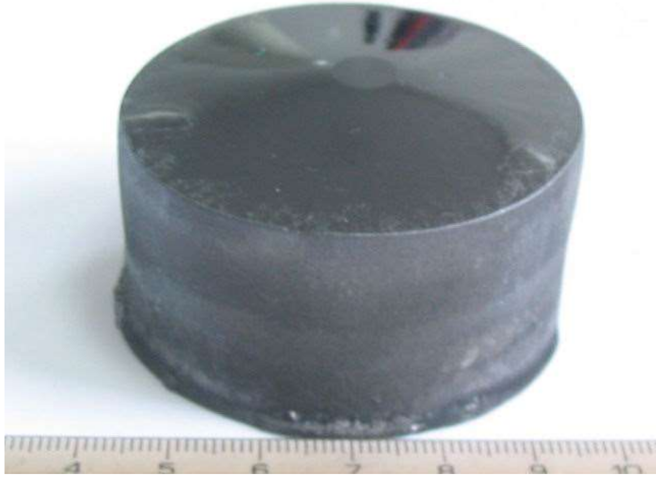
Software for Modeling of Long-Term Growth of Wide-Bandgap Crystals and Epilayers from Vapor

Virtual Reactor



2018
STR Group, Inc.

Virtual Reactor – Family of Software Tools

STR Virtual Reactor (VR™) is a family of stand-alone 2D software tools designed for the simulation of long-term growth of bulk crystals and epilayers from vapor

Virtual Reactor editions:

- Physical Vapor Transport
  - For growth of SiC: **VR™-PVT SiC**
  - For growth of AlN: **VR™-PVT AlN**
- Hydride Vapor Phase Epitaxy: **HEpiGaNS™**
  - For growth of GaN
  - For growth of AlN and AlGaN
- Chemical Vapor Deposition
  - For growth of SiC: **VR™-CVD SiC**
- Metal-Organic Chemical Vapor Deposition
  - For growth of GaN, AlN, InGaN, AlGaN, and AlInN: **VR™-Nitride Edition**
  - For growth of AlAs, AlP, GaAs, GaP, InAs, InP, AlGaAs, InGaAs, InGaP and AlInGaP: **VR™-III-V Edition**

VR^{TM}-III-V Edition

Software for Modeling of
Epitaxial Growth of Group-III Arsenides and Phosphides by
Metal-Organic Chemical Vapor Deposition

