CROSSLIGHT

Software Inc.

Crosslight Device Simulation Software Information

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About Crosslight Software Inc.

Crosslight Software Inc. (formerly Beamtek Software Inc.) is the leading supplier of semiconductor device and process simulation software. It is an international company established in 1992 with head office in Canada and branch offices and distribution/support centers in many countries around the world.

Its flagship product PICS3D, for the 3D simulation of semiconductor optoelectronic devices, won the commercial technology award from trade journal Laser Focus World in 1998. Since the award, Crosslight's research team has been working even harder to provide state-of-the-art device/process simulation software for the semiconductor industry.

Crosslight Software is the world leader in providing commercial physical models of semiconductor optoelectronic/electronic devices. Crosslight's customers include tens of major manufacturers of semiconductor electronic and optoelectronic components and systems.

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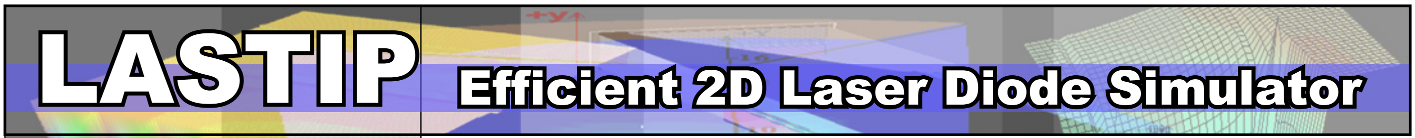
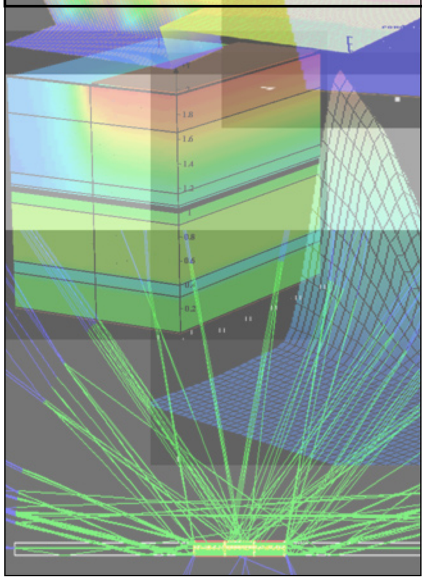




What is LASTIP

LASTIP (LASer Technology Integrated Program) is a powerful device simulation program designed to simulate the operation of a semiconductor laser in two dimensions (2D). Given the structural and material properties, it produces a large amount of simulation data to describe the lasing characteristics. Based on well-established physical models, it provides the user with a quantitative insight into various aspects of a semiconductor laser.

It can be used as a computer aided design (CAD) tool to optimize existing lasers or to assess new designs. With the physical models and advanced capabilities of LASTIP, the user can concentrate on device optimization and design while leaving all the numerical modeling work to the computers.

Applications

LASTIP can be used to model the electrical and optical behaviors on a 2D cross section of all types of semiconductor lasers emitting at any wavelength and from any semiconductor material. It is most suitable for Fabry-Perot (FP) type of laser diode where variations of physical quantities in the longitudinal dimension are relatively less important than other types of lasers.

Physical Models and Advanced Features

In an arbitrary two-dimensional (2D) cross section a semiconductor laser, LASTIP solves the following basic equations under continuous wave (CW) or transient conditions.

Poisson's equation describes the potential charge relation in a semiconductor with heterojunctions.

The time-dependent electron and hole current continuity equations govern the carrier flux-recombination relation. The Thermionic emission model has been used to describe carrier transport across a graded or abrupt heterojunction, or a quantum well.

The complex wave equation yields the optical field distribution in the transverse and lateral directions based on the arbitrary complex refractive index distribution. Several advanced numerical techniques allow the user to obtain multi-lateral mode solutions.

The time-dependent photon rate equation is solved to relate the optical power with modal gain and recombination.

The Finite element method (FEM) is used to discretize the basic differential equations. The FEM is ideal for treating arbitrary laser geometries.

AC small signal model can be used on CW solutions to extract high frequency characteristics such as modulation response and AC capacitance.

To obtain accurate simulation data, LASTIP has implemented the following physical models.

- Quantum well subbands are solved to accurately compute the carrier concentrations and optical gain. Strained quantum wells are treated using a k.p theory. LASTIP allows the user to incorporate valence band mixing effects into the 2D simulator for both zinc-blende and wurtzite material systems. We closely follow the work of S.L. Chuang (Rev. B, vol. 43, pp. 9649-9661, 1991. IEEE J. Quantum Electron., vol. 32, No. 10, pp. 1791-1800, 1996.)

- The Optical gain function for quantum well or bulk material is computed starting from material parameters such as effective masses and bandgaps. Sophisticated gain broadening models include Lorentzian and Landsberg types. Intraband scattering mechanisms involving carrier-carrier and carrier-phonon scattering are taken into account to estimate the broadening parameter. Interband optical transition based on integral over k.p non-parabolic subbands are also available.
- Carrier recombination models include SRH (Shockley-Read-Hall) recombination, Auger recombination and recombinations due to stimulated and spontaneous emissions.
- Deep level trap and trap dynamic models are implemented to allow for an accurate model of semi-insulating semiconductor materials. The Poole-Frenkel model of field induced impurity ionization is implemented for an accurate model of II-VI compound material used in blue lasers.
- Interface states may be modeled using surface deep level traps, surface recombination centers, or fixed surface charges. The piezo-electric surface charge may be modeled using fixed surface charges.
- Fermi statistics are used for the accurate computation of bulk and quantum well carrier concentrations.
- Incomplete ionization model is used to accurately describe the charge states of doped impurities.
- Field-dependent mobility model is implemented in various analytical forms.
- The Far-field emission pattern is computed based on complex near field distribution obtained from the 2D wave equation.
- A Non-linear gain suppression model is included in both CW and transient simulations.
- Temperature dependent models enable the user to investigate temperature effects due to all possible causes. All material parameters are allowed to vary with temperature.
- A Low-temperature simulation can be performed down to 77K and below.
- A large number of material models have been implemented. These include GaAs/ AlGaAs, InGaAs/ AlGaAs, InGaAsP, InGaAlAs, InGaAlP, InGaAsP/InGaAlAs-InP GaSb/AlAsSb, ZnSe-based II-VI, GaN-based materials (InGaN and ALGaN), and InGaAsN. For GaN-based materials, a **wurtzite** band structure is considered.
- Flexible format for material parameter input enables the user to modify existing material models or create his/her own material models.
- A Fully coupled Newton method is used for the self-consistent solution of the basic equations. This ensures good stability and convergence.

Another unique feature of LASTIP is its numerical stability against mesh points regardless the structure of the device. For a minimal amount of mesh points, the simulator runs smoothly for a device with structural variation from a few nano meters in one direction (such as quantum wells) to hundreds of micron meters in another direction and it is still able to produce reasonable results. When the simulator can afford to use fewer mesh, the speed is up. Such stability is extremely important especially in an initial stage of a simulation project when device engineers need to go through many trial-and-error cycles. We are pleased that many years of innovation in linear and non-linear numerical techniques results in praises from users of LASTIP.

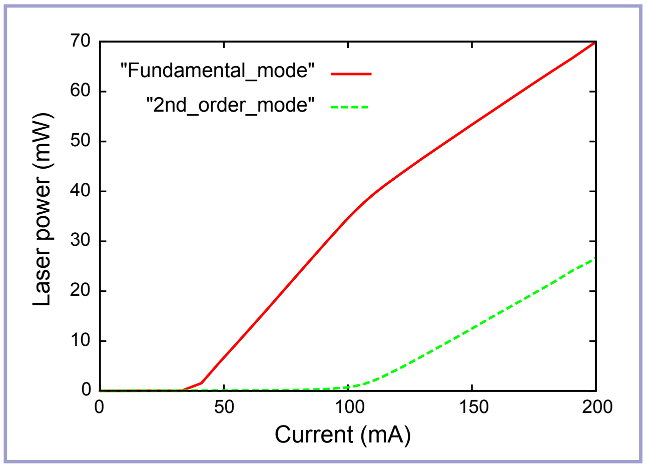
Output Data

LASTIP is capable of generating large amount of output data including, but not limited to, the following.

1. Structural 2D distribution of many physical quantities at selected biases. These include potential, electron concentration, electric field and current distributions. Detailed band diagram may be plotted to provide information such as band alignment, quasi-Fermi levers, quantum subband levels and wave functions.
2. Bias dependence of most critical quantities such as Light

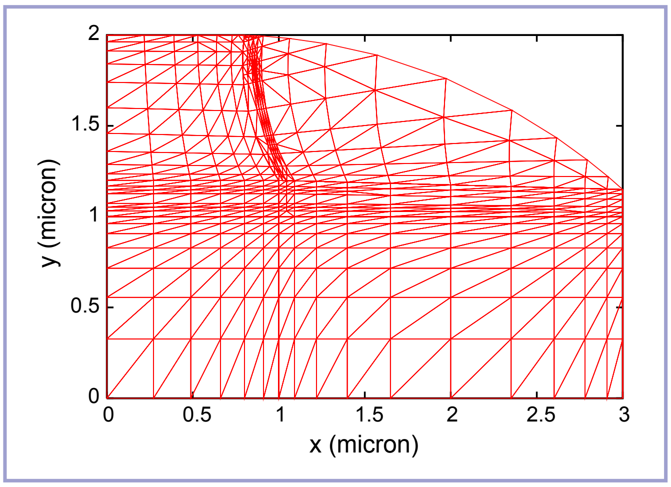
versus current (L-I) characteristics, current versus voltage (I-V) characteristics and modal gain versus current.

3. Spectral data at selected biases for modal gain, spontaneous emission and refractive index change.
4. Far-field distribution.
5. Time dependent simulation with output similar to those of bias dependent CD simulation. Fourier transform can be used to convert results into spectral domain.
6. High frequency characteristics from AC small signal analysis.
7. All of the above at different temperatures.

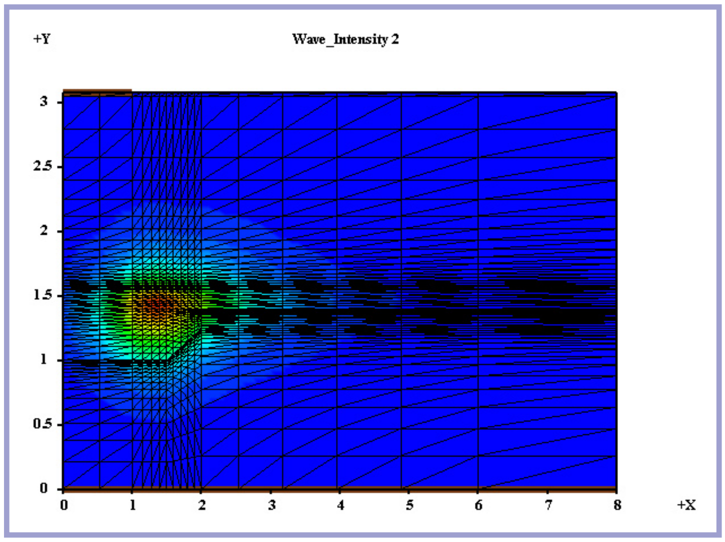


Simulated light-current characteristics for a quaternary InGaAsP laser indicating lateral mode competition effect.

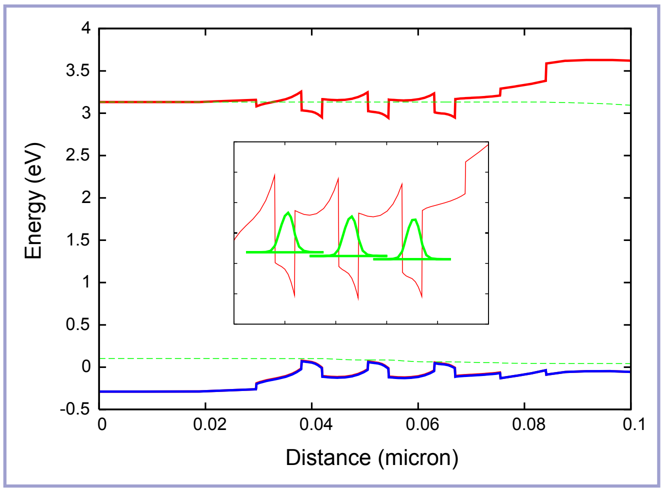
Sample Results of LASTIP

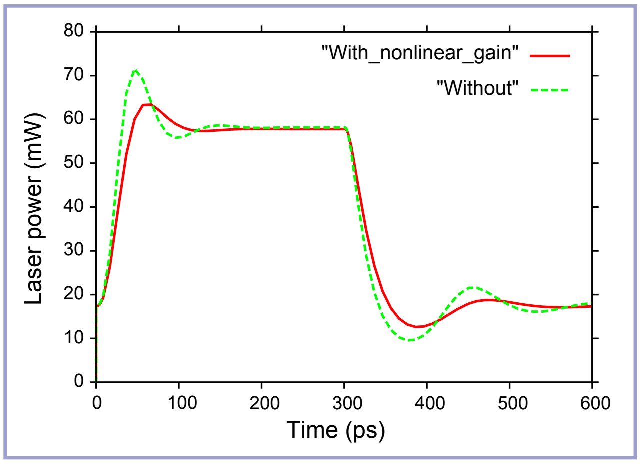


Unstructured mesh generated to fit the material boundaries with curvatures.

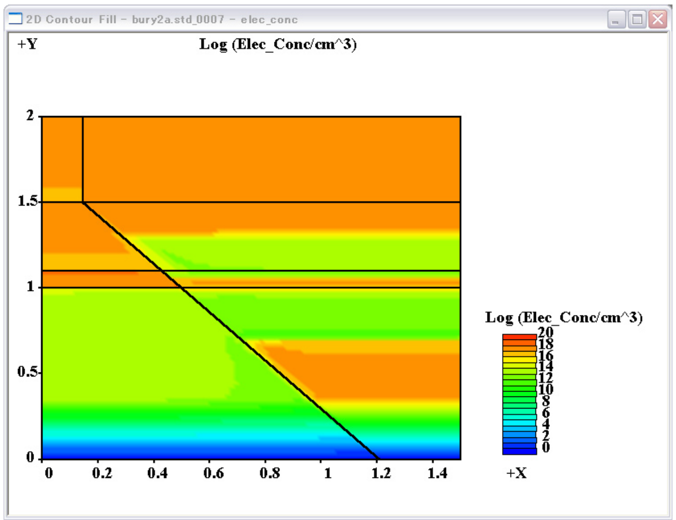


Second order mode intensity distribution simulated by LASTIP

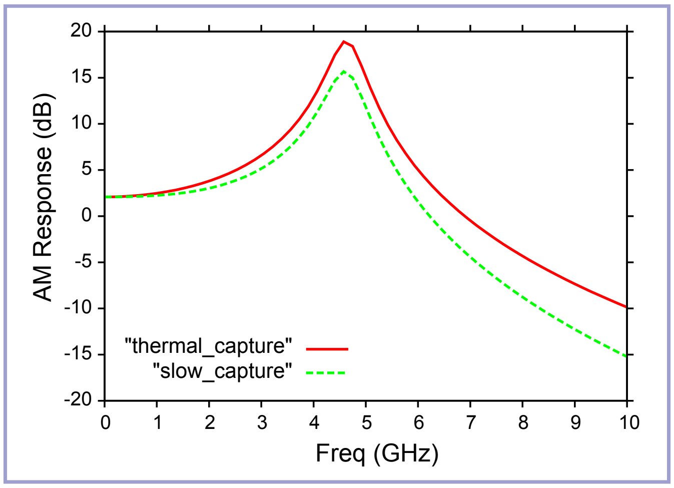




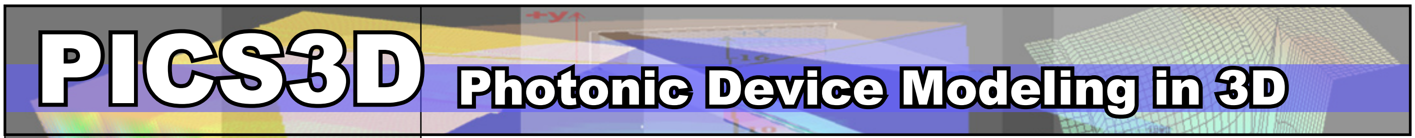
Simulated laser output power as a function of time. The difference between the two curves is due to different non-linear gain suppression effects.

