PROCOM-Process Simulation Software for Compound Semiconductor Growth by MOCVD

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Contents

0.1 What is PROCOM

PROCOM (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, PROCOM 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. PROCOM can help shorten such an improvement cycle and reduce overall manufacturing cost.

PROCOM 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.

0.2 Applications

The PROCOM 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).

Convenient simulation examples have been set up for GaN, InP, GaAs, InN, AlN, InGaN, AlGaN, AlGaAs, InGaAs, InGaAsP and many combinations of ternaries and quaternaries. PROCOM may also be used to study incorporation of dopants and impurities into the compounds.

0.3 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 PROCOM.

- **Chemical kinetics models** using experimental or theoretical gas and surface reaction rates for a large number of chemical species.
- **Mass transport/conservation equations** involving detailed chemical reaction between gas mixtures and surface species. Multiple component chemical species diffusion and convection are the main mechanisms of mass transport.
- **Navier-Stokes fluid dynamic equations** (momentum conservation) governing the convection flows of the overall gas species.
- **Heat transfer equation** (energy conservation) is solved to determine the temperature distribution within the reactor. Since all reaction rates are strong functions of temperature, accurate temperature distribution is critical.
- **Complete chemical species library** has been prepared and chemical data and transport property parameters are stored in user-accessible formulas so that customization may be done as soon as new data are available.
- **Transient and steady state simulations** can be performed for different deposition conditions. For example, a combination of transient and steady state simulation may be used to simulate the growth of multiple quantum wells in opto-electronic applications.
- **Different levels of models** may be used in process design analysis. At the lowest level, a quick chemical analysis may be performed to determine the end products of a reaction system assuming all species are well mixed (or well stirred). This will be an idea situation if all chemical species are quickly transported to the deposition surface. At the next level, a 2D mesh may be set up to study mass and heat transport. At the highest level, a 3D simulation may be used to mimic a real MOCVD growth process.

0.4 Capabilities

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

- **SimuProcom** graphic user interface (GUI) program is used as a general control panel to drive different components of PROCOM. 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 involed 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 PROCOM. 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.

- **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.

0.5 Sample Input/Output

- 1) Figure 1 illustrates the use of GeoEditor to set up a test structure of a horizontal MOCVD reactor. Gas inlet/outlet, substrates and hot/cold wall are treated as boundaries.

- 2) 2D mesh corresponding to the test structure is displayed in Figure 2.

- 3) A screen capture of SimuProcom (GUI) control program is shown with a display of chemical species using the graphic tool CrosslightView in Figure 3.

- 4) An example display of a GUI tool called ChemEditor with a user-accessible chemical species macro library in Figure 4. Large selection of chemical data have been collected in PROCOM.