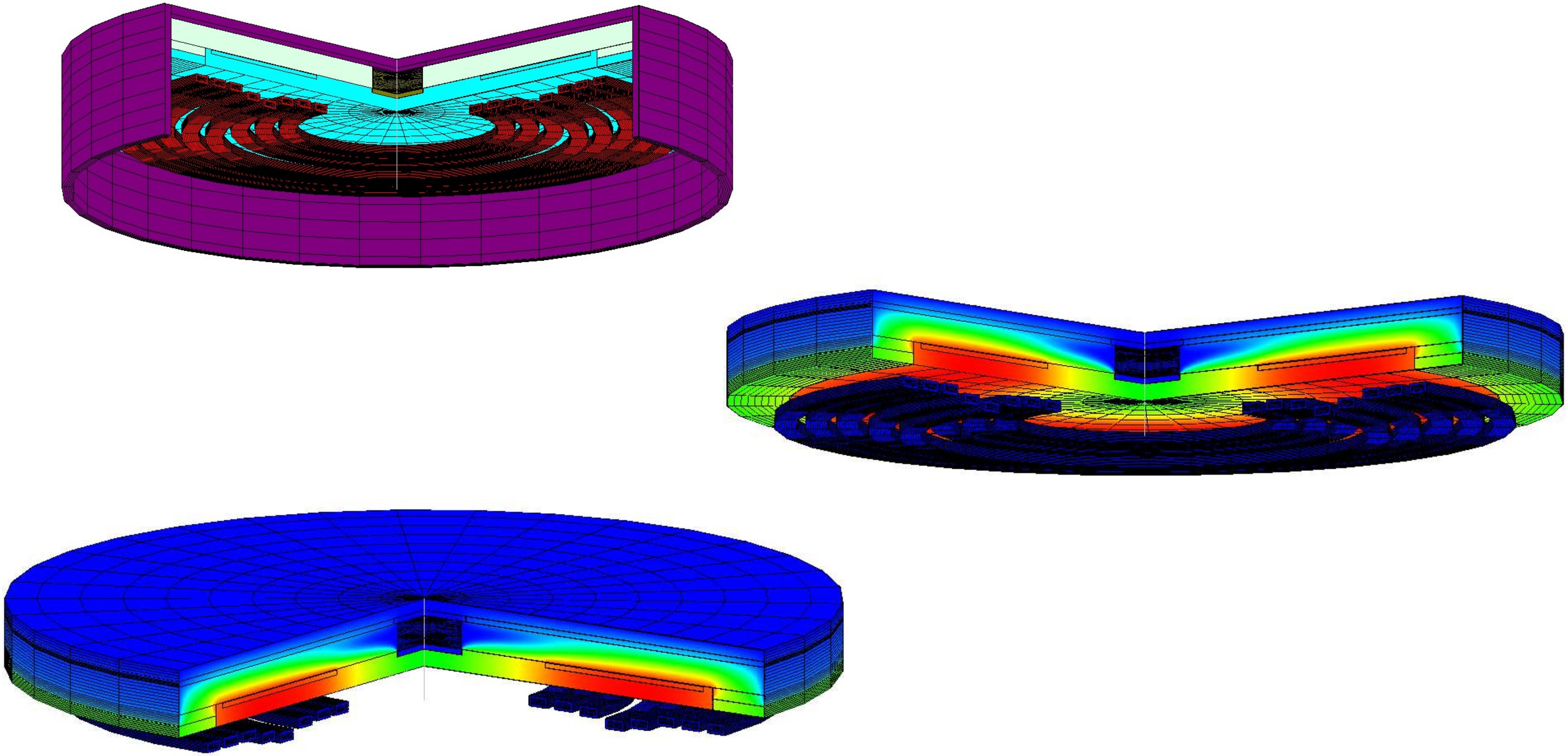
VR™-III-V Edition

- ✓ **AlAs**
- ✓ **AlP**
- ✓ **GaAs**
- ✓ **GaP**
- ✓ **InAs**
- ✓ **InP**
- ✓ **AlGaAs**
- ✓ **InGaAs**
- ✓ **InGaP**
- ✓ **AlInGaP**

- Prediction of the growth rate and composition uniformity over the large wafers.

- Parasitic deposition on the walls and injectors (low temperature growth kinetics).

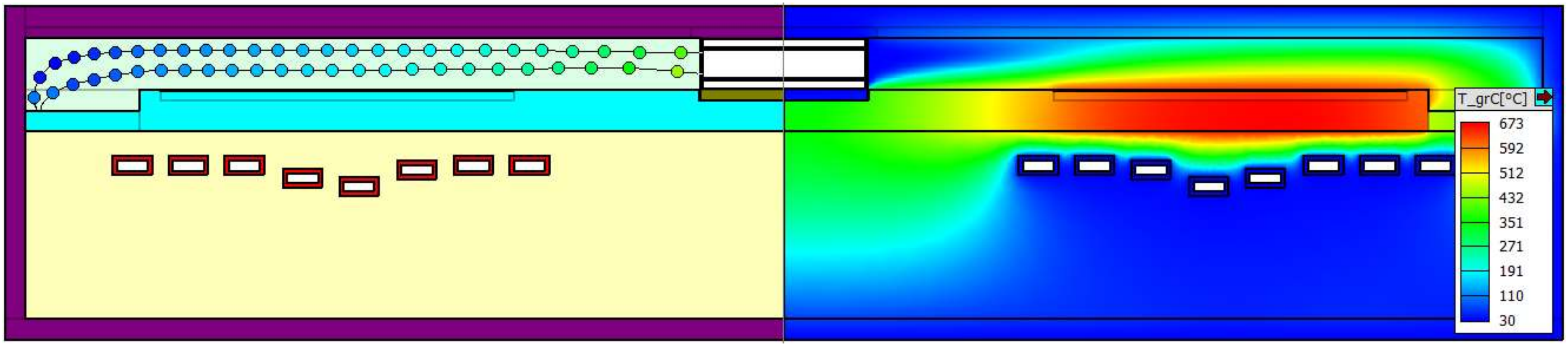
Example of Planetary Reactor with RF Heating



Materials and Temperature Distribution: 3D View

Heat Transfer and the Flow Patterns

- Conductive heat transfer in solid blocks;
- Radiative heat transfer in transparent gas blocks. The view-factor technique is used to model the radiation heat exchange;
- Heat transfer and gas mixture flow, including multi-component diffusion with the Soret effect;
- Heat conductivity and viscosity of the mixture are calculated in terms of molecular kinetic theory. The diffusion of reactive species is modeled using the Wilke approximation.