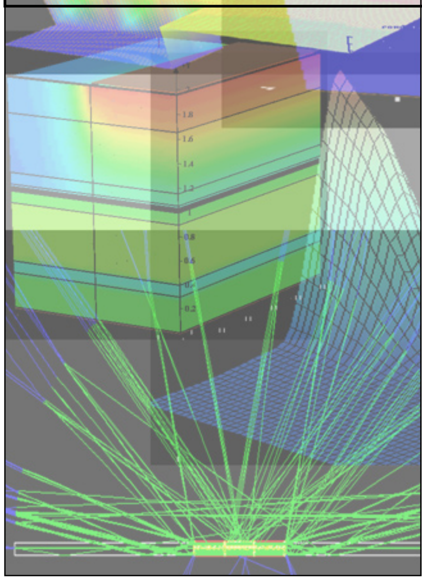


Distribution of electron concentration in a buried-heterostructure laser



Laser diode modulation response extracted from CW simulation data using small signal analysis technique. The results here demonstrate the effect of quantum capture.





What is PICS3D

PICS3D (Photonic Integrated Circuit Simulator in 3D) is a state of the art 3D simulator for laser diodes and related photonic devices. Its primary goal is to provide a 3D simulator for edge and surface emitting laser diodes. It has also been expanded to include models for other components integrated with or related to the laser emitter. PICS3D is a more advanced simulator that extends the physical models of LASTIP from 2D to 3D.

Applications

PICS3D may be used for any type of active or passive waveguide semiconductor devices. It is also suitable for vertical cavity surface emitting lasers (VCSEL). Applicable devices include but are not limited to the following:

1. Edge lasers including Fabry-Perot, DBR, DFB lasers. Both first order and second order gratings can be treated in DFB/DBR lasers. Multiple sectional devices combining active and passive sections can be simulated routinely.
2. Quantum well and bulk electric-absorption modulator (EAM).
3. Semiconductor optical amplifiers (SOA).
4. Waveguide photo-detectors (WPD).
5. Optically pumped edge emission lasers.
6. Vertical cavity surface emitting lasers (VCSEL).
7. Optically pumped VCSEL's. External cavity lasers.

Introduction to 3D Laser Model

A semiconductor laser is a unique three dimensional (3D) device, in that both the lateral and longitudinal dimensions are crucial to the operation of the device as a light emitter. The lateral dimension provides the important mechanisms of optical gain, spontaneous and stimulated recombination while the longitudinal dimension provides the amplification of the spontaneous emission and produces the emission characteristics of the device.

Missing either the lateral or longitudinal dimension is a handicap for any laser simulator. Our LASTIP package provides detailed modeling capability for the material and layer geometry in the lateral dimension (x and y directions) while the longitudinal dimension (z-direction) is a simplified rate equation assuming uniform distribution in the z direction and a single longitudinal mode.

The longitudinal spatial hole burning effect is ignored. As a result, it is not possible to properly treat cases where longitudinal behavior is crucial. Common examples of this type are DFB, DBR and VCSEL lasers where the distributed effect in the longitudinal direction plays an important role.

PICS3D is capable of performing simulation in time, spectrum as well as in the three spatial dimensions. It gives us a full view of a laser diode in operation at a price: longer computation time. The computation time problem is being reduced with increasing computing power of new generations of computer hardware and updated operating systems.

Since the basic physical models and capabilities of PICS3D on the lateral/traverse dimensions are the same as those for LASTIP, we shall only describe our treatment of longitudinal modes and the z-dimension in this product description.

Longitudinal Mode Models

The numerical approach for solving the longitudinal modes is based on a combination of transfer matrix and the complex Green function method. The transfer matrix method divides the longitudinal cavity into subsections and propagates waves from one subsection to the next. The complex Green function method is a rigorous analytical method that can be used to compute the optical power of a multiple longitudinal mode system accurately. Both coupled-mode theory and multi-layer optics theory can be used for treatment of grating structures in DFB, DBR and VCSEL laser diodes.

The dynamic equations derived from such an approach allow us to compute the large and small signal responses of the multimode laser diode system.

Advanced Techniques for 3D Simulation

To achieve maximum computation speed and efficiency, we have invented a new technology for numerical simulation of laser diodes in 3D. Our new technology divides the tasks of 3D simulation into a combination of 2D and 1Dz (1D in z-direction, the longitudinal direction) simulations (quasi-3D approach). The 2D and 1Dz modules are carefully coordinated so that coupling of physical models in the 2D and 1Dz modules are not lost.

As an option, the 2D module mentioned above may be replaced by a full 3D carrier transport model which allows for a more realistic description of the photonic device. The full 3D option is used at a cost of much increased computation time as compared with the quasi-3D approach.

Timing

As described in the previous section, PICS3D turns on and off the 2D solver and the PICS1D modules self-consistently and exchanges information between the two packages dynamically. Therefore the computation time should be the sum of the two packages plus some administrative overheads. For a high-end PC the following timing is typical:

1. For a PICS3D simulation of edge emitting laser treating only the y-z dimensions (the x-direction is uniform as in broad area lasers), the longitudinal dimension is cut up into 20 or so sections. The CW simulation takes approx. 10 minutes.
2. Consider a 3D simulation of strained multiple quantum well laser (edge type). We cut up the z-dimension into 20 or so sections. The CW simulation takes about 30 minutes.
3. For a VCSEL with simple geometry and no heat transfer, 1/2 hour or so is expected.
4. For a VCSEL simulation with heat transfer, 2 hours or so is expected.

Therefore, with PICS3D, one expects to spend typically 10 minutes to 2 hours for each simulation. PICS3D is perfectly suitable for IBM PC's that everybody is using these days.

PICS3D Output Capabilities

PICS3D has all of the data output capabilities of LASTIP for any specific x-y plane of an edge type laser. In addition, PICS3D is capable of producing the following data.

1. Coupling coefficients for waveguide gratings(1st and 2nd order grating).
2. Longitudinal distribution of carrier density, optical gain and optical wave intensity for the main and side longitudinal modes. For second order grating DFB, PICS1D can compute the distribution of surface emitting modes.
3. The current bias and time dependence (CW and transient large signal analysis) of the following quantities can be produced: Emission power and frequency change (chirping) for different longitudinal modes, sidemode suppression ratio, linewidth and linewidth-power product, effective alpha, 2nd harmonic distortion and surface emitting power (for 2nd order grating DFB).

4. Mode emission spectrum at different bias condition and from different laser facets.
5. Mode emission spectrum at different bias and time.
6. FM small signal modulation response spectra at different bias.
7. FM and RIN noise spectra at different bias.
8. Second harmonic distortion spectra

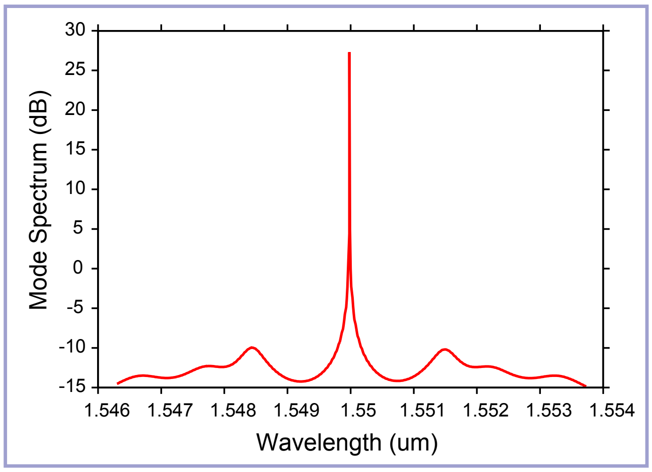
Choice of LASTIP or PICS3D

The stronger capability of PICS3D does not imply that PICS3D renders LASTIP obsolete. LASTIP is still the most powerful and efficient simulator if only layer design and material properties are concerned for a Fabry-Perot laser. Due to the complexity of the advanced physical models incorporated into PICS3D, its use requires more simulation skills and is recommended for advanced users who already have some experience of LASTIP or APSYS.

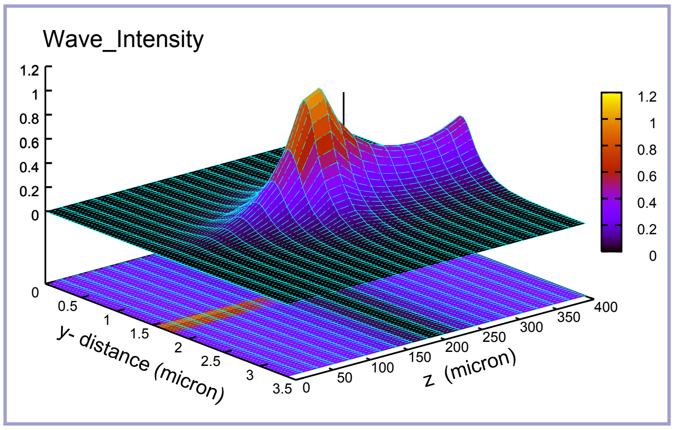
Due to the different treatment of optical models in the longitudinal direction, LASTIP is capable of generating more efficient and stable solution in multi-lateral mode solutions. Usually PICS3D is recommended only when LASTIP can not provide an accurate description of the longitudinal variation of the optical/electrical properties.

Therefore, in deciding which simulator to use, our users are advised to discuss their needs with Crosslight Software experts.

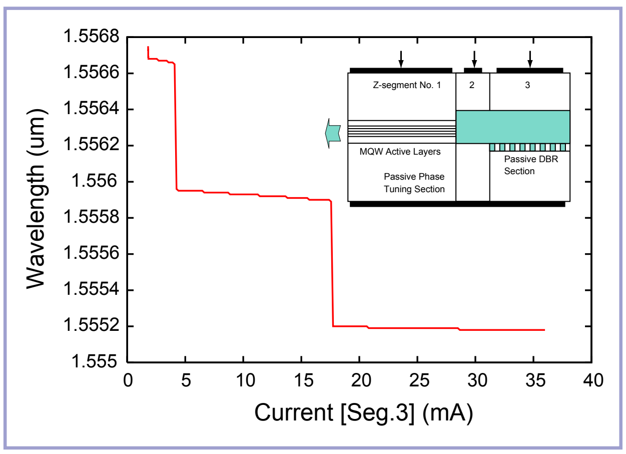
Selected Results of PICS3D



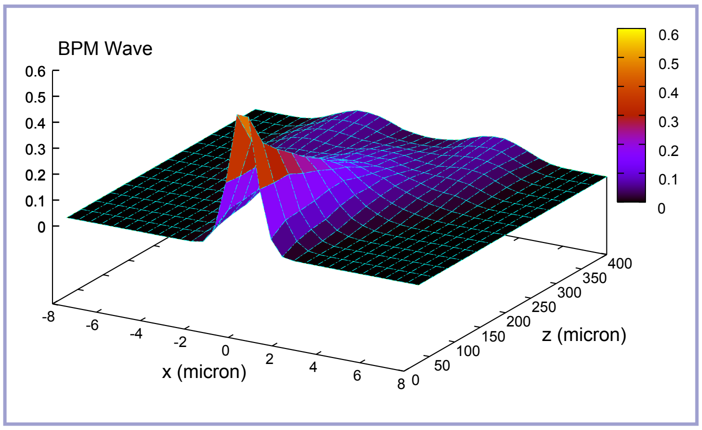
Simulated emission power spectrum from the InGaAsP MQW DFB laser with 1/4 wave shift in middle section.



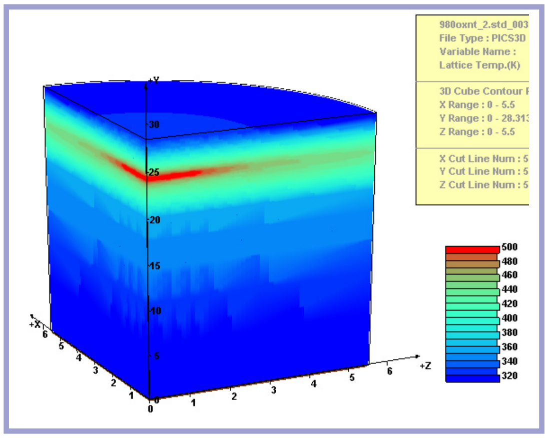
Simulated traveling optical wave intensity distribution within an InGaAsP MQW DFB laser with 1/4 wave shift in middle section.



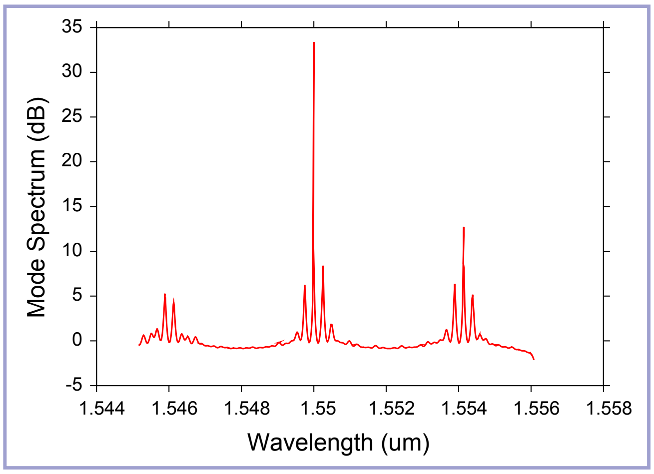
Tuning characteristics of a 3-section DBR laser simulated by PICS3D.



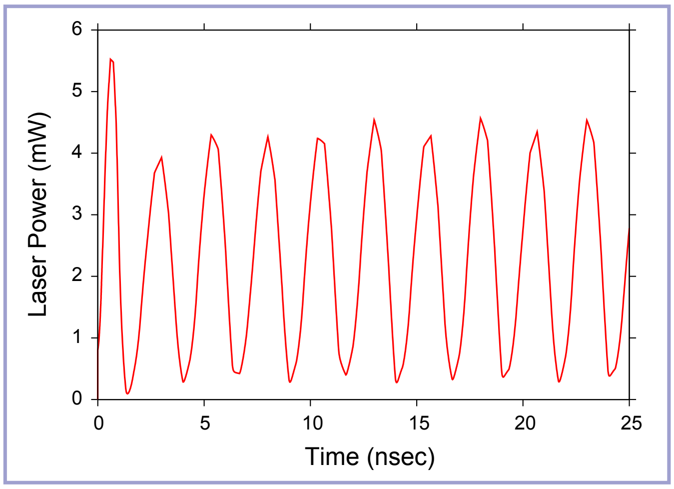
Simulated wave intensity in a tapered semiconductor optical amplifier (SOA) using the beam propagation method (BPM) which is coupled to the main module of PICS3D.