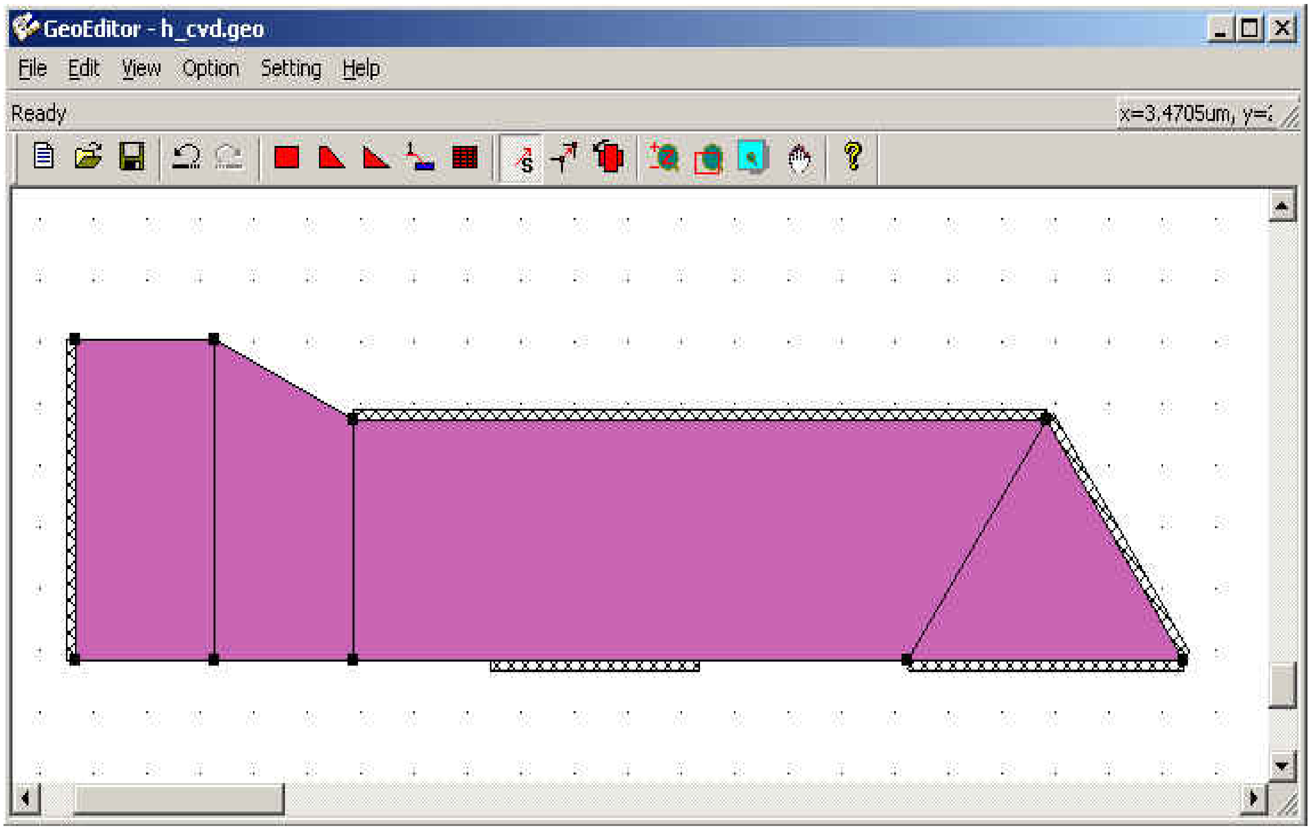

Figure 1: Use of GUI program GeoEditor to set up a simple test structure of a horzontal MOCVD reactor.

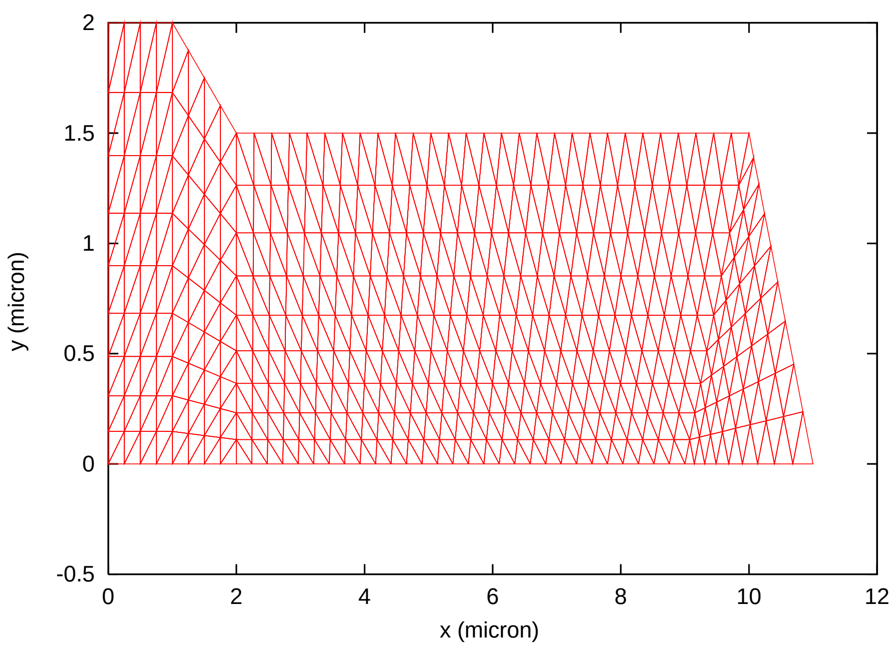

Figure 2: Finite element mesh used by PROCOM for a test structure of a horizontal reactor.

