

PROCOT

Process Simulation Software for Compound Semiconductor by MOCVD

What is PROCOT

PROCOT (PROcesses of COMpounds) is a 2/3-dimensional process simulation software package for compound semiconductor growth by Metal-Organic Chemical Vapor Deposition (MOCVD). Given the deposition reactor geometry, chemical species and growth condition parameters, PROCOT predicts the semiconductor film growth rate, composition, thickness uniformity, dopant incorporation and defect distribution based on detailed chemical kinetics and mass/heat transfer models. Due to the complexity of the chemical and transports mechanisms involved in MOCVD, theories and predictions of MOCVD growth have been difficult and device manufacturers traditionally rely heavily on experimental approach. Most manufacturers have their own secret recipes of MOCVD growth while improvement in growth procedures is achieved at high cost by means of trial-and-error. PROCOT can help shorten such an improvement cycle and reduce overall manufacturing cost. PROCOT is intended for two types of end-users: 1) MOCVD growers wishing to develop new growth procedures or improve their existing deposition process parameters; 2) MOCVD equipment manufacturer wishing to improve reactor design.

Applications

The PROCOT software is a general purpose MOCVD reactor simulator and does not have any limits on the type of reactor geometry/design or the number of chemical species involved in a deposition process. However, emphasis and demo examples are mostly in the area of compound semiconductor thin films with

application in electronic and optoelectronic devices such as laser diode (LD) and light-emitting diodes (LED).

Physical Models and Advanced Features

In an arbitrary two-dimensional (2D) cross section or a full 3-dimensional description of the MOCVD reactor, finite element method is used to solve a number partial differential equations governing the chemical and physical processes. The following advanced models and features are implemented in the PROCOT.

Physical Models & Advanced Features

- Chemical kinetics models.
- Mass transport/conservation equations.
- Navier-Stokes fluid dynamic equations.
- Heat transfer equation.
- Complete chemical species library.
- Transient and steady state simulations.

Capabilities

Convenient graphic user interface (GUI) may be used to setup and input MOCVD deposition parameters and to view simulation results. PROCOT offers the following input capabilities.

SimuProcom graphic user interface (GUI) program is used as a general control panel to drive different components of PROCOT. It activates a set of tools (the WIZARD) to offer online help with available commands and to reduce the amount of typing needed. ChemEditor is a new graphic user interface (GUI) program used to create and maintain the chemical reaction models involved in a reactor.

GeoEditor is a GUI program used to define arbitrary reactor geometry. Any number of gas inlet/outlet may be defined within this GUI.

A large selection of output variables may be generated by PROCOT. These include the following.

Chemical species distribution in 2/3 D may be produced for both gas and surface species.

Gas chemical reaction rates distribution in 2/3 D.

Flow velocity distribution in 2/3 D.

Temperature distribution in 2/3 D.

Film deposition rate as a function of position in the 2/3D model. Deposition rate as a function of temperature in the quick analysis of level 1 (well-mixed model) may be used to determine the optimal growth temperature.

APPLICATIONS

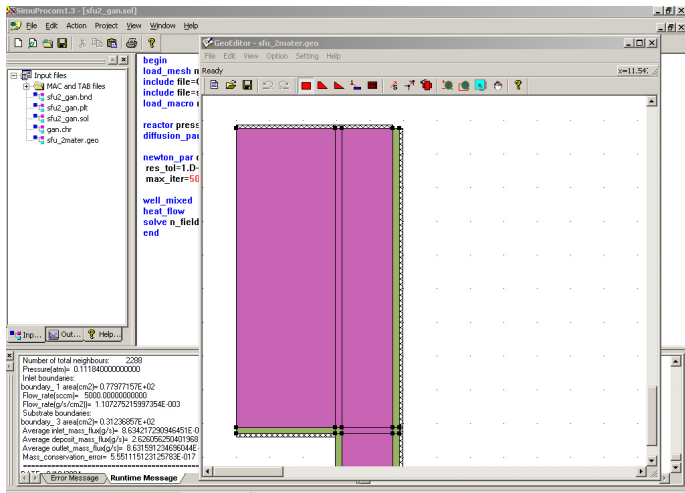
Compound semiconductor thin films

Laser diode(LD)
Light-emitting diode(LED)

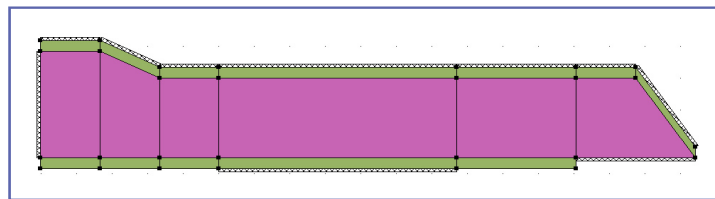
GaN	InP	GaAs
InN	AlN	InGaAs
AlGaAs	AlGaAs	
InGaAs	InGaAsP	

and more ternaries & quaternaries...