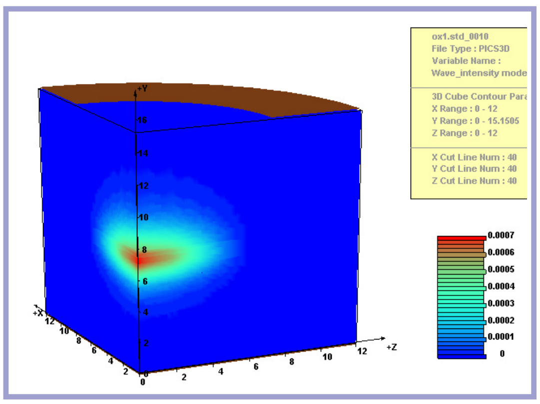
Simulated temperature distribution within a VCSEL with oxide aperture.



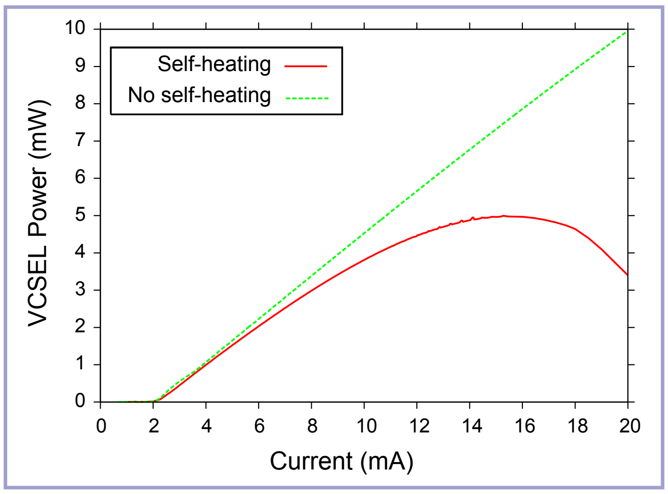
Emission power spectrum of a sampled grating DBR laser simulated by PICS3D.



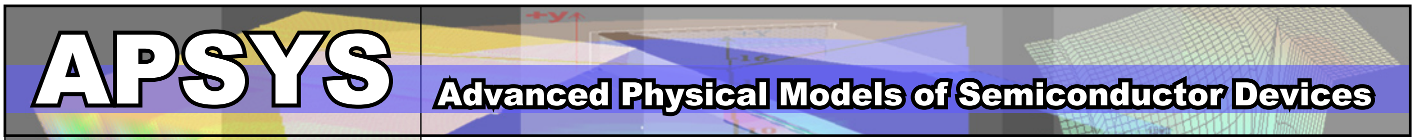
Power output of a self-pulsation laser simulated by PICS3D.

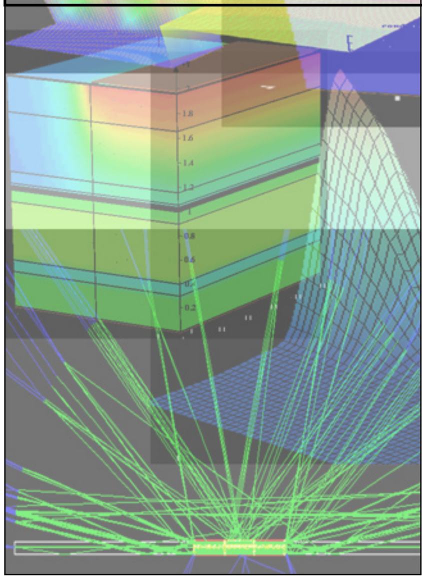


Optical wave intensity distribution within a VCSEL with oxide aperture.



Typical AlGaAs MQW VCSEL output power characteristics simulated by PICS3d.





What is APSYS

APSYS is a general purpose two-dimensional (2D) finite element analysis and modeling software program for compound semiconductor devices (with silicon as a special case). It includes many advanced physical models and offers a very flexible modeling and simulation environment for compound semiconductor devices. Advanced features include hot carrier transport, heterojunction and quantum well models. Optionally, 3D finite element analysis can be used (APSYS-3D option).

The simulation software is designed in such a way that user participation in developing his/her own physical models is encouraged. For example, the composition and temperature dependence of all of the physical parameters (bandgap, mobility, etc.) are located in a user accessible macro library with formulas written in syntax of C/FORTRAN. These formulas are parsed and incorporated into the simulation software only at run-time (at a small cost to simulation speed) so that the user can modify and fine tune these formulas any time. Such an approach to physical parameters meets the need of computer aided design (CAD) for a new generation of semiconductor devices when the search for new material and new structures never seem to stop.

Another unique feature of APSYS is its numerical stability against mesh points regardless the structure of the device. For a minimal amount of mesh points, the simulator runs smoothly for a device with structural variation from a few nano meters in one direction (such as quantum wells) to hundreds of micron meters in another direction and it is still able to produce reasonable results. When the simulator can afford to use fewer mesh, the speed is up. Such stability is extremely important especially in an initial stage of a simulation project when device engineers need to go through many trial-and-error cycles. We are pleased that many years of innovation in linear and non-linear numerical techniques results in praises from users of APSYS.

Applications

APSYS can be applied to the modeling and analysis of almost all devices except semiconductor lasers (which are simulated by our other products LASTIP and PICS3D). These include the following devices based on silicon and compound materials.

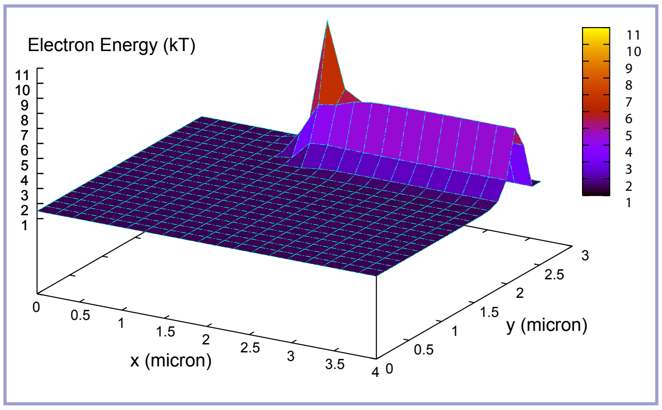
1. Silicon devices including MOSFET's, bipolar transistors and JFET's.
2. All types of Photodetectors (PD's) including MSM PD's, APD's and waveguide PD's.
3. Solar cells.
4. HBT's of any compound including SiGe, AlGaAs, InGaAsP and InGaN/AlGaN.
5. High electron mobility transistors (HEMT's) and GaAs MESFET's.
6. Light emitting diodes (LED's)
7. Resonant tunneling diodes (RTD's).
8. Traveling wave semiconductor optical amplifiers (SOA's).

Physical Models and Advanced Features

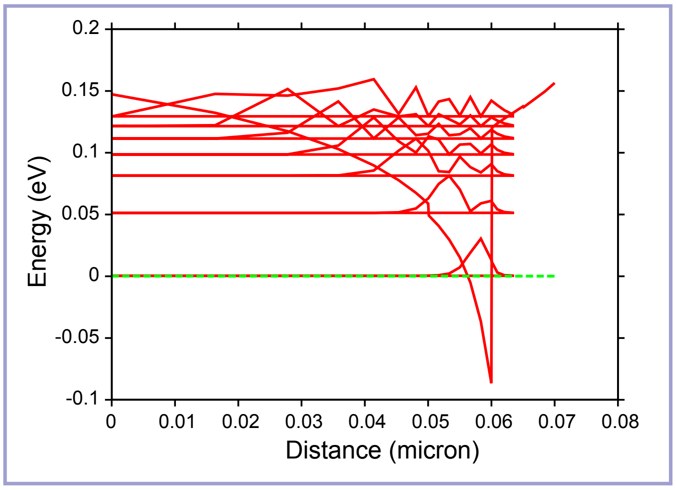
APSYS is a full 2D/3D simulator which solves, self-consistently, the Poisson's equation, the current continuity equations, the carrier energy transport equations (hydrodynamic model), quantum mechanical wave equation, and the scalar wave equation for photonic waveguiding devices (such as waveguide photo-detectors). APSYS includes the following physical models and advanced features:

1. Hydrodynamic models for hot carriers with either field or energy dependent mobility.
2. Heat transfer equations with flexible thermal boundary conditions and arbitrary temperature dependent parameters.
3. Thermionic emission model for carrier transport across a graded or abrupt heterojunction, or a quantum well.
4. Impact ionization model with either field or energy dependent impact ionization coefficients.
5. Deep level trap and trap dynamic models are implemented to allow for the accurate model of semi-insulating and insulating materials.
6. Interface states are modeled accurately to take into account the surface Fermi level pinning, interface recombination and interface fixed charges.
7. Frenkel-Poole model of field induced impurity ionization is implemented for some new compound materials.
8. Low-temperature simulation can be performed down to 77K and below.
9. Guided optical modes (multimode model) may be solved for arbitrary complex refractive index distribution.
10. Quantum well subbands are solved using a k.p theory for strained or unstrained well/barrier.
11. A large number of material models have been implemented. These include Silicon, AlGaAs, InGaAs, SiGe, InGaAsP, InGaN, AlGaN, ZnSe, InGaAlAs, InGaAlP and many others new compound materials still being investigated.
12. Flexible format for material parameter input enables the user to create his/her own material models using standard syntax of Fortran and C.
13. Finite element method (FEM) is used to treat arbitrary device geometry.
14. A cylindrical coordinate system may be used to model devices with cylindrical symmetry.

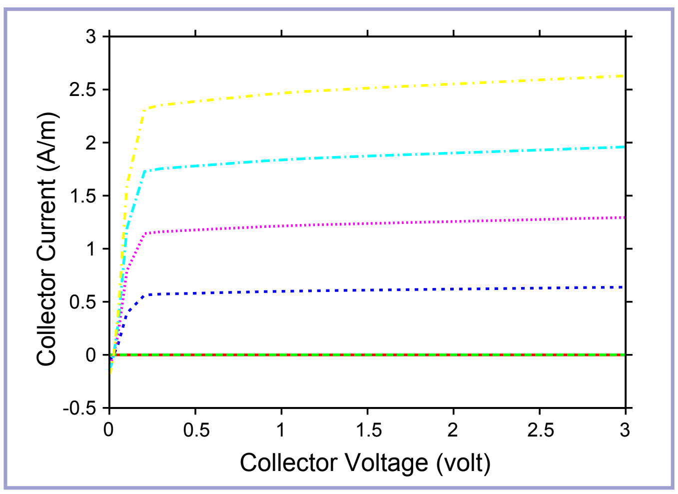
Many other advanced features and options as described in the Chapter **Modules and Options** in this brochure.



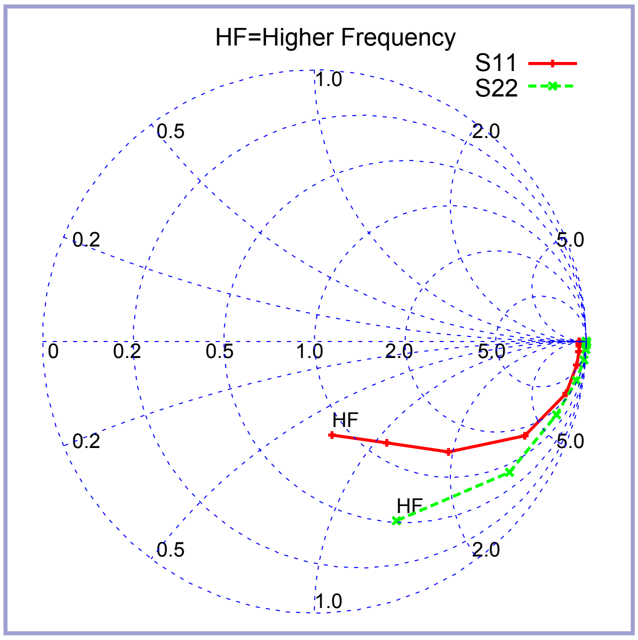
2D distribution of electron energy from the hydrodynamic model of APSYS in an N-MOSFET. The peak of the energy is located near the drain.



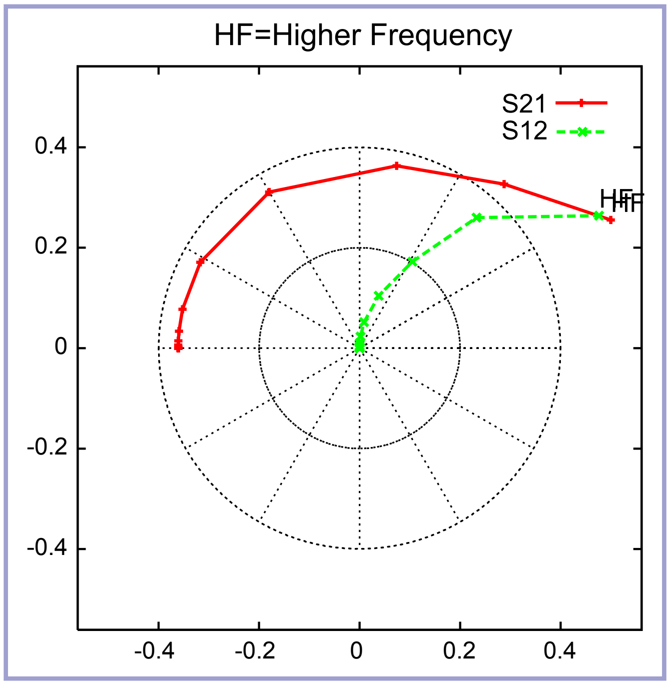
Electron wave function in the 2D gas system of a GaN-based high electron mobility transistor (HEMT).