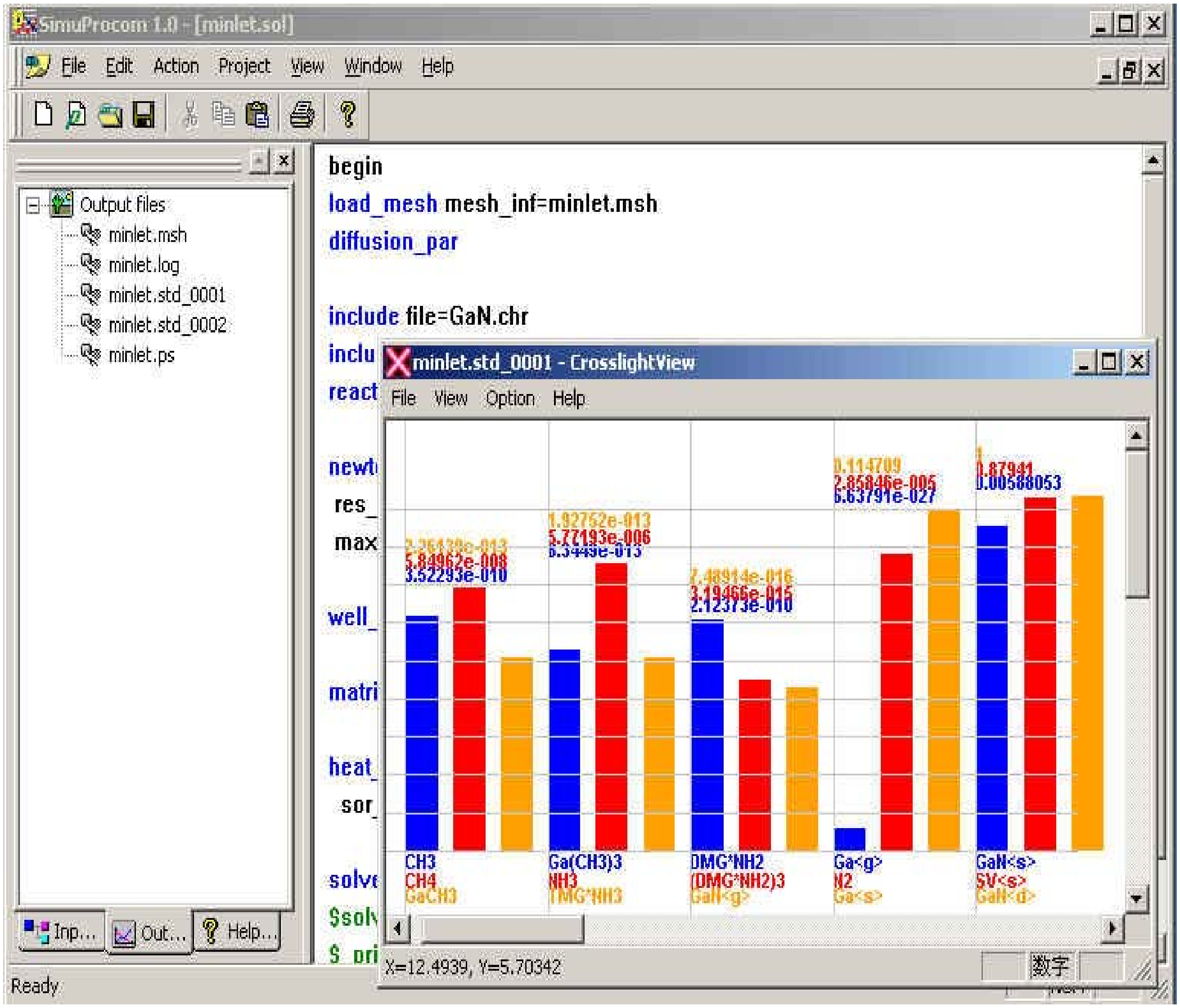

Figure 3: SimuProcom graphic user interface is used to create and control the simulation involved in a GaN growth.