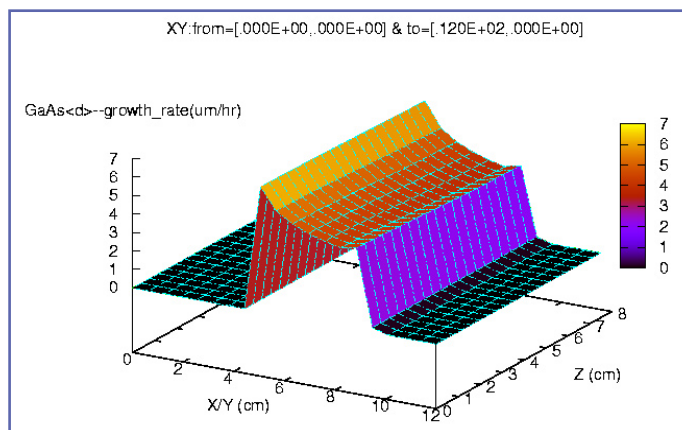
Film composition as a function of position (uniformity analysis).
Dopant and/or other impurities distribution may also be simulated.
The 2/3D data may be viewed by a graphic user interface program called CrosslightView to generate color images in 2/3 dimensions or by a public domain graphic software called GNUPLOT.



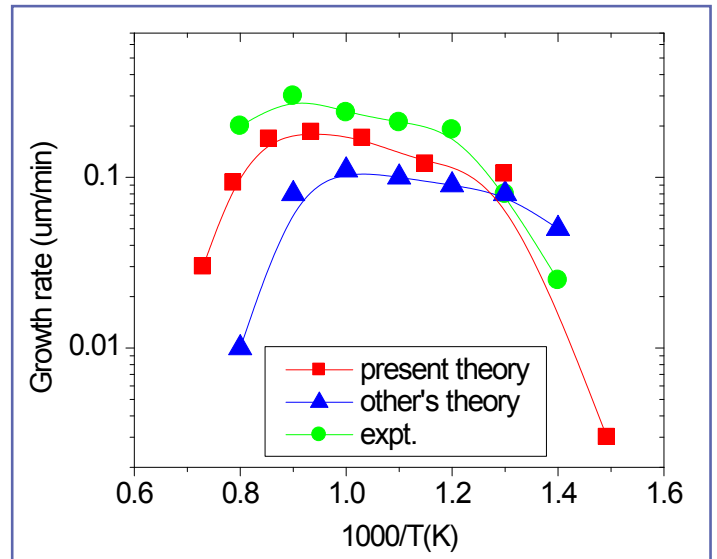
User friendly GUI environment SimuProcom.



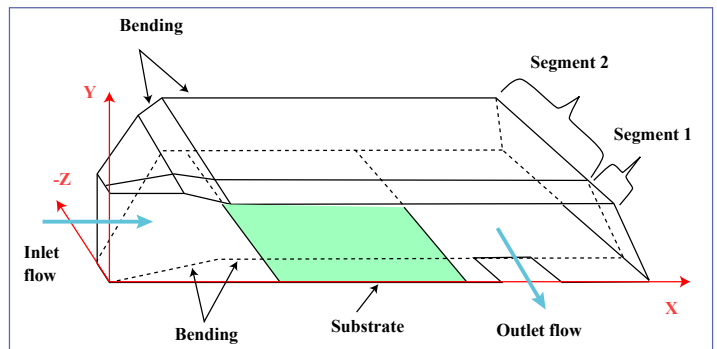
Geometry of horizontal reactor



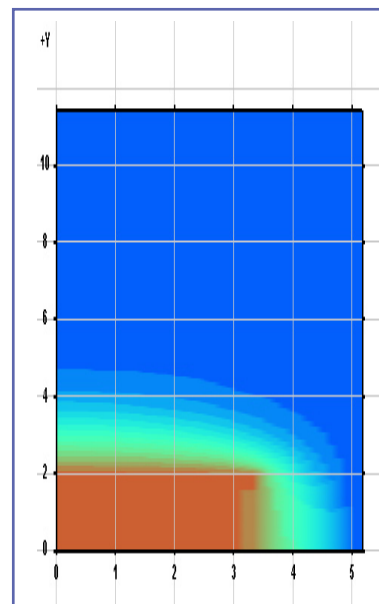
GaAs growth rates in 3D



Growth rate versus temperature



Reactor model in 3D, only half of it is shown because of symmetry of the reactor



Temperature distribution in vertical reactor