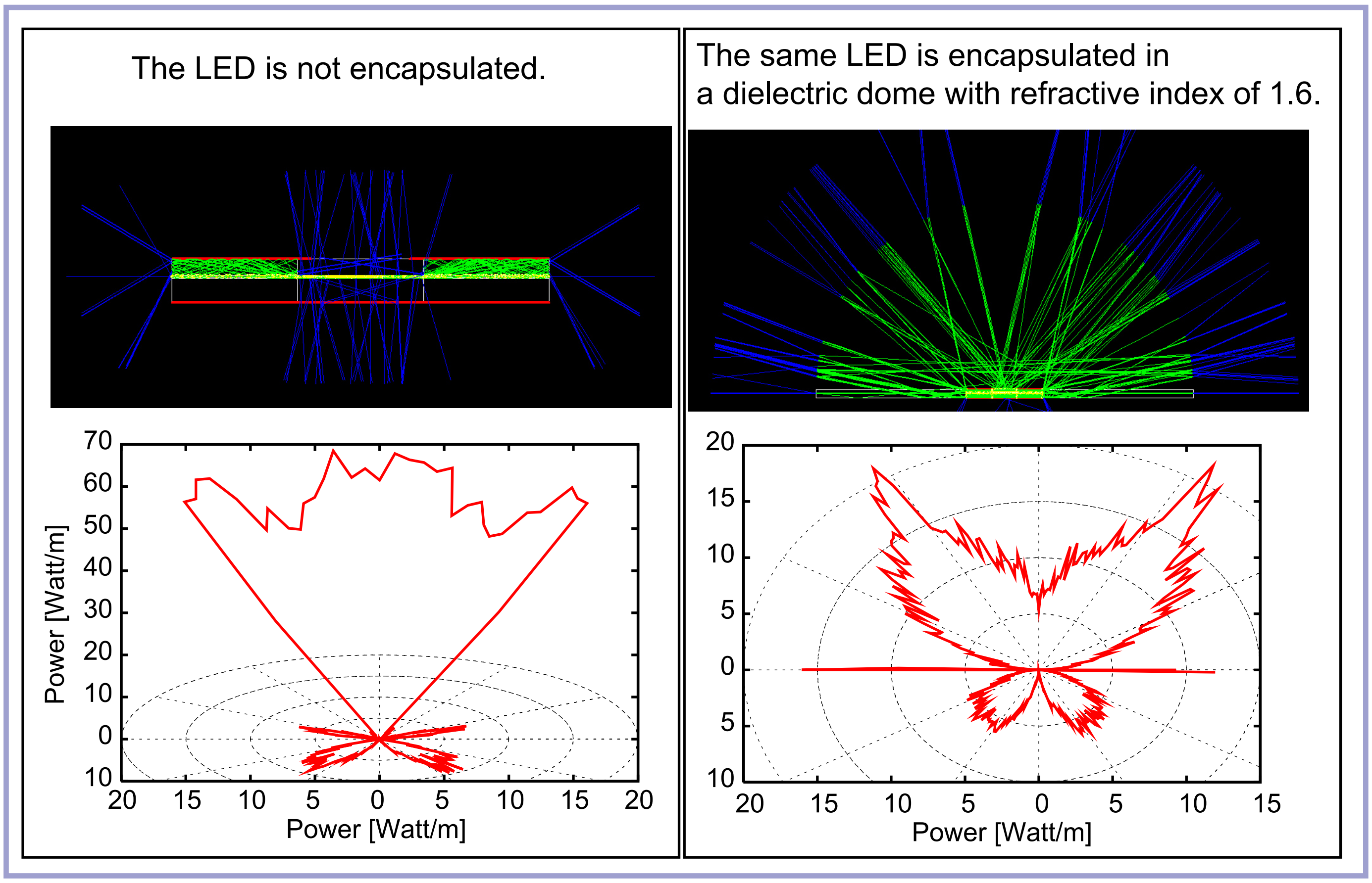
Curves of the Ic-Vc characteristics of a bipolar junction transistor (BJT) can be conveniently produced by APSYS at different base current levels.



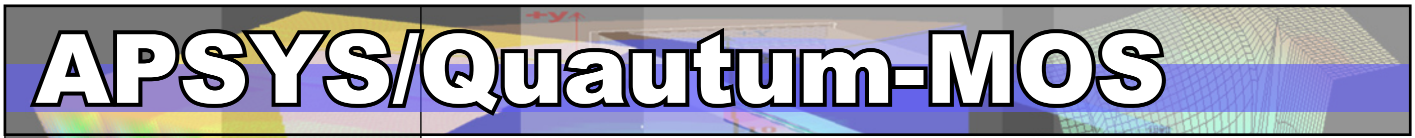
Simulated high frequency parameters S11 and S22 from AC analysis can be plotted on Smith chart or on linear plots.

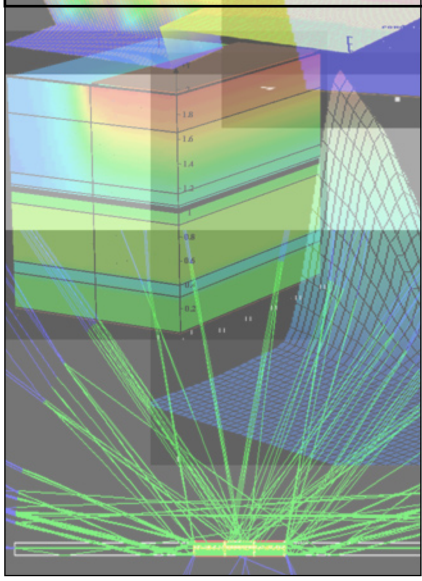


Simulated high frequency parameters S21 and S12 from AC analysis can be displayed on polar or linear plots.



Use of ray-tracing technique to study the light extraction from an LED with and without an encapsulated dielectric dome.





What is APSYS/Quantum-MOS

APSYS is a new generation semiconductor device simulator from Crosslight Software Inc. (www.crosslight.com). It is a general-purpose 2/3D finite element analysis program with numerous advanced features such as physical models for quantum wells and quantum tunneling. It has been successfully applied to novel optoelectronic compound semiconductor devices such as GaN-based blue light emitting diodes (LED's).

APSYS/Quantum-MOS is a special edition of the APSYS simulator with small scale (around 0.1 micron) silicon MOS device application in mind. It combines several advanced options of APSYS together to provide an accurate model of the quantum effects associated with submicron MOS silicon devices with ultra-thin gate oxide. The options include quantum-MOS, self-consistent, complex MQW, and quantum tunneling. The combination is intended to offer a package deal with value and affordability for a specialized application of APSYS.

Quantum Drift-Diffusion Model For Silicon

It has been well known that when MOS device is scaled down and oxide thickness is reduced, carriers in the conducting channel may tunnel through the oxide to become gate leakage current. To make things more complicated, the tunneling carriers are initially confined in a quantum well formed between the oxide and the silicon channel.

To provide a realistic physical model, APSYS/Quantum-MOS divides the MOS device into a classical region and a quantum one with the latter being a narrow region under the gate oxide.

In the quantum region, 2D quantum well density of states prevails whereas in the classical region, conventional bulk carrier statistics applies.

Quantum mechanical wave equations are solved for the confined states taking into account the effect of valley splitting for the conduction band within the quantum inversion layer. At the current version, inversion layer in the planes of 100, 110 and 111 have been demonstrated. Valley degeneracies arising from the six-valleys have been taken into account. For confined hole states, separate heavy hole (HH) and light hole (LH) subbands are considered.

The simulation engine of APSYS-QMOS combines quantum mechanical model with the drift-diffusion equation solver (the quantum drift-diffusion model) to provide both accuracy and efficiency needed for design and analysis of small scale silicon devices.

The oxide is no longer treated as a pure insulator. It is treated as a semiconductor with a huge bandgap over 7.5 eV. The quantum particles described by wave functions penetrate into the oxide and escape into the gate via thermionic emission.

The MOS can be cut up into multiple segments along the conduction channel, each of which is treated by a 1D quantum well model. This way the potential variation along the channel is fully taken into account.

In addition to providing an accurate quantum mechanical picture, APSYS/Quantum-MOS offers all features and capabilities available in a commercial silicon device simulator and more. The following is a partial listing.

- Hot carrier effects using a hydrodynamic model.
- Heat transfer model.
- Quantum transport model for graded and abrupt heterojunctions including thermionic emission,
- quantum capture, intraband and interband quantum tunneling.
- Impact ionization model applicable for both silicon and compound semiconductors.
- Deep level trap and trap dynamic models. Photo-excited
- deep trap model is also included.
- Low-temperature simulation down to 77K and below.
- Guided optical modes for optoelectronic applications.
- k.p theory for quantum well subbands of compound semiconductors.
- A large number of material models including silicon, strained-silicon, AlGaAs, SiGe, InGaAsP, GaN-based wurtzite material and others new compound materials.
- Flexible input format for material/physical parameters to enable user-defined models with syntax of C and Fortran.

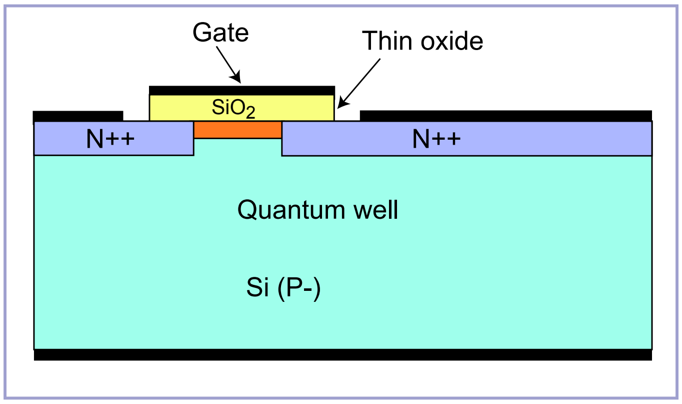
Modeling Mobility Enhancement in Strained Silicon

When silicon is strained, fundamental changes occur in the band structure: conduction and valence band valleys split and effective masses changes as a function of strain. The situation is more complicated when carriers are confined in a strained silicon quantum well and one needs a comprehensive model like APSYS-QMOS to fully describe the behavior of conduction carriers.

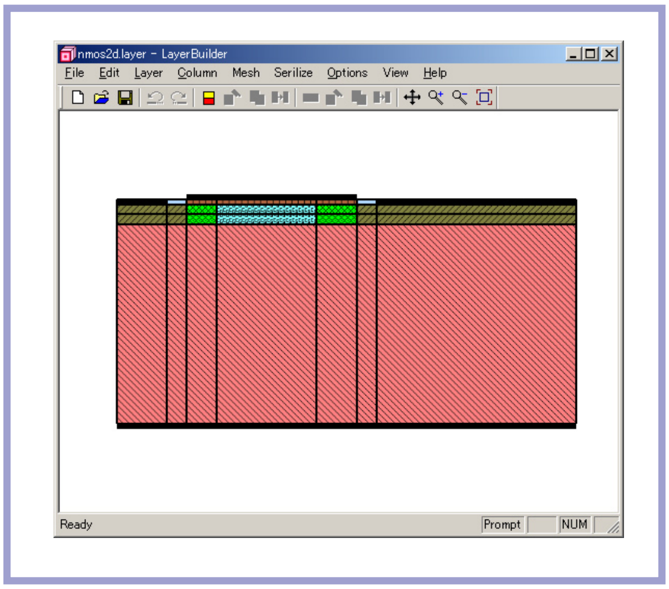
APSYS-QMOS has an extremely flexible and powerful material model for strained silicon and SiGe structures. The material macro language system allows for a detailed description of splitting of the six conduction band and the two valence band valleys (LH and HH) as a result of strain and/or quantum confinement.

Mobility enhancement in APSYS-QMOS is based on calculation of averaged conduction mass and inter-valley phonon scattering within the environment of quantum confined MOS conduction channel. Mobility enhancement comes from reduced conduction mass and decreased phonon scattering as a result of quantum confined valley splitting in both the conduction and the valence band. The basic effects are included in our quantum drift-diffusion simulator and runs like a regular silicon device simulator. Usually, such type of mobility enhancement model would be based on Monte-Carlo simulation and this would be highly inefficient.

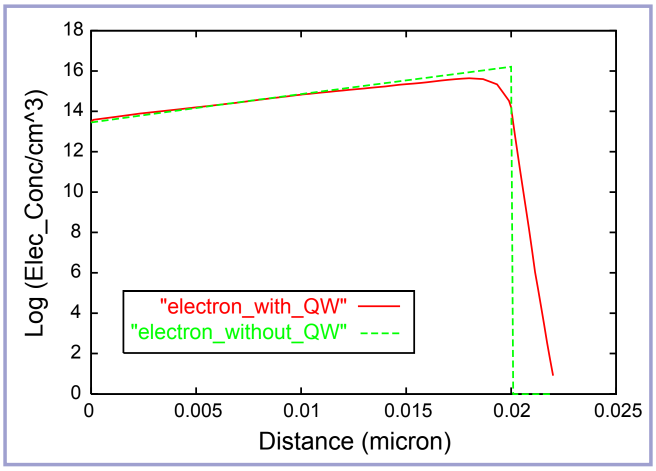
Simulated mobility enhancement effects for both electrons and holes agree reasonably well with experiment. Strained Si and SiGe channels under both biaxial and unaxial types of strain have been taken into account. Our flexible macro language provides a convenient platform on which various types of mobility enhancement mechanisms can be studied.



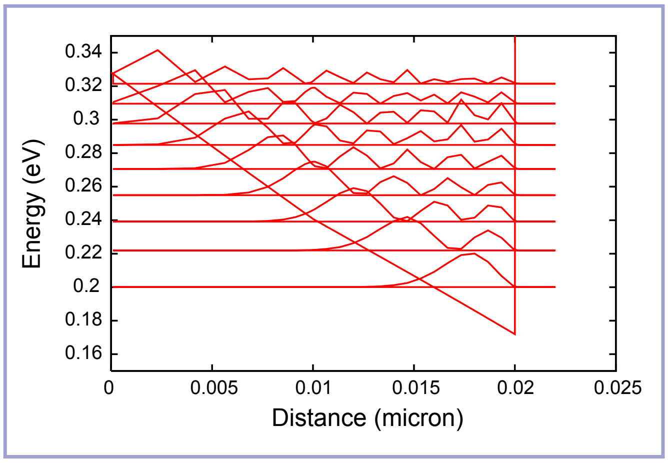
A simple n-channel MOS device with an oxide thickness of 2 nm.



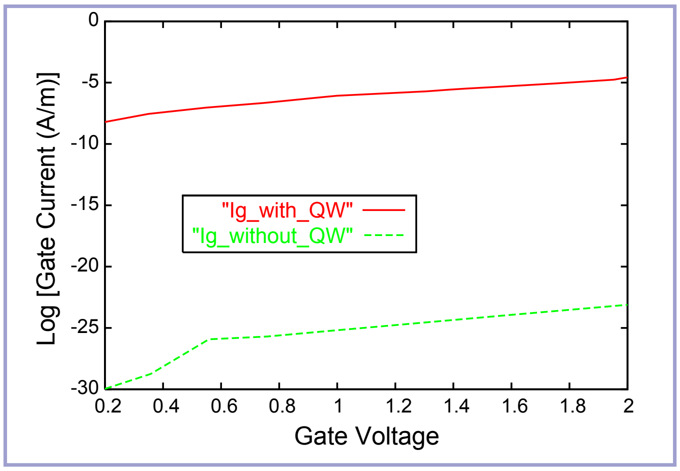
The n-channel MOS device as set up by the Crosslight GUI program LayerBuilder.



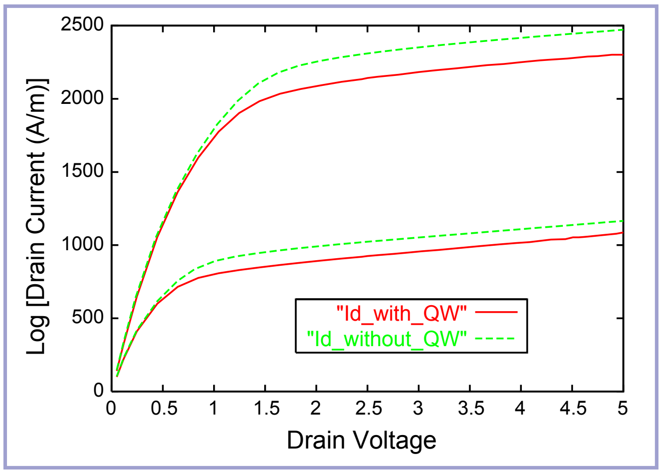
Electron distribution in a 1D cut under the gate with and without quantum effects.