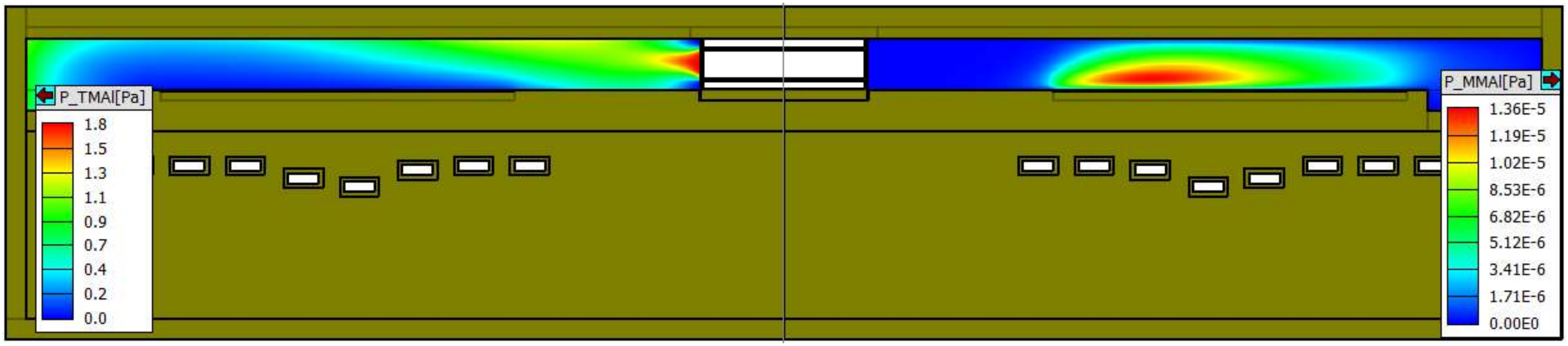
Materials

Stream Traces and Temperature Distribution

2D View

Gas-Phase Chemistry

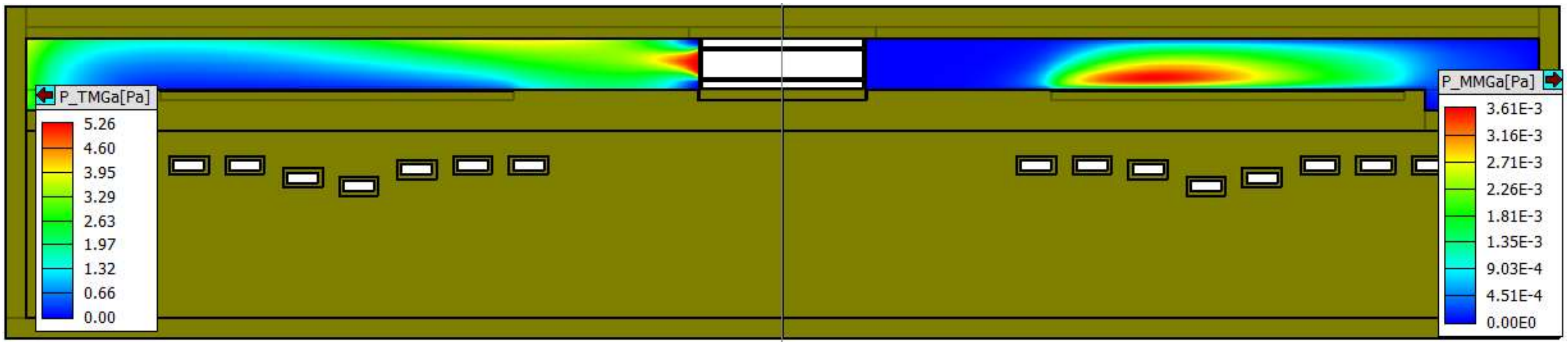
- Gas-phase chemistry is relatively simple compared to VR Nitride Edition (lower temperatures);
- Ga/In/Al chemistry: first-order decomposition of the MO precursors;
- As/P chemistry: actually no or little gas-phase decomposition of group-V hydride precursors;
- Second-order reactions usually can be neglected.