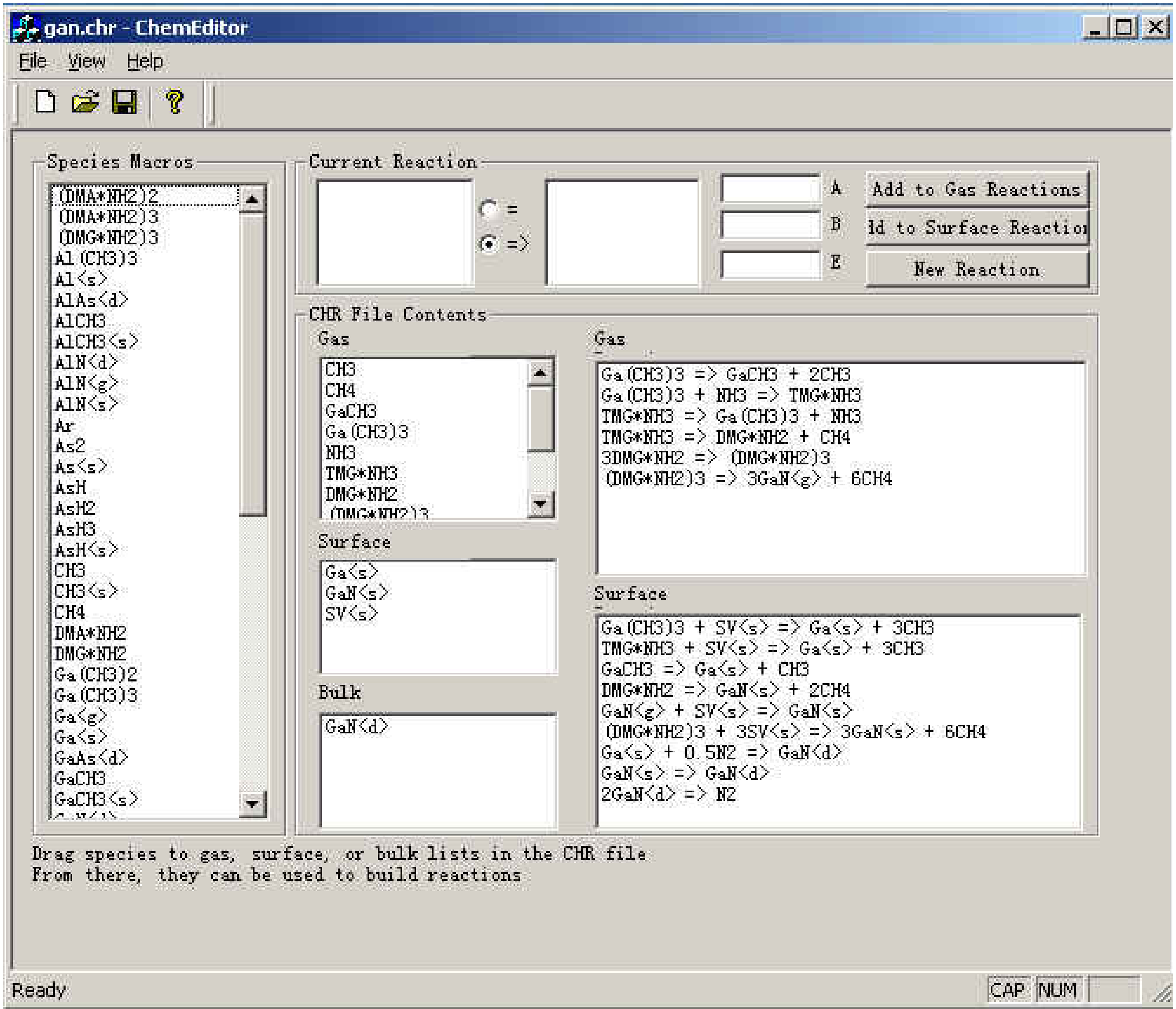

Figure 4: ChemEditor may be used to create and edit complex chemical reactions involved in a reactor simulation.