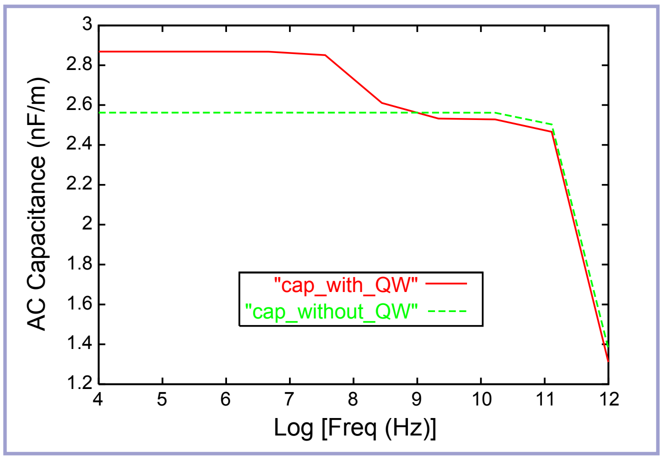
Confined electron subbands with corresponding wave functions under the gate oxide.



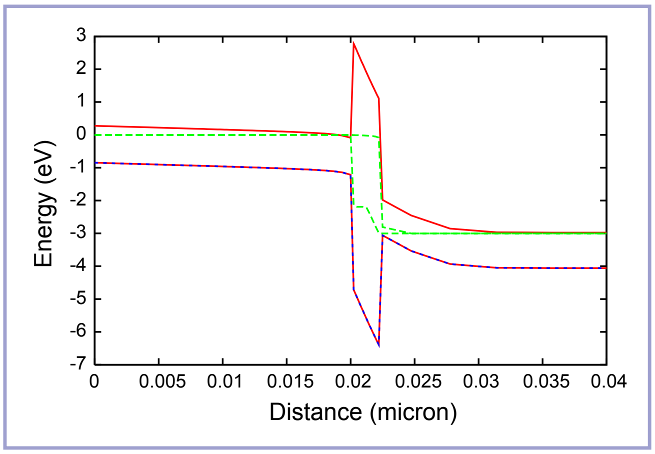
Gate leakage current with and without quantum effects.



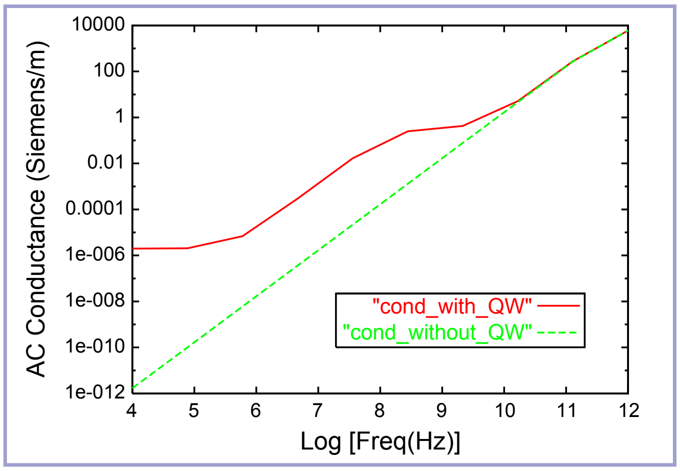
Drain currents with and without quantum well model. The reduced current with QW indicates less amount of conducting electrons in the channel for the same voltage bias when there is QW.



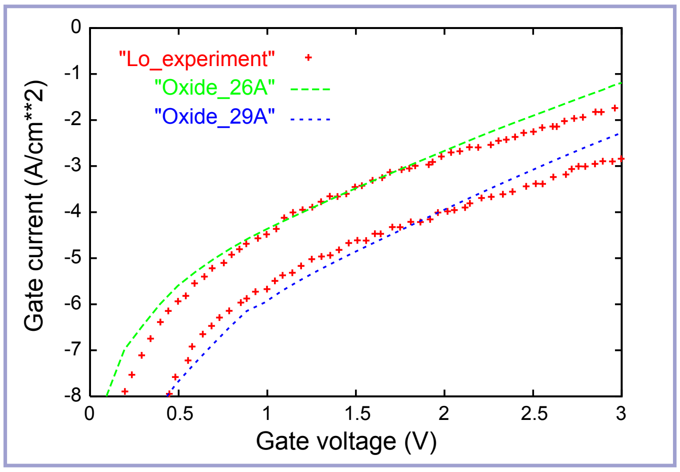
Comparison of the AC gate capacitance with and without quantum effects. The reason for a larger AC capacitance with QW



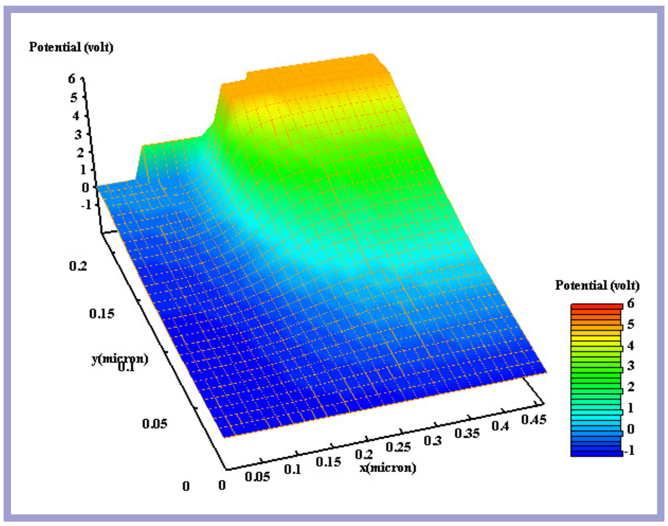
The quantum-MOS model can be used for polysilicon gate structure as well as metal gate. Here is the band diagram of the npoly-gate quantum MOS at a gate bias of 3 volts.



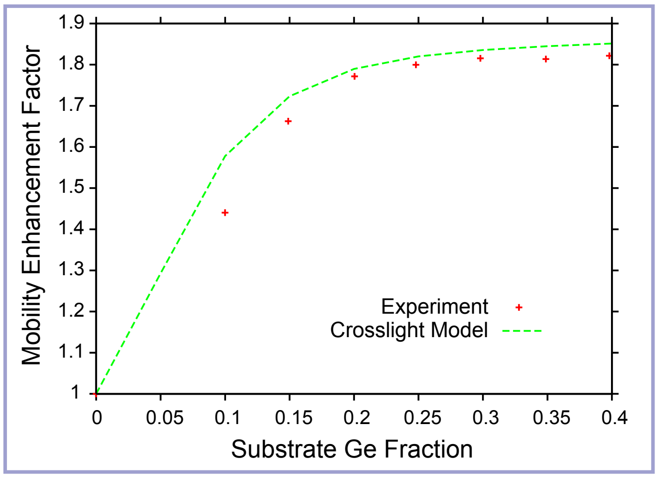
AC gate conductance with and without quantum well.



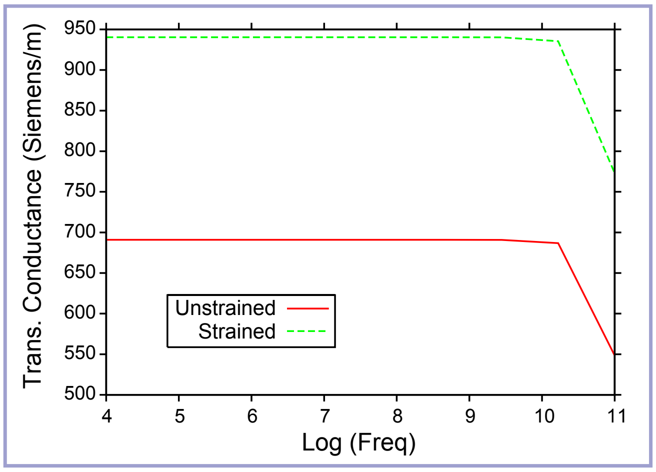
Comparison of simulated gate current with published measurement data.



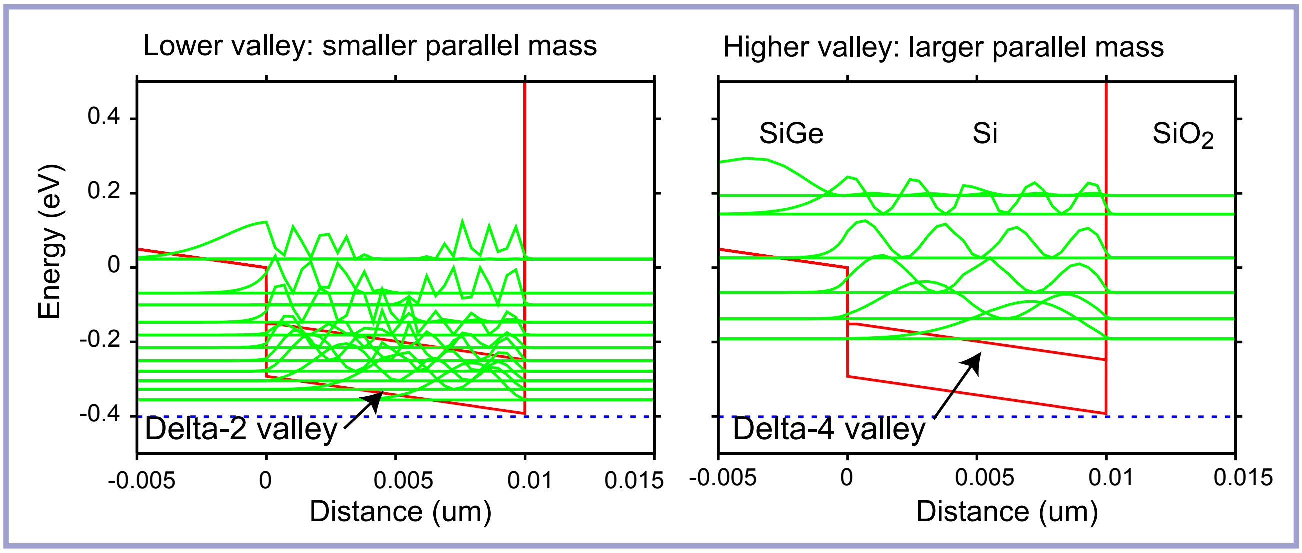
Distribution of potential in the MOS device as drawn by the Crosslight GUI program CrosslightView.



Electron mobility enhancement factor calculated from conduction mass averaged over confined subbands. Effects from reduced inter-valley phonon scattering has also been taken into account.



Simulated transconduction of a MOSFET with and without uniaxial strain along the conduction channel. Device gate length is 0.17 micron and gate bias is -1 volt. Gate oxide thickness is 20 A.



Quantum confined subbands and envelop wave functions for strained silicon grown on relaxed SiGe. The left hand side figure shows subbands for the lower Δ_2 valley of the conduction band and the right hand side shows those for the higher Δ_4 valley.

Simulator Modules and Options

Introduction to Simulator Modules

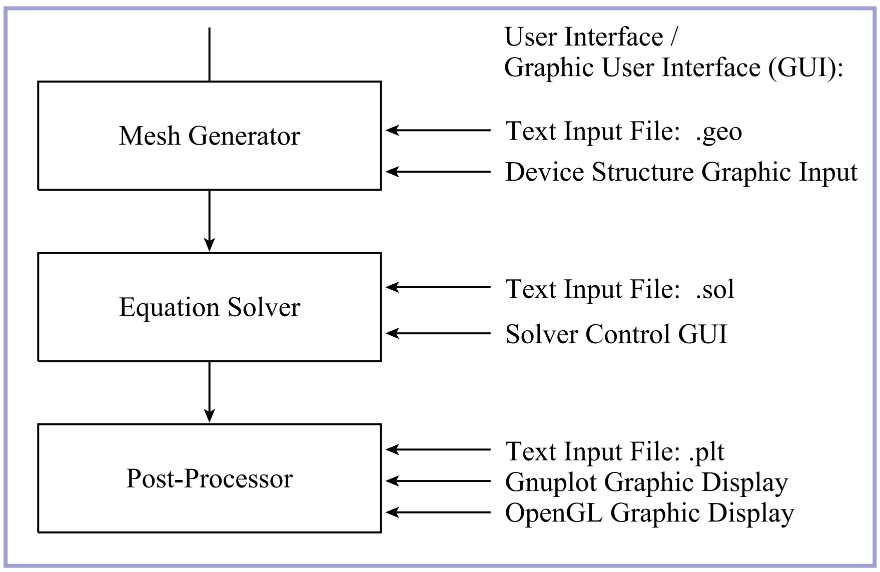
Each of the device simulation package (LASTIP, PICS3D or APSYS) from Crosslight consists of a basic package plus a number of options suitable for specific device applications. Additional price is charged for each option and potential users are advised to obtain free-consultation from Crosslight on what options are most suitable for their specific needs.

The basic design of our simulators is very simple. Each of the device simulation software package LASTIP, PICS3D or APSYS consists of the following modules:

a) Core Simulator: The simulation software uses 2D/3D finite element method (FEM) to solve the partial differential equations (PDE) appropriate for semiconductor lasers. The core software can be divided into three sub-modules: The pre-processor (or 2D/3D mesh generator), the main equation solver and the post-processor (or data plotting program). The core software uses text-based ASCII input files. The chargeable options are part of the core simulation module.

b) Setup Utility Programs: These include SetupLayer, SetupLastip, SetupPics3d and SetupApsys. They can be used to simplify the creation of ASCII input files to be used by the Core Simulator. These auxiliary programs are interactive and prompts the user to answer questions on text-based computer terminals. They will generate the ASCII input files acceptable to the core software. The Setup Utility Programs come with the basic packages.

c) Graphic User Interface: Graphic user interface (GUI) programs are available to create a more user-friendly environment for using the core software. These programs are developed for the Windows computer platforms. The GUI programs can also be divided into pre-processing and post-processing GUI programs, corresponding to the pre-processor and post-processor of the core software. All GUI programs come with the basic packages.

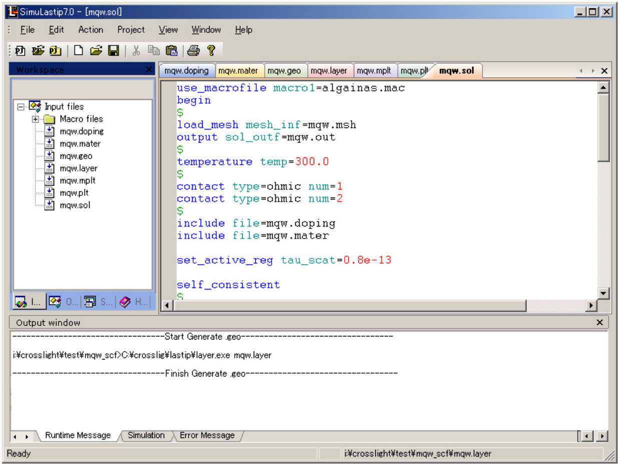


The general architecture of the core software

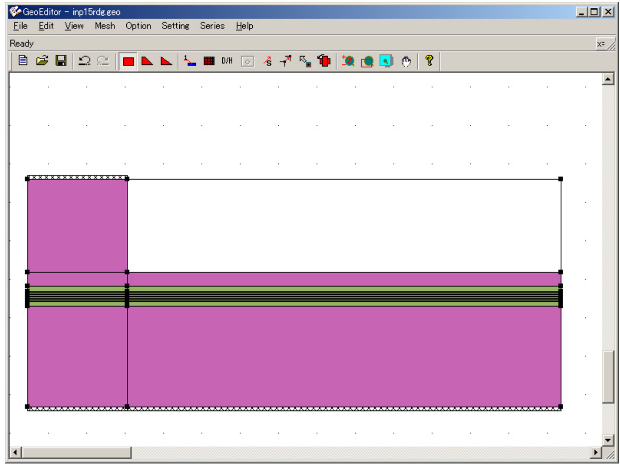
Graphic User Interface

All of our simulation software packages LASTIP, PICS3D and APSYS come the following graphic user interface (GUI) programs:

a) Simulation Centers: These GUI programs are named SimuLastip, SimuPics3d and SimuApsys (also referred to as SimuCenters). Each of the GUI program can be regarded as a control panel to activate various modules of the simulation software. For example, using the SimuLastip, you can activate the LayerBuilder program to set up the layer structure, use the setup utility program SetupLayer to set up a new simulation input file, run the main simulator and plot the results. All of these steps can be realized from menu buttons within the SimuLastip GUI program.