TMAl Partial Pressure

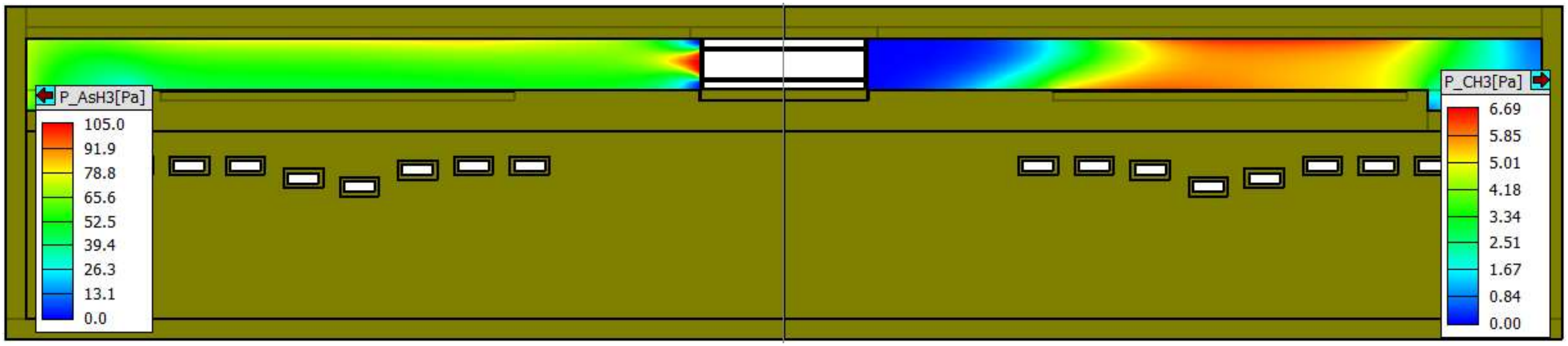
MMAl Partial Pressure

Gas-Phase Chemistry



TMGa Partial Pressure

MMGa Partial Pressure

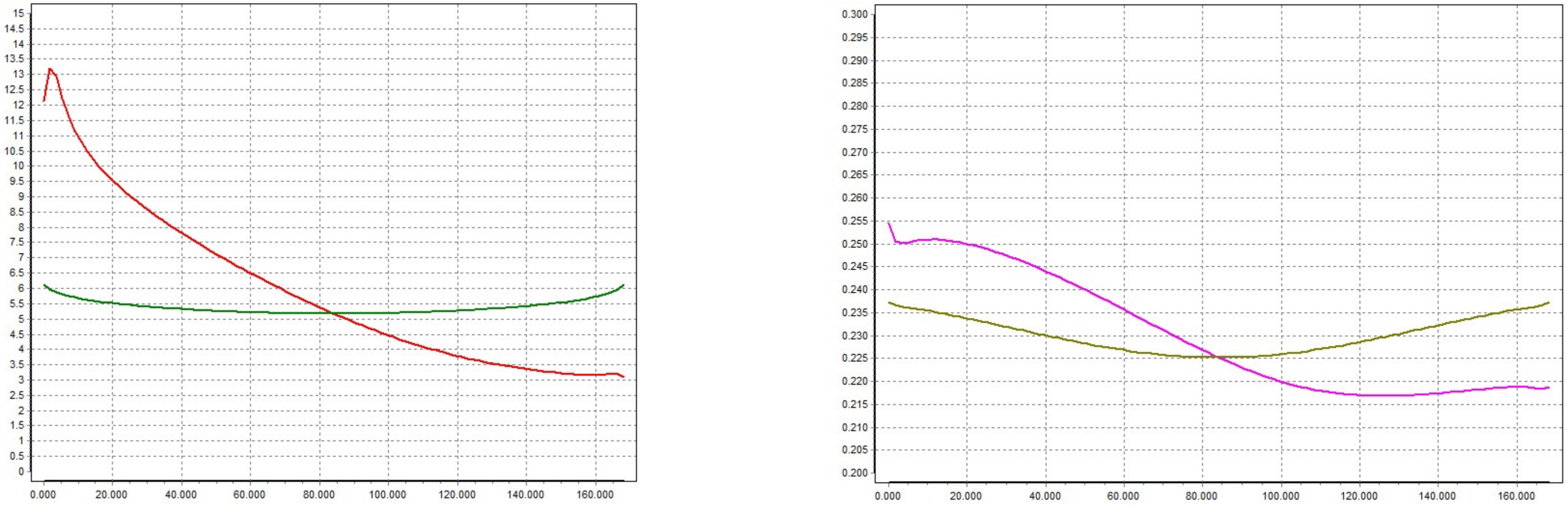


AsH_3 Partial Pressure

CH_3 Partial Pressure

Surface Chemistry

- Ga/In/Al chemistry: adsorption and incorporation of group-III atoms;
- As/P chemistry: adsorption, incorporation, and desorption of excess group-V species as dimers and tetramers;
- Desorption of group-III species is normally weak;
- Low temperatures: strong kinetic limitations, different ranges of temperatures for In-, Ga-, and Al-containing materials