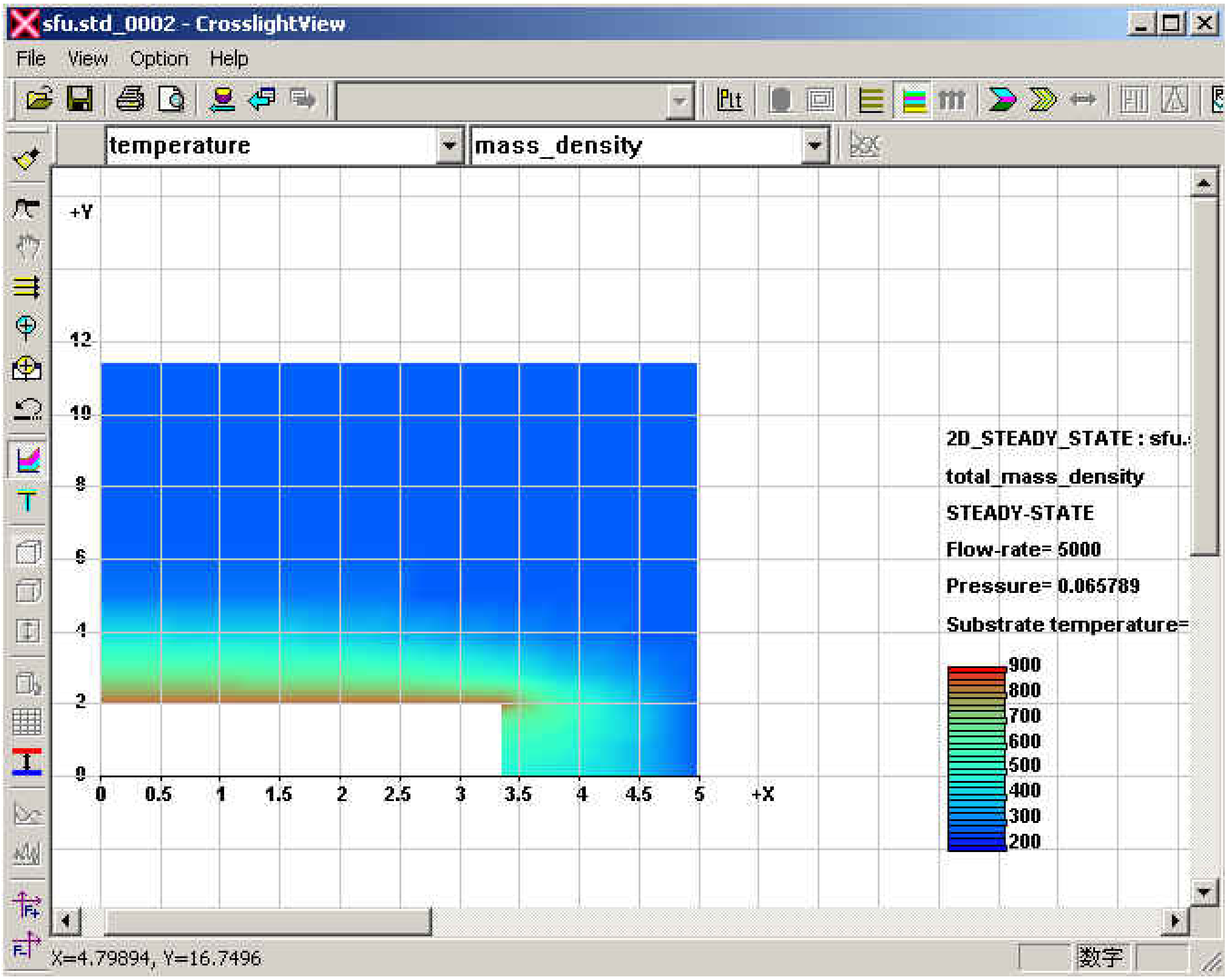

Figure 5: Simulated temperature distribution in a vertical reactor with symmetric axis on the left.