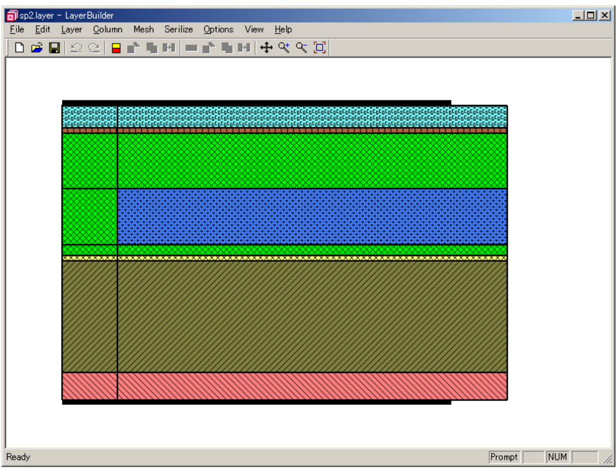


The SimuPics3d program is used as a general control panel to active various program modules of the PICS3D program.



The GeoEditor program can be used to draw devices with arbitrary geometry.

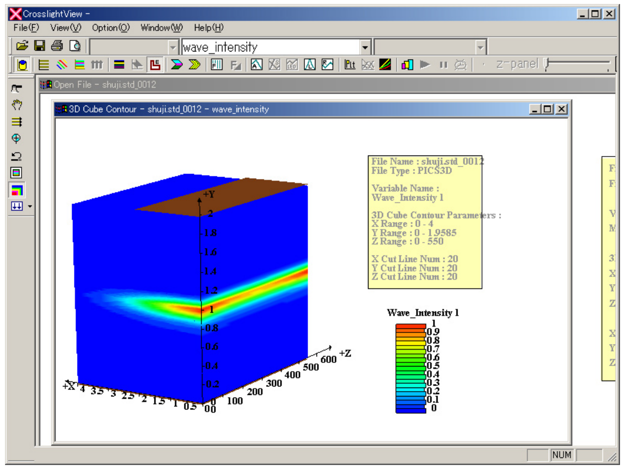
b) LayerBuilder: This GUI program can be used to build a layered device structure using visual means. Its output is compatible with the .layer input file format. It is most convenient for building devices with all material boundaries parallel to each other. The **Microsoft Excel** format input file can be imported or exported by this GUI program.



The LayerBuilder program is best suited for building devices with parallel layers. It is compatible with Microsoft Excel file format.

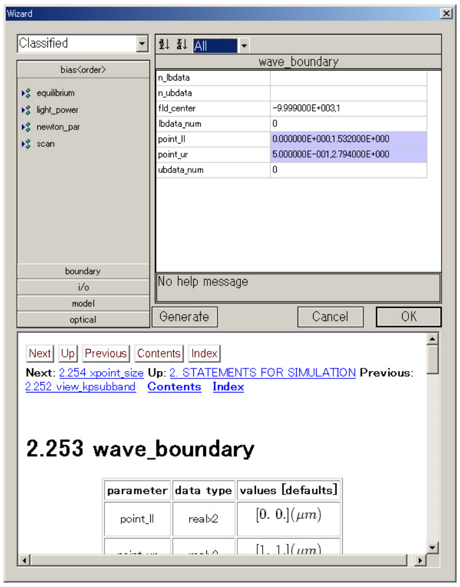
c) GeoEditor: A device drawing CAD tool that can be used to set up a device with arbitrary geometry. Its output is compatible with the .geo input file format.

d) CrosslightView: Based OpenGL or JavaGL, this GUI program can be used to view the simulation data in 3D color graphics and animation movies.



The CrosslightView program displays 3D simulation in color 3D graphics.

e) CrosslightEdit: is a customized smart editor designed for the user to edit any input files of the core simulator. The user can modify or create input commands by clicking on a list of valid parameters instead of using tedious typing. It also provides online helps explaining meanings of each parameter.



The CrosslightEdit program provides an efficient way to edit the input files. The online help function enables the user to get keyword definitions with just a simple click. This GUI has been integrated into the SimuCenter->Edit menu.

Device Specific Recommendations

It may be confusing for a beginner to decide which package (option) to use for a specific application because one package (option) may be used to simulate many devices and a single device may be simulated by more than one package (option). Since each application is different in device structure and purpose, it is difficult to give a complete list of recommended options. Recommendations can only be made on some common device design applications and a potential user is advised to go through the description of each option to decide if it is beneficial to use such an option. Here are some recommendations for common cases:

1. Edge emitting lasers of any kind, with well isolated symmetric quantum wells, when optimization of layer/material for the reduction of threshold and enhancement of efficiency is the main purpose, especially suitable for Fabry-Perot lasers: LASTIP basic package.
2. High power edge emitting FP lasers: LASTIP basic package with thermal option.
3. Edge lasers with strong longitudinal variation of physical variables including DBR, DFB and multiple section lasers: PICS3D basic package.
4. Quantum well electric-absorption modulator (EAM): PICS3D basic, photon-absorbing waveguide option and self-consistent MQW option.
5. Bulk electric-absorption modulator (EAM): PICS3D basic, photon-absorbing waveguide option and Franz-Keldysh model option.
6. Semiconductor optical amplifiers (SOA): PICS3D basic and 3D semiconductor optical amplifier option. Add BPM option if taper is involved. Add thermal option if high power is required. Add vectorial wave option if bulk SOA is used for polarization insensitive applications. For high speed impulse response study of SOA, APSYS basic with the 2D traveling wave SOA option may also be considered.
7. Waveguide photo-detectors (WPD): PICS3D basic and photon-absorbing waveguide option.
8. Optically pumped edge emission lasers: Optically pumped laser option with LASTIP basic or PICS3D basic, depending on if longitudinal variation is important.
9. Vertical cavity surface emitting lasers (VCSEL): PICS3D-VCSEL edition basic package. Add thermal option if thermal roll-off by self-heating is to be studied.
10. Optically pumped VCSEL's: Same as 9. above except with optically pumped laser option added.
11. External cavity lasers: PICS3D basic and fiber-grating/external cavity option.
12. Common silicon based devices including MOSFET's, bipolar transistors and JFET's: APSYS basic. Add 3D current flow option if full 3D simulation is desired. Add thermal option if self-heating is important.
13. Deep submicron MOS with thin gate oxide and FinFET's: APSYS Quantum-MOS edition. Add 3D current flow option if full 3D simulation is desired.
14. All types of Photodetectors (PD's) including MSM PD's, APD's and waveguide PD's: APSYS basic. Add waveguide model option for wavegide PD's. Add 3D current flow option if full 3D simulation is desired.
15. Solar cells: APSYS basic. Add 3D current flow option if full 3D simulation is desired.

16. HBT's of any compound including SiGe, AlGaAs, InGaAsP and InGaN/AlGaN: APSYS basic with quantum tunneling option. Add 3D current flow option if full 3D simulation is desired.
17. High electron mobility transistors (HEMT's): APSYS basic with complex-MQW, self-consistent MQW and quantum tunneling options. Add 3D current flow option if full 3D simulation is desired.
18. Light emitting diodes (LED's) APSYS basic with LED and ray-tracing options. Add self-consistent MQW options if InGaN/AlGaN (wurtzite) based material systems are involved. Add 3D current flow option if full 3D simulation is desired. Add thermal option is self-heating is important.

Thermal Option

Introduction

Crosslight Software is proud to offer a state of the art thermal (or heat transfer) modeling option for all of our base simulators (LASTIP, PICS3D and APSYS). It is well known that the heating effect is very important for semiconductor lasers in almost all applications. The heat generated by a semiconductor laser often forces the designer to include an additional cooling systems, thereby increasing the cost of the application. The heating effect is more important for high power semiconductor lasers where the device temperature determines the maximum power.

In the basic version of our simulators, thermal effects were included as a simple temperature dependent model. The lattice temperature of the device was assumed to be uniform and was set by the user. This simple model is useful for the evaluation of temperature sensitivity of the laser. However, in a realistic application environment, the temperature distribution within a device is unknown *a priori*. The temperature is determined by the optical power, the current flow and also by the thermal environment.

From the point of view of simulation and modeling, the concern is two-fold. First, we must determine the temperature distribution from all possible heat sources. This involves a much larger simulation area than the small region near the p-n junction. We must consider how the heating power flows though the whole substrate as well as from any wire bonds. Secondly, we must consider how the heating affects the laser performance. This means we must accurately evaluate the degradation of power, efficiency, *etc.*, due to the non-uniform temperature distribution. This is not a trivial task because virtually all variables and material parameters are temperature dependent. The thermal option provides a thermal modeling environment so that all possible temperature dependencies can be taken into account.

The theoretical basis of our thermal model is well established and can be found in Refs. [1], [2], [3] and [4]. The model involves solving the following heat flow equation:

$$C_p \rho \frac{\partial T}{\partial t} = \nabla \cdot \kappa \nabla T + H$$

where Cp is the specific heat and ρ is the density of the material. κ is the thermal conductivity and H is the heat source. For semiconductor lasers, it is crucial that we include all heat sources accurately. We have included the following the heat sources:

1. Joule heating due to the bias current.
2. Joule heating due to optical absorption. This is associated with intraband absorption or the internal loss. This is a major heat source in lossy material or in high power lasers.
3. Recombination heat. When an electron-hole pair recombines, heat is released for most recombination processes.
4. Thomson heat caused by the change in thermoelectric power when an electron-hole pair recombines.
5. Peltier heat due to the spatial gradient of the thermoelectric power in a semiconductor material.
6. Radiation heat source associated with exchange of photon energies with the device.

A spatial gradient in the temperature also causes a thermal diffusion current of the form $-q\mu_n n P_n \nabla T$ and $-q\mu_p p P_p \nabla T$ for electron and hole currents, respectively, where P_n and P_p are the thermoelectric powers.

Flexible thermal boundaries

We have implemented very flexible boundary conditions to handle many thermal environments. Three types of thermal contacts are included:

1. Fixed temperature at a contact. This may be used to simulate a semiconductor attached to a heat sink.
2. Controlled heat flow out of a contact. This may be useful if we know the cooling power of a contact.
3. A thermal contact attached to thermal conductor, which is then connected to a heat sink. This may be used to simplify a simulation area by a thermal conductor. Self-heating due to Joule effect is included for the thermal conductor.

Using type 3) contact above, it is also possible to divide the device into an electrical-thermal area and a purely thermal area on the outside. The outer thermal area may be solved using an auxiliary thermal program so that completely different mesh system can be used. The finer mesh inside the electrical-thermal area does not propagate to the purely thermal area outside. Use of this auxiliary program can speed up the simulation when a device is attached to a larger thermal environment.

User-defined temperature dependent parameters

The material macro facility in our simulators allows the user to define all material parameters as temperature dependent according to the formulas provided by the users. These user-defined parameters are updated (or re-calculated) every time a new temperature distribution is found by the thermal model. For example, the user may define the temperature dependence of the bandgap as follows:

```
function(y,temper)
shift=-4.1E-4*temper**2 /(temper+136)+8.46E-2;
1.347 - 0.778*y + 0.149*y**2+shift
end_function
```

The syntax follows that of C/FORTRAN.

Option currently available for product: LASTIP, PICS3D, APSYS.

[1] G.K. Wachutka, “Rigorous thermodynamic treatment of heat generation and conduction in semiconductor modeling", IEEE Trans., vol CAD-9, pp. 1141-1149, 1990.

[2] A. Marshak and K. van Vilet, “Electrical current in solids with position dependent band structure", Solid State Electron., vol. 21, pp. 417-427, 1978.

[3] L. Liou, J. Ebel, and C Huang, “Thermal effects on the characteristics of AlGaAs/GaAs heterojunction bipolar transistors using two dimensional numerical simulation", *IEEE Trans.*, vol. ED-40, pp. 35-43, 1993.

[4] R. Stratton, “Semiconductor current flow equations (diffusion and degeneracy)", *IEEE Trans.*, vol. ED-19, pp. 1288-1292, 1972.

Quantum Tunneling Option

In highly doped heterojunction or Schottky contacts, an important current transport mechanism is the quantum tunneling effect. The quantum barriers are so thin that a significant amount of tunneling current goes through the barriers. It is also the key transport mechanism in realistic Ohmic contact which is essentially a highly doped Schottky contact [1]. The tunneling effect is also the key transport mechanism in devices such as resonant tunneling diodes (RTD's).

The standard modeling tools for commonly used semiconductor devices has been the Drift-Diffusion (DD) model which is implemented as the core module in Crosslight Software simulators. The DD model accounts for most of the mechanisms of how a semiconductor device works (pn-diodes, transistors, LDs). However, finite element analysis based on the DD model has drawbacks in treating the quantum tunneling effects. The reason is that the DD model must assume that the carriers are localized like a particle whereas tunneling model requires the carriers be treated like a propagating wave.

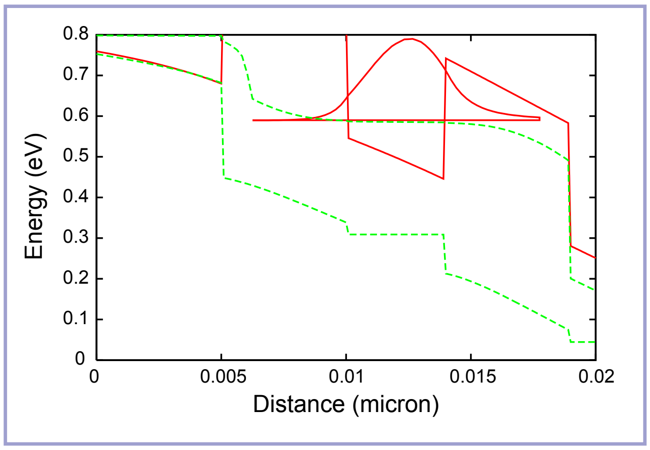
Our simulators have successfully combined the wave and particles natures together to offer a realistic tunneling transport model. The numerical approach in the region of tunneling is based formulas of Grinberg and others [2].

For heavily doped reverse biased junction, the interband tunneling model (also known as Zener breakdown effect) based on first principle quantum physics is also implemented. Many new devices designs depends on tunneling junctions and this option will be helpful.

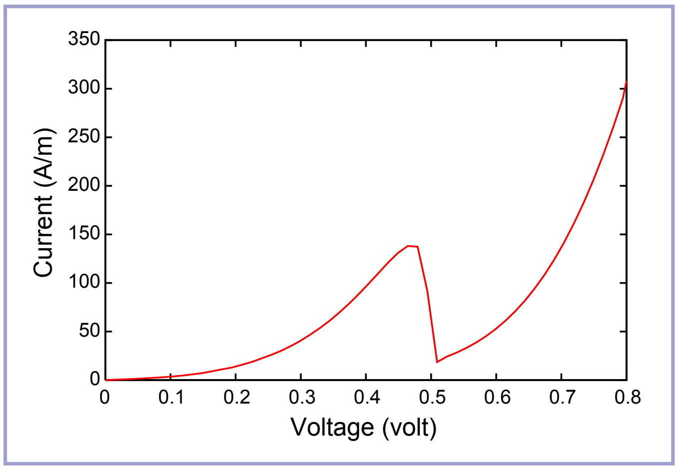
Option currently available for products: LASTIP, PICS3D, APSYS.

[1] S. M. Sze, "Physics of semiconductor devices'', 2nd ed. John Wiley & Sons (1981).

[2] A.A. Grinberg, M.S. Shur, R.J. Fischer, and H. Morkoc, "An investigation of the effect of graded layers and tunneling on the performance of AlGaAs/GaAs heterojunction bipolar transistors," IEEE Trans. Electron Device, vol. ED-31, pp. 1758-1765, 1984.



Band diagram of a simple double barrier resonant tunneling diode simulated by APSYS. The wave function and quantum level are also indicated. (Tunneling option).



Simulated I-V characteristics for a double barrier RTD.

Complex MQW Option

In the basic package of our simulator, we treat MQW system assuming the wells are uncoupled and both the left and right barriers are equal. This treatment is sufficient for most device designs. To go beyond the basic quantum well structure, we need the complex MQW option.

There are circumstances in which we need to go beyond the single square quantum well model. In some device design, we may need to consider quantum levels in the barrier region if the well is within another larger well. We may also need to treat a case where the well has uneven barriers. When MQW's are close enough to each other, we must consider the interaction of MQW's.

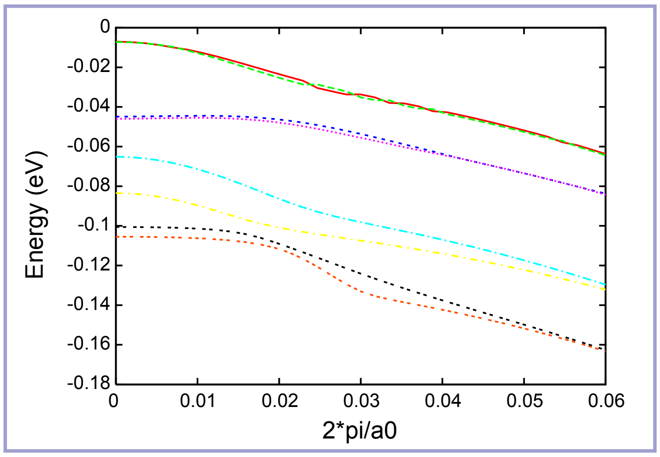
The complex MQW option enables us to treat quantum wells with uneven barriers and/or quantum wells coupling to each through thin barriers. In the complex MQW option, we must resolve a number of issues relating to the wave nature of quantum mechanics. Consider the simple case of two wells. As the two wells are brought closer together, the degenerate subbands start to split. From the viewpoint of wave mechanics, the wave function of each energy level belongs to both wells. However, drift-diffusion theory (classical theory) requires that we must know where the carriers are located.

Therefore, we face the task of deciding for each coupled confined state, which well the carrier belongs. Similarly, for optical interband transition, the process takes place in the whole coupled complex structure. But again, we must decide for each transition, which well it takes place.

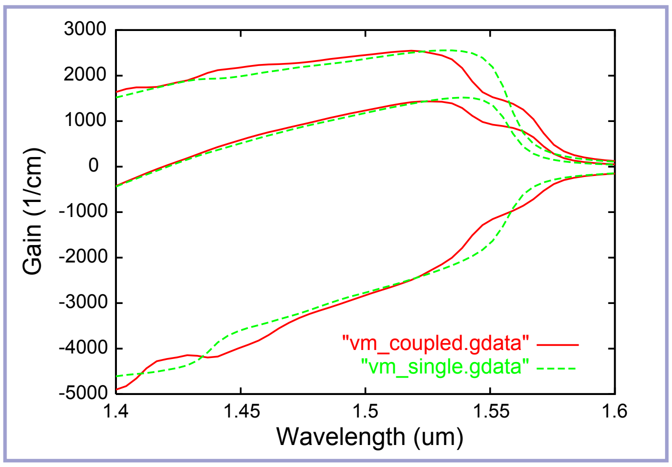
The situation is like quantum tunneling where we have a contradiction: the wave nature in a quantum theory versus the particle nature in drift-diffusion theory. We must create a reasonable method to bridge the gap.

In the complex MQW option, we again use the semi-classical approach to combine the wave nature in quantum mechanics with the particle nature in drift-diffusion theory.

Option currently available for product: LASTIP, PICS3D, APSYS.



Subbands of coupled QW showing the splitting of subband energies due to interaction between quantum wells. (**complex-MQW option**).



Comparison of optical gain spectrum from single and coupled quantum wells. (**complex-MQW option**).

Self-Consistent MQW Option

The standard model of MQW laser diodes is that of a flat band model, i.e., the electrical field assume to be negligible. For forward biased junctions, such as in laser diodes under lasing condition, this is a good approximation since band is almost flat. In the following cases however, the electrical field effect is not negligible:

1) In GaN-based MQW system, the piezo-electrical surface charge causes a large internal electrical field that tilted the quantum wells strongly to one side. This not only affect the carrier confinement but also affect the interband optical transition energy and momentum.
2) In electro-absorption modulators (EAM's), the applied electrical field is the key operating modulation force.
3) In HEMT's, the 2D electron gas is confined by the electrical field caused by the one-sided barrier of a heterojunction.

When the electrical field interacts with confined carriers, a rigorous self-consistent approach must be adopted.

The **Self-Consistent MQW** option enables the quantum mechanical wave equation to be solved together with the classical drift-diffusion equations in a self-consistent manner in order to provide an accurate description of the device.

Applicable package(s): LASTIP, APSYS, PICS3D.

VCSEL Option

VCSEL model is different from that of conventional edge emitting lasers with the following different theoretical treatments. 1) A cylindrical coordinate system is set up to treat the drift-diffusion (DD) problem in a 3D simulation. 2) A cylindrical coordinate system is also set up to treat the heat transfer equations. 3) The solution of the lateral optical modes on the reduced 2D plane (xy or rz_r-plane) is different because the direction of wave propagation is also on the reduced 2D plane. 4) A multiple longitudinal mode model is solved on the same reduced 2D plane.

We have successfully implemented the cylindrical coordinate system in our VCSEL model. The strained MQW structures are modeled using a k.p theory to solve for the quantum well subband structures and for the optical gain spectrum. The gain spectrum is computed at every bias points to ensure self-consistency.

For simplicity, we decouple the longitudinal and lateral mode models at the present stage of our model. Since the DBR mirrors of the VCSEL region consist of relatively smaller number of grating layers, we use the 2x2 matrix method commonly used in multiple layer optics. We use a transfer matrix technique (following [1]) to computer the frequency dependent round trip gain of the VCSEL cavity. Once the round trip gain is computed, we search for its roots on the complex frequency plane which correspond to the longitudinal modes [2]. The complex frequencies can be used in Green's function method to compute the optical power spectrum and longitudinal photon distribution [2].

For the solution of lateral modes, we have implemented two types of numerical models. The first is the fiber-like effective index method (fiber-like EIM), in which we assume that the wave distribution in the VCSEL is such that the top cylinder determines the optical confinement in the lateral direction and the lower cylinder only contributes an effective index change in the lateral cladding region. Then we are able to treat the optical modes just like in an optical fiber.

In the second method, a more complex effective index method [3] has been implemented. This is suitable for VCSEL's with oxide aperture confinement.

Option currently available for product: PICS3D. This option has also been incorporated into PICS3D as a special VCSEL-only PICS3D edition referred to as the PICS3D-VCSEL edition. The purpose of this special edition is to enable VCSEL-only users to avoid paying the regular PICS3D-basic for edge lasers.

[1] T. Makino, IEEE J. Quantum Electron., vol. 29, No. 1 (1992).

[2] C. H. Henry, J. Lightwave Technol., vol. LT-4, 288-297, March 1986.

[3] G. R. Hadley, et. al., IEEE J. Quantum Electron., vol., 32, No. 4, pp. 607-616,1996.

Vectorial Wave Option

The basic versions of our laser diode simulator solve the scalar wave equation for the transverse/lateral optical modes. This is sufficient for most applications since the dimensions of the laser are usually large relative to the wavelength and the index confinement is not too strong. The need for vectorial wave solver arises in some cases where index confinement is strong in the direction of polarization. The vectorial wave option deals with such a situation.

We follow the vectorial formulation of Stern as in the following reference.

M. Stern, "Finite difference analysis of planar optical waveguides", Chapter in Progress In Electromagnetics Research, PIER 10, pp.123-186, Editor W.P. Huang, EMW Publishing, 1995.

Option currently available for product: LASTIP, PICS3D, APSYS.

PML/EEIM Option and Radiative Mode

Enhanced Effective Index Method

In the standard effective index method (EIM), all boundaries are assumed to be zero or decaying exponentially. As a result, radiative modes are excluded. Our simulators offer an extension of the EIM that allows us to treat radiative modes as well as confined modes. We shall refer to this extension as the enhanced effective index method (EEIM).

We follow the solution approach of Ref. of

G. R. Hadley, D. Botez, and L. J. Mawst, "Modal discrimination in leaky-mode (antiguided) arrays", IEEE J. Quantum Electronics, vol. 27, No. 4, April 1991, pp. 921-930.

For an arbitrary device structure, we divide it into columns and rows. The confined modal basis in y-direction is solved using standard methods with confined boundary. The radiative solution in the x-direction is obtained by a propagation matrix method with confined y-modes as basis.

Perfectly Match Layer

The finite element (FEM) discretization of the wave equation results in an eigen value matrix problem of the order of the number of mesh points (for scalar equations). The matrix problem can easily be set up if the modes are well confined within a finite region and their intensities decay as a function of distance from the mode centers. We can obtain a well defined eigen matrix by deleting the nodes of the boundary assuming zero wave intensities there. The situation for leaky modes is more complicated for finite element analysis: there is no simple way to truncate the mesh to establish a well defined eigen matrix.

The idea of perfectly match layer (PML) is to create an artificial material medium layer to absorb the radiating wave without reflecting it back. Since the wave decays to zero intensity within the PML, we have converted the problem into one of confined modes if our mesh extends into the PML boundary.

We have implemented a model of anisotropic PML due to Sacks and others [Z. S. Sacks, D.M. Kingsland, R. Lee, and Jin-Fa Lee, ``A perfectly matched anisotropic absorber for use as an absorbing boundary condition," IEEE Trans. Antennas Propagat., vol.43, (no.12), IEEE, pp.1460-1463, Dec. 1995.] In the anisotropic PML model, the artificial PML has an complex anisotropic dielectric constant. If the complex anisotropic dielectric constant is chosen properly, the PML method should enable us to apply FEM to radiative mode solutions which are more accurate and powerful than EEIM.

Applicable package(s): LASTIP, APSYS, PICS3D.

Waveguide Model Option

Passive semiconductor devices such as waveguide photodetectors and electro-absorption modulators involve interaction of semiconductor with guided optical modes. The guided optical mode solver is already included in the LASTIP and PICS3D laser diode simulators as standard features since optical modes are an inherent part of the laser diode operation. The guided optical mode solver is an option for APSYS when it is necessary for dealing with interaction between electrical current and optical modes. This option includes the following mode solvers for guided optical modes on a finite element mesh:

1) SOR iterative mode solver efficient for single optical mode devices.
2) Effective index method suitable and efficient for multi-lateral mode devices with slow variation of index in the x-direction.
3) Arnoldi sparse eigen mode solver as a general purpose multi-mode solver on a finite element mesh.

All of the above solvers are designed to work with a complex refractive index distribution.

Applicable package(s): APSYS.

Full 3D Current Flow Option

Introducing the full 3D model

With all the simulation power and sophistication, Crosslight software packages are mostly written for a two-dimension cross section of a semiconductor device or a waveguide. We usually take a cross section where physical quantities vary the most. We created sophisticated techniques to vary the mesh density and grid boundaries to fit all types of device geometries.

In basic versions of our simulator such as PICS3D, the optical wave is allowed to interact in all three dimensions. However, current flow in z-direction is forbidden. The isolation of current flow allows us to decouple the drift-diffusion equation and save a substantial amount of computation time.

With increasing computing power and decreasing cost of modern computers (especially high end PC's), our next natural step is to lift the limitation for current flow and to create a full 3D model for drift-diffusion and energy transport equations.

The 3D current flow option (or 3D-flow option) adds a whole new dimension to device modeling as compared with conventional 2D simulators. The 3D flow option enables our users to extend their device modeling power well into the future.

Setup and solve a full 3D structure

For any 3D simulator to be practical, it must be easy to set up. In another word, it must be easy to describe or input the 3D device structure to the simulator. In a 2D environment, it is relatively straightforward to describe everything using a pair of coordinates (x,y). In 3D, the additional variation in z makes it difficult. For example, how do you describe a part of the device that has doping variation on x-y plane but also has boundary and doping variation along the z-direction?

In the 3D flow option, we input the geometry and material information based on a description of many 2D segments since we already know how to input the 2D structure. We also know how to create and refine the 2D mesh.

The basic idea for 3D mesh generation is to let the user (with the help of the simulator) generate and refine mesh for each 2D segment while the 3D mesh connecting different 2D meshes are generated automatically. We have created a sophisticated algorithm to automatically generate prisms and tetrohedrons connecting the 2D planes. 3D heat flow may also be enabled if thermal option is activated.

Option currently available for product: APSYS and PICS3D.

3D Semiconductor Optical Amplifier Option

The simulation of a semiconductor optical amplifier (SOA) differs from that of a laser diode in the following.

1) The wavelength of the system is determined by external source instead of by the material and structure of the optical cavity.
2) The lack of reflection of light due to the AR coatings.
3) No need to consider spontaneous emission as far as light power is concerned. The stimulated recombination is critical and responsible for longitudinal spatial hole burning.

The set up of 3D amplifier option is very simple and can be run just like a laser diode. Therefore, all the sophisticated physical models we have been using in laser diode simulation (such as k.p theory for optical gain model) can be used for 3D amplifier without modifications.

Option currently available for product: PICS3D.

Light Emitting Diode Option

LED versus laser diodes

The modeling of a light emitting diode (LED) is significantly different from that of a laser diode for the following reasons.

1) LED operates well below lasing threshold while theories of lasers almost always assumes lasing condition; 2) Absence of simulated recombination in LED; 3) Continuous emission spectrum must be considered for LED while longitudinal modes of laser only requires a limited number of lasing wavelengths; 4) The randomness of spontaneous recombination in LED in contrast to the coherence of laser modes which affects the near and far-field models.

Theoretical basis

The problem of LED is as follows. Consider a piece of semiconductor of arbitrarily shape. The system can be regarded as an optical cavity containing spontaneous emission, which is considered random and continuous. The light may be reflected by the material boundaries and absorbed by the lossy material before emitted outside.

Such a problem was previous solved by Henry [1] using the Green's function method for laser diode and semiconductor optical amplifiers. We find that the same theories are also applicable for LED's and we have implemented it into the LED option. Since the Green's function approach is analytical, only simplified 1D light extraction model can be treated. For realistic 2/3D device simulation this option should be regarded as an entry level model to study the basics of LED such as internal efficiency and emission spectrum.

For more sophisticated models of light extraction from LED with full 2/3D effects, we recommend the ray-tracing option which is described separately in this document.

LED related capabilities

The following output capabilities of the LED option may be of particular interests to LED designers:

1) Emission spectrum in different directions.
2) Internal and external emission efficiencies in different directions.
3) Turn on/off (transient) characteristics.
4) Temperature dependence of above quantities.
5) Temperature distribution when used together with the thermal option.

Option currently available for product: APSYS.

[1] C. H. Henry, "Theory of spontaneous emission noise in open resonators and its application to lasers and optical amplifiers", J. Lightwave Technol., vol. LT-4, pp.~288--297, March 1986.

Organic Light Emitting Diode Option

Conduction and recombination in OLED

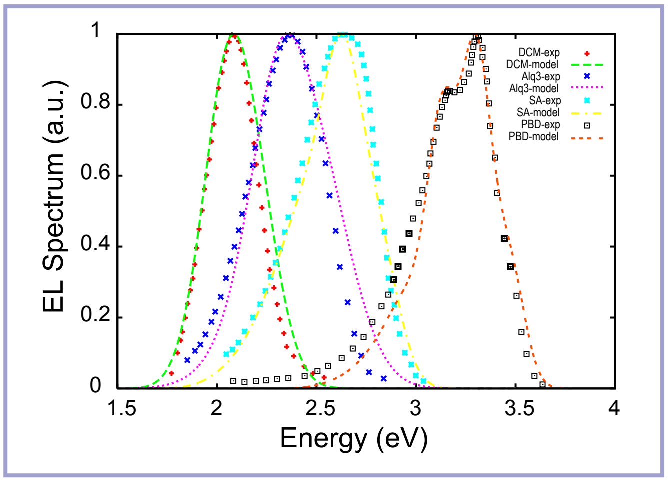
Carrier conduction and recombination mechanisms in organic semiconductor are different from those in conventional semiconductor. Carrier conduction and bi-molecular recombinations are usually described in the form of Poole-Frenkel-like model (see for example, B. Ryhstaller and S.A. Carter, S. Barth, H. Riel, and W. Riess, "Transient and steady-state behavior of space charges in multilayer organic light-emitting diodes," J. Appl. Phys., 15 April, 2001, Vol. 89, No. 8, pp. 4575-4586). The quantum drift-diffusion model in APSYS has been adapted to describe electron/hole behavior in an organic light emitting diode.

The advatage of using APSYS-OLED model is that all available features of quantum tunneling and quantum confinement effects can be used just like in a conventional quantum well semicondutor device.

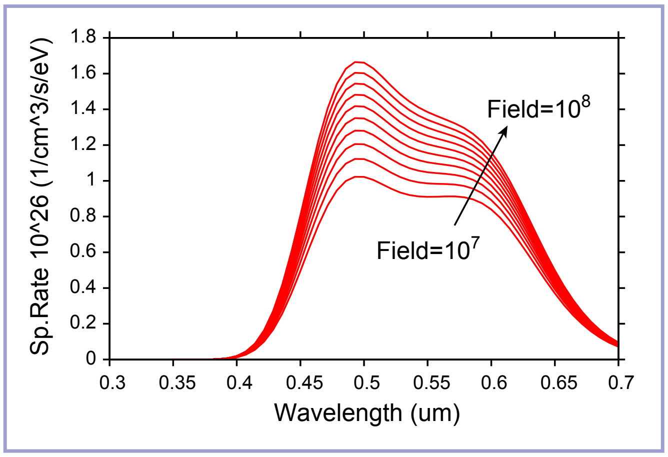
Electroluminescent and absorption spectra Model

Organic semiconductor emits light via Frenkel exciton recombination. Conventional semiconductor theories based on free-carrier/many-body interband transition are no longer valid. We have established an optical spectrum model based on a Hamiltonian including intra-molecular and inter-molecular electronic and vibronic interactions. A phonon cloud of several unit cells is used to represent exciton-phonon interaction. All excited states of the molecular crystal are solved and optical transition dipole moments computed between all states.

Our model is similar to that in Ref: Vragovic, R. Scholz and M. Schreiber, Europhysics Letters,vol. 57 (2), pp. 288-294, 2002.



Comparison of simulated EL spectra and experiment.



Simulated EL spectrum from DCM doped Alq3 organic material. Different external applied field is indicated.

Ray-Tracing Option

In the basic models of light emitting diode (LED), the emission direction is simplified in one of three orthogonal directions and any edge effects are neglected. This causes significant error when the shape of the LED is different from a broad-area device. For emission from arbitrary geometry of an LED, the ray-tracing option of APSYS may be used.

The ray-tracing option is treated as a post-processing step after the spontaneous recombination intensity distribution is determined by the APSYS simulator. Due to randomness of the spontaneous emission, we divide up the continuous spontaneous emission profile into discretized emission centers with each emission center radiating rays of geometric light. We trace these rays through their paths within and device until they are either completely absorbed or emitted to outside of the device.

In simple LED with dimensions larger than the wavelength, it is sufficient to consider the rays as purely geometric and non-interfering. For complex devices that use the interference effects such as LED with DBR stacks, we take into account the wave nature of the rays we are tracing. In such a case, we tackle issues such as light channeling and corner effect as exceptions to our wave treatment.

Photon recycling effect can be taken into account by importing the photon distribution generated during a previous ray-tracing analysis while generating new ray-tracing data for the next round of simulation. This process can be re-iterated to achieve self-consistency when photon-recycling effect is desired.

The ray-tracing option has been implemented for 2D and 3D applications.

Applicable package(s): APSYS.

Fiber-Grating/ External Cavity Option

Use of fiber-grating as part of the external cavity of a laser diode has gained popularity recently as a cost effective way of controlling and tuning the laser wavelength. However, a couple of outstanding issues are always associated with this type of laser: longitudinal mode hopping and coupling losses. This option allows the user to address issues related to external cavity lasers in general and fiber-grating lasers in particular.

The fiber-grating/external cavity option allows the user to define explicitly the air-gap and passive-fiber sections. Optical lateral modes in the fiber are computed as scalar fiber modes if a fiber is defined as part of the longitudinal structure. The grating of a fiber is specified by the coupling coefficient (kappa).

Applicable package: PICS3D.

2D Traveling Wave Optical Amplifiers

The traveling wave optical amplifier option offers the capability of simulating high speed (pico-second scale) semiconductor optical amplifiers (SOA) in a 2D cross section parallel to the direction of propagation.

Modeling of high speed SOA is not a trivial task even with our existing laser diode (LD) simulators for the following reasons.

1) A SOA with input signal of a pico-second pulse has a wave packet length substantially shorter than the device length. Therefore, the transient traveling wave effect must be taken into account while conventional laser simulators ignore the traveling wave effect.

2) The signal amplification process must be modeled on the x-z plane instead of on the x-y plane as for edge emitting lasers. This means much of the software for LD must be re-written.
3) Since the stimulated recombination associated with the gain or absorption processes determines the shape of the output pulse, we must treat the drift-diffusion equations and the traveling wave equation in a self-consistent manner. Numerically, this means solving the drift-diffusion equations and the wave equation using coupled method.

Using this option, we are able to quantitatively model the propagation process of the optical pulse being amplified. It can be used to study the effect of current injection on the profile and the speed of the optical pulses. It is also possible to shine a background light with a different wavelength than the input light. The background light can be used to control and modify the carrier/light interaction within the SOA.

Option currently available for product: APSYS.

Second Order Grating Option

When the grating period of a DFB laser is 1/2 of the emission wavelength, we have a first order grating structure. In such a structure, the forward wave only couples with the backward wave in 180 degrees.

A grating structure with a period equal to the wavelength is a second order grating. The forward wave experiences a first order diffraction in 90 degrees (which causes radiation loss) and a second order diffraction in 180 degrees (or the backward wave).

The second order grating option evaluates the coupling coefficients and uses a modified coupled wave equations for the longitudinal modes. Our theoretical basis comes from the following reference.

R.F. Kazarinov and C.H. Henry, "Second-order distributed feedback lasers with mode selection provided by first-order radiation losses,'' IEEE Journal of Quantum Electronics, vol. 21, No. 3, pp. 144-153, 1985.

Option currently available for product: PICS3D

Beam Propagation Method Option

In the basic version of our simulator, we assume that the optical field lateral profile can be solved in an x-y cross section after the wave equation variables are separated. This is a good approximation if the geometry of the optical waveguide does not vary in the longitudinal direction. If substantial variation is present, such as in the case of tapered waveguides, separation of variables is not possible.

When considering interaction of laser with other devices, it is important to know the phase profile of the emitted wave. BPM option can provide accurate phase profile unavailable using other methods.

In the current version of PICS3D, we have an option to use the 3D Fast Fourier Transform Beam Propagation Method (FFT-BPM). The problem is posed as follows: We start with a know solution

on one z-plane. For example, we can use the effective index method for the lateral profile on a plane, then we propagate the wave after Fourier transforming both the wave equation and the wave function into wave vector space. It is straight forward to advance the wave solution by a small distance after FFT. Then, we perform an inverse FFT to recover the wave in a new plane. The procedure can be repeated until we reach the end of the waveguide. The numerical methods are based on the following references.

[1] E. Yamashita, ``The beam propagation method,” in Analysis methods for electromagnetic wave problems, Boston, MA: Artech, pp.341-369 1990

[2] G.P. Agrawal, “Fast-fourier-transform based beam-propagation model for stripe-geometry semiconductor lasers:inclusion of axial effects." J. Appl. Phys., vol. 56, pp. 3100-3109, 1984.

[3] J.M. Burzler, S. Hughes, B.S. Wherrett, ``Split-step fourier methods applied to model nonlinear refractive effects in optically thick media.” Appl. Phys. B62, pp.389-397, 1996

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Applicable package: PICS3D

Optically Pumped Laser Option

In the option of optically pumped laser, the active region operates under two different wavelengths: the shorter wavelength for the pump and the longer wavelength for laser emission.

Our accurate optical gain spectrum model is evaluated at every mesh point of the active regions (or passive regions declared as "active") which respond to different optical wavelengths to treat them either as a pump or emitter. The refraction and absorption of the incident pump light passing through the device is processed as plane wave passing a multiple optical layer system. The simulator figures out the correct amount of carriers generated by the pump which in turn causes population inversion and lasing action.

It is also possible to apply this option to VCSEL's. The simulator accepts input pumping power in the form of single wavelength or of user-defined continuous spectrum.

Applicable package(s): PICS3D, LASTIP.

Manybody/Exciton Option

Coulomb interaction between electrons and holes confined in an active region of laser diodes can significantly enhance it's optical gain value and influence the emission spectrum. In particular, it has been reported that, Coulomb enhancement is stronger in short wavelength blue-green ZnCdSe and InGaN quantum well lasers compare to the long wavelength III-V lasers, due to the lower value of dielectric constant in wide-bandgap materials.

The role of Coulomb interaction between electrons and holes confined into an active region of laser diode can be explained within a simple physical picture; while Coulomb force attracts electrons and holes at a closer distance, e-h radiative recombination rate increases, which manifests in enhancement in intensity of spontaneous emission as well as in gain magnitude. In addition Coulomb interaction modifies spontaneous emission and gain spectra of laser diodes by shifting the gain peak towards lower energies.

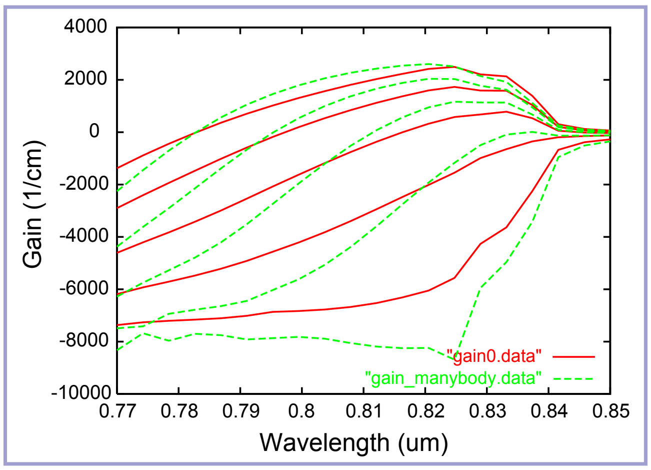
One of the inherent characteristics of electron-hole plasma is screening of the Coulomb potential. Using a modified, screened Coulomb potential, we have improved the accuracy of optical gain spectrum calculation of our device simulators.

It is well known, from semiconductor physics, that an inter-band light absorption is not a simple derivative of a free electron-hole (e-h) pair generation. Both e-h energy, as well as their motion are affected by mutual Coulomb attraction. In extreme cases, strongly correlated, hydrogen atom-like, bound electron-hole state, called exciton, can be formed in semiconductors.

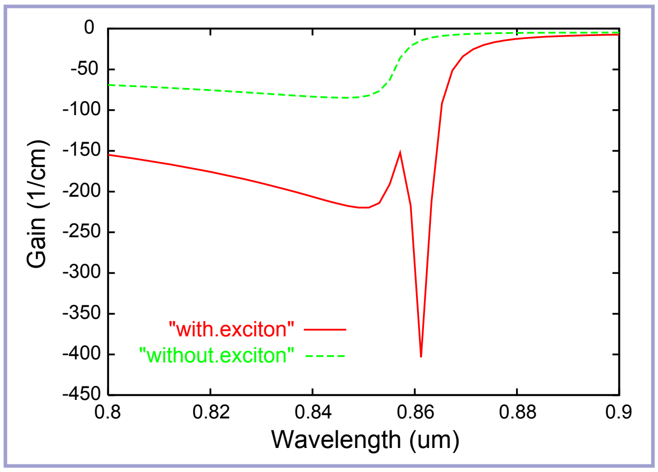
Again, screened Coulomb potential must be considered in any realistic exciton model when carrier density is significant.

Exciton model has found it application in electro-absorption modulator (EAM). In the APSYS package, the exciton model can be used to simulate the modal absorption spectrum. In the PICS3D package, such a spectrum may be used to simulate a complete EAM with longitudinal absorption/spatial hole burning.

Option currently available for products: LASTIP, PICS3D, APSYS.



Comparison of the optical gain spectrum with and without the manybody gain enhancement effect. (**Manybody/exciton option**).



Comparison of absorption spectra with exciton absorption (red curve) and without (green curve) for an EAM under reverse bias. (**Manybody/exciton option**).

Photon-Absorbing Waveguide Option

The option of Photon-Absorbing Waveguide (PAW) is similar to the 3D semiconductor optical amplifier (3D-SOA) option in that they both model a wave propagating in one direction in a waveguide containing active layers. The main difference is that the PAW operates with a voltage controlled reverse bias while the 3D-SOA with a current controlled forward bias. Use of different bias mechanism means a different simulation technique in a 3D or quasi-3D environment.

In the case of electro-absorption modulator (EAM) and waveguide photo-detector, the active waveguide is under reverse voltage bias. The device is in a photo-absorbing attenuation mode instead of a amplification mode.

Option currently available for product: PICS3D

Arizona (Koch) Gain Table Option

A special data interface to import optical gain table computed from the microscopic many-body gain/index/PL model by a research group from Arizona State University. This gain table is also referred to as the "Koch gain table", a result of collaboration with Drs. S.W. Koch, J. Hader and J.V. Moloney.

Option currently available for product: LASTIP, PICS3D and APSYS.

Franz-Keldysh Model Option

The Franz-Keldysh model option allows the computation of absorption spectrum as a function of electrical field in bulk semiconductor. It is implemented with bulk electro-absorption modulator (EAM) application in mind.

Option currently available for product: LASTIP, PICS3D and APSYS.