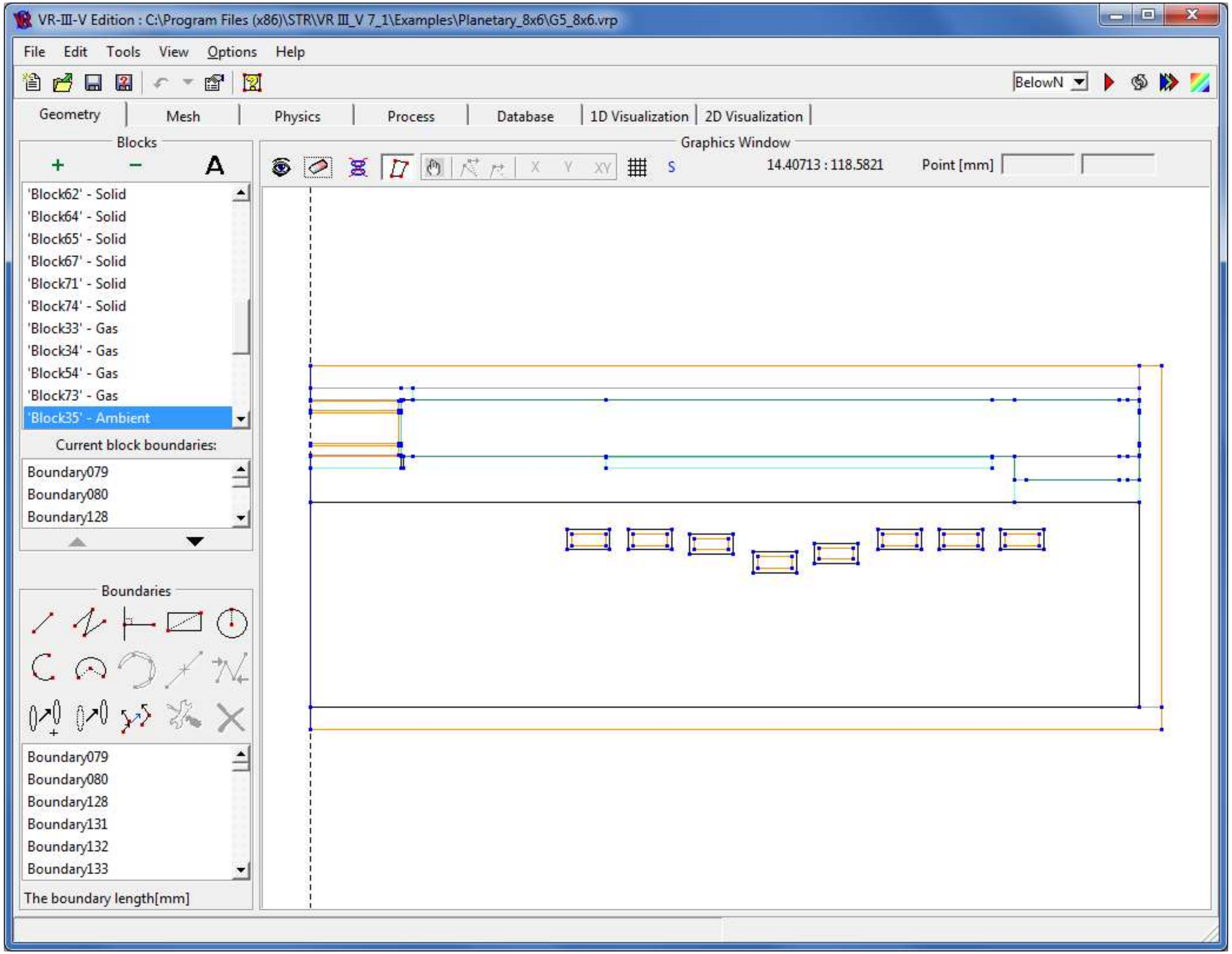


Distribution of instantaneous and rotation-averaged growth rate (left) and AlAs content in Al$_x$Ga$_{1-x}$As (right) across the susceptor

