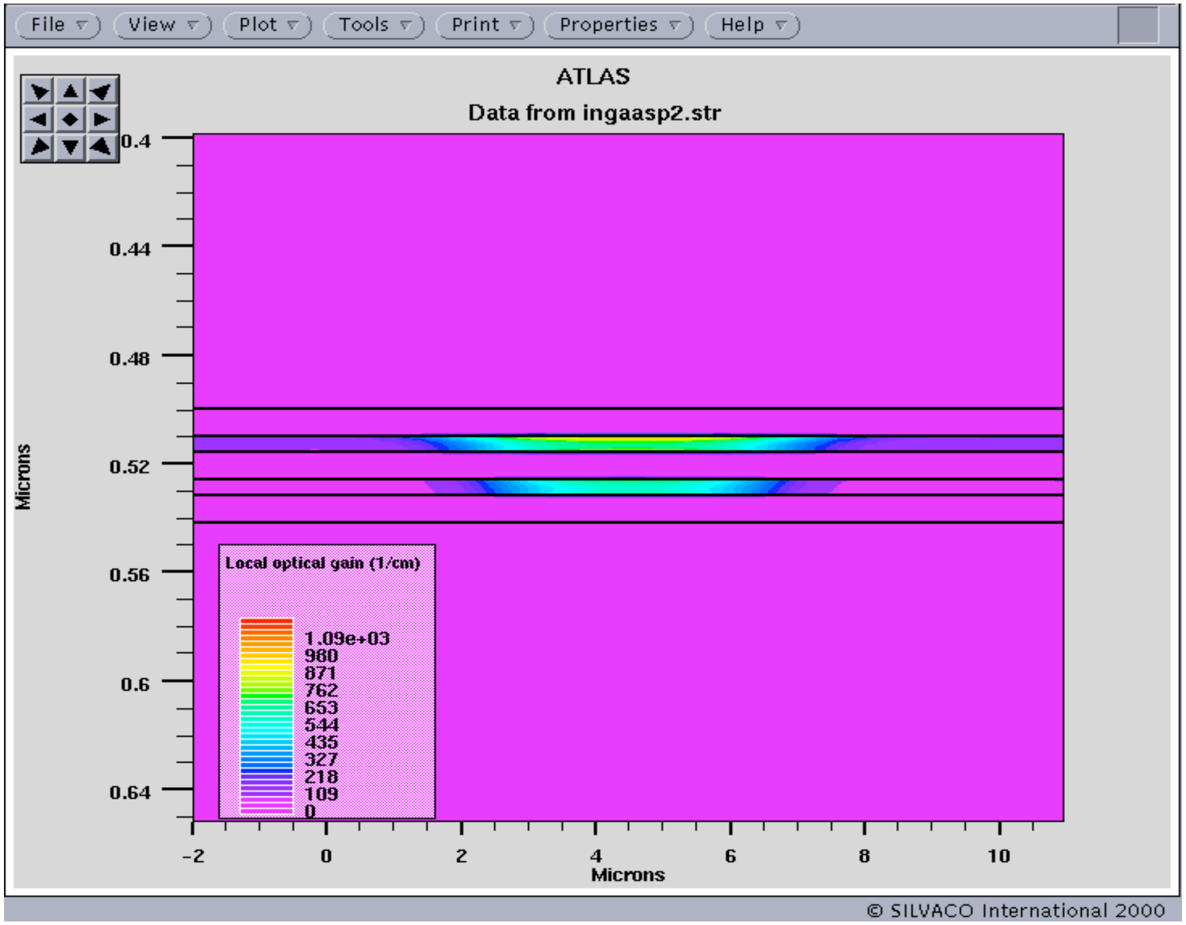
Transient Response of Laser Output Power to Turn-on Voltage Pulse



Multiple Quantum Well Laser Diode



Optical Gain for MQW Laser Diode



Conclusions: Laser

- By solving the Helmholtz equation with optical gain models Laser allows accurate simulation of laser diode
- Multiple quantum well and strained MQW laser diodes
- Analysis of the effects of structures design and material parameters is straightforward
- Near field and far field patterns allow improved laser diode designs to be made
- Seamless integration into Blaze allows users to quickly implement laser device simulations and study results with TonyPlot