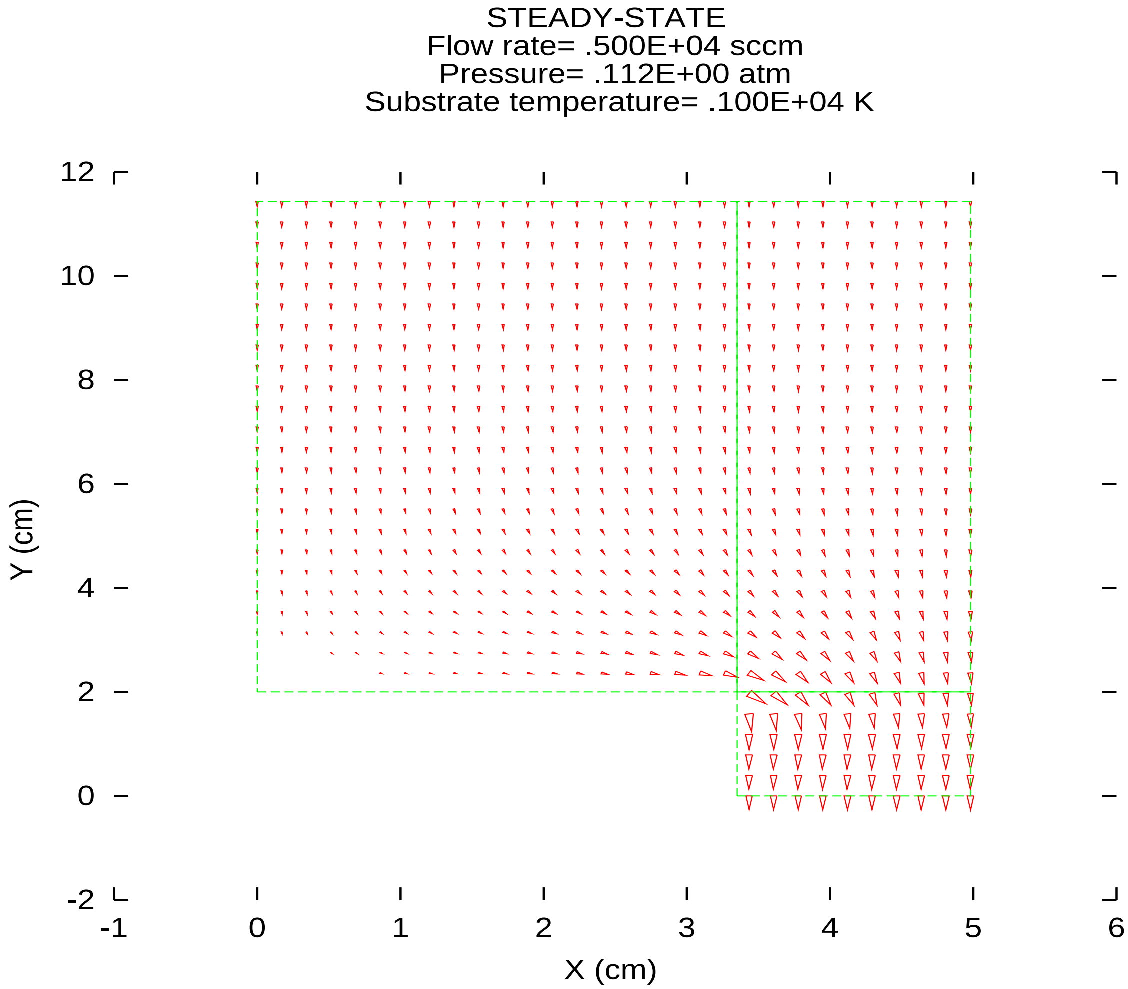

Figure 6: Simulated convection flow distribution in a vertical reactor with cylindrical symmetry axis on the left.

- 5) Simulated temperature color contours in a vertical reactor are showed in 5
- 6) Convecton flow distribution can be simulated in a vertical reactor (with cylindrical symmetry) as shown in Figure 6
- 7) Growth-rate of GaN as a function a position in a horizontal reactor is given in Figure 7.
- 8) distribution of TMGa species in a vertical reactor (with cylindrical symmetry on the left) in a GaN deposition example is given in Figure 8.

0.6 About Crosslight Software Inc.

Crosslight Software Inc. (formerly Beamtek Software Inc.) is an international company established in 1992 with head office in Canada. Initially a spin-off company from the National Research Council of Canada, it now has branch offices and distribution/support

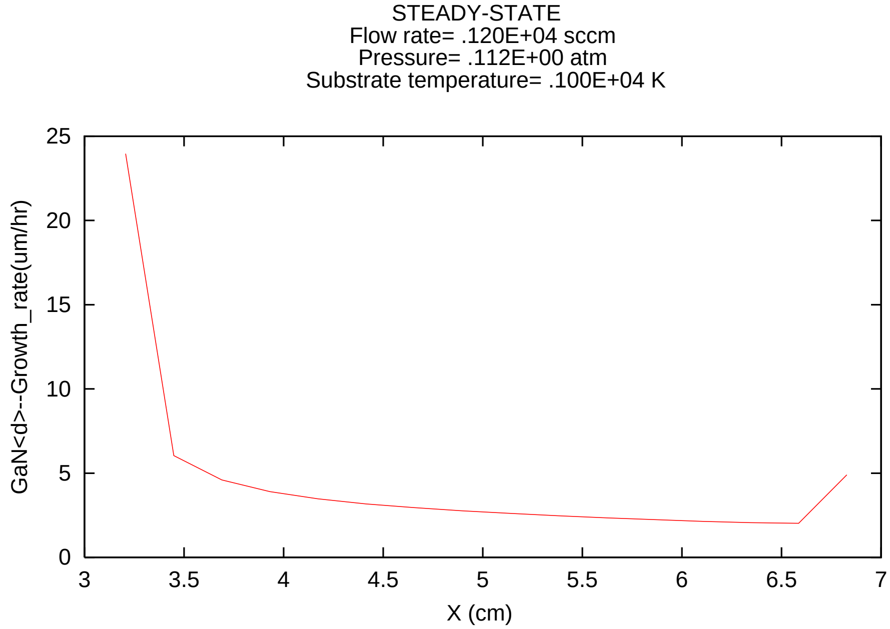

Figure 7: Growth-rate vs. position plot may be used to optimize the efficiency and uniformity of the growth.