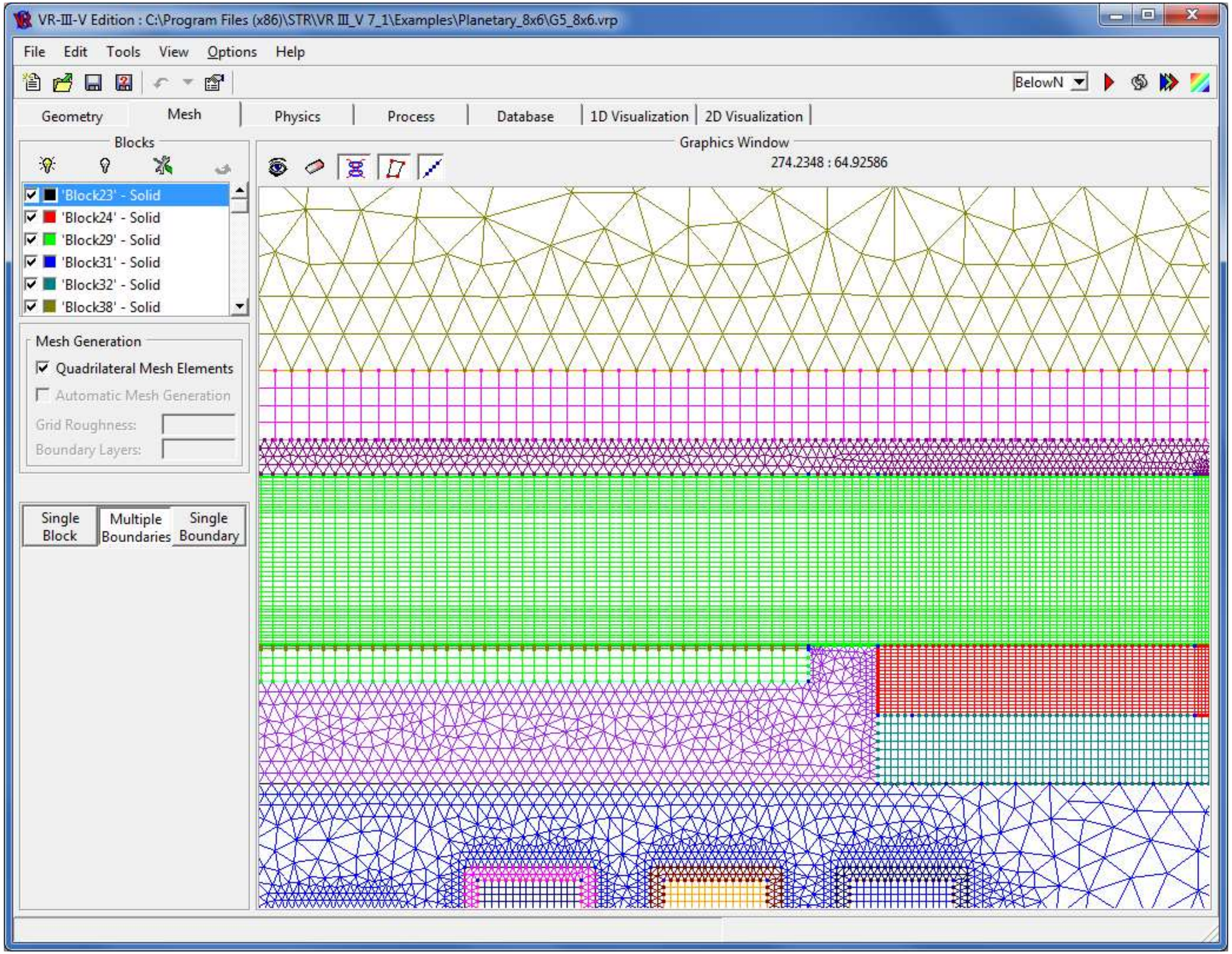
VR™-III-V Edition

Graphical User Interface

Specification of the Reactor Geometry



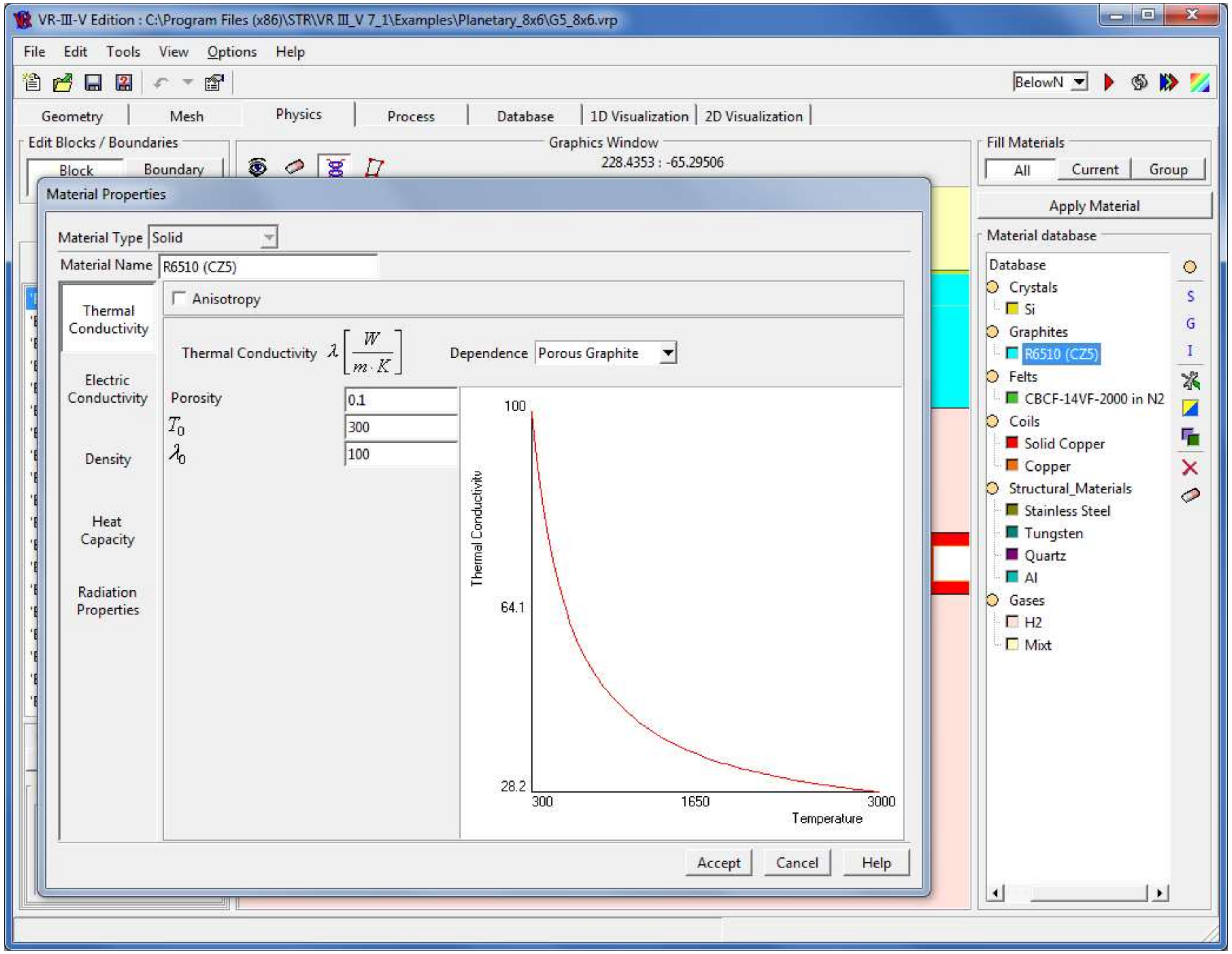
Mesh Generation



☑ 🟥 'Block23' - Solid
☑ 🟥 'Block24' - Solid
☑ 🟩 'Block29' - Solid
☑ 🟦 'Block31' - Solid
☑ 🟦 'Block32' - Solid
☑ 🟫 'Block38' - Solid

☑ Quadrilateral Mesh Elements
☐ Automatic Mesh Generation
Grid Roughness:
Boundary Layers:

Specification of the Materials Properties



VR-III-V Edition : C:\Program Files (x86)\STR\VR III_V 7_1\Examples\Planetary_8x6\G5_8x6.vrp

Graphics Window 228.4353 : -65.29506

Material Properties

Material Type: Solid

Material Name: R6510 (CZ5)

☐ Anisotropy