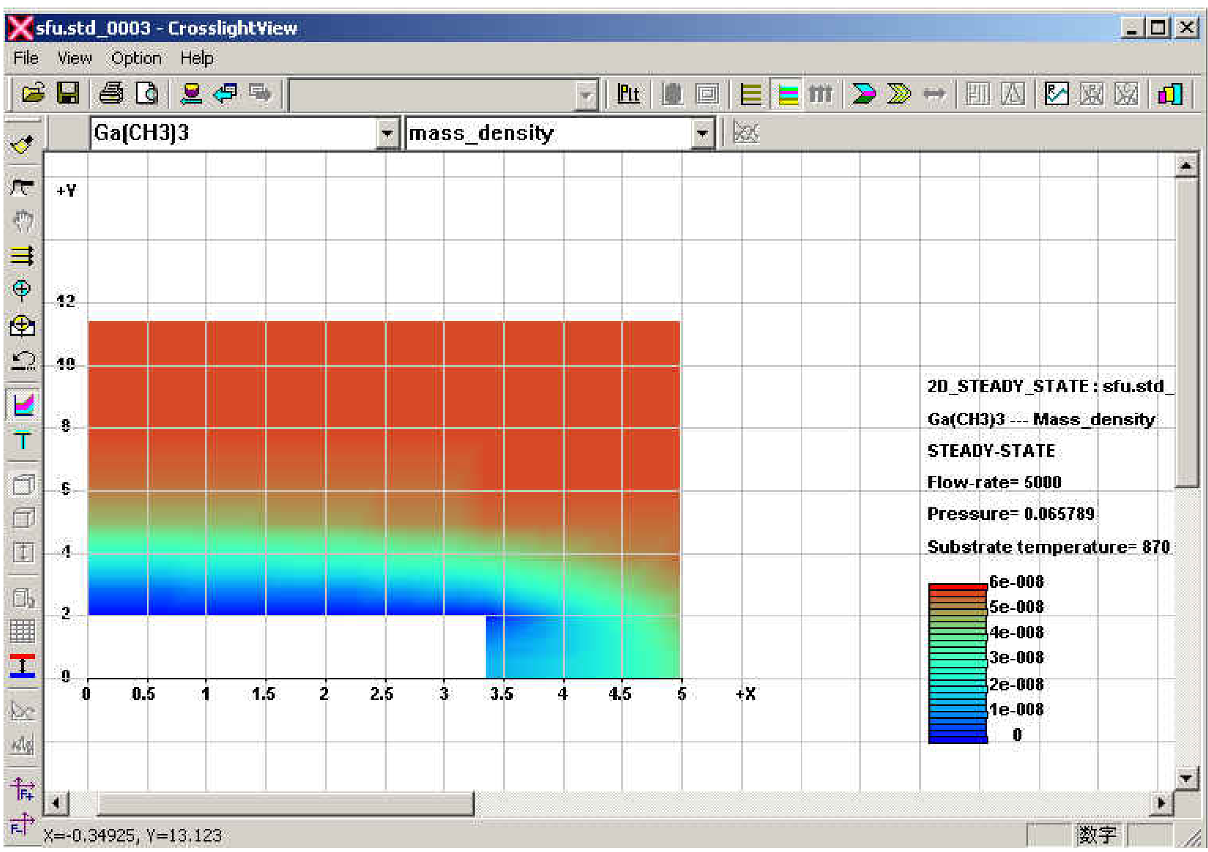

Figure 8: Distribution of TMGa density in a GaN deposition simulation.

centers in many countries around the world. Some of its simulators had won international software awards over the years.

Crosslight Software is the leader in providing commercial physical models of semiconductor optoelectronic/electronic devices. Crosslight's customers include tens of major manufacturers of semiconductor electronic and optoelectronic equipments. With the availability of the PROCOM software, Crosslight offers one-stop shopping for semiconductor device manufacturers requiring both device and process simulation tools. For details about Crosslight, please visit www.crosslight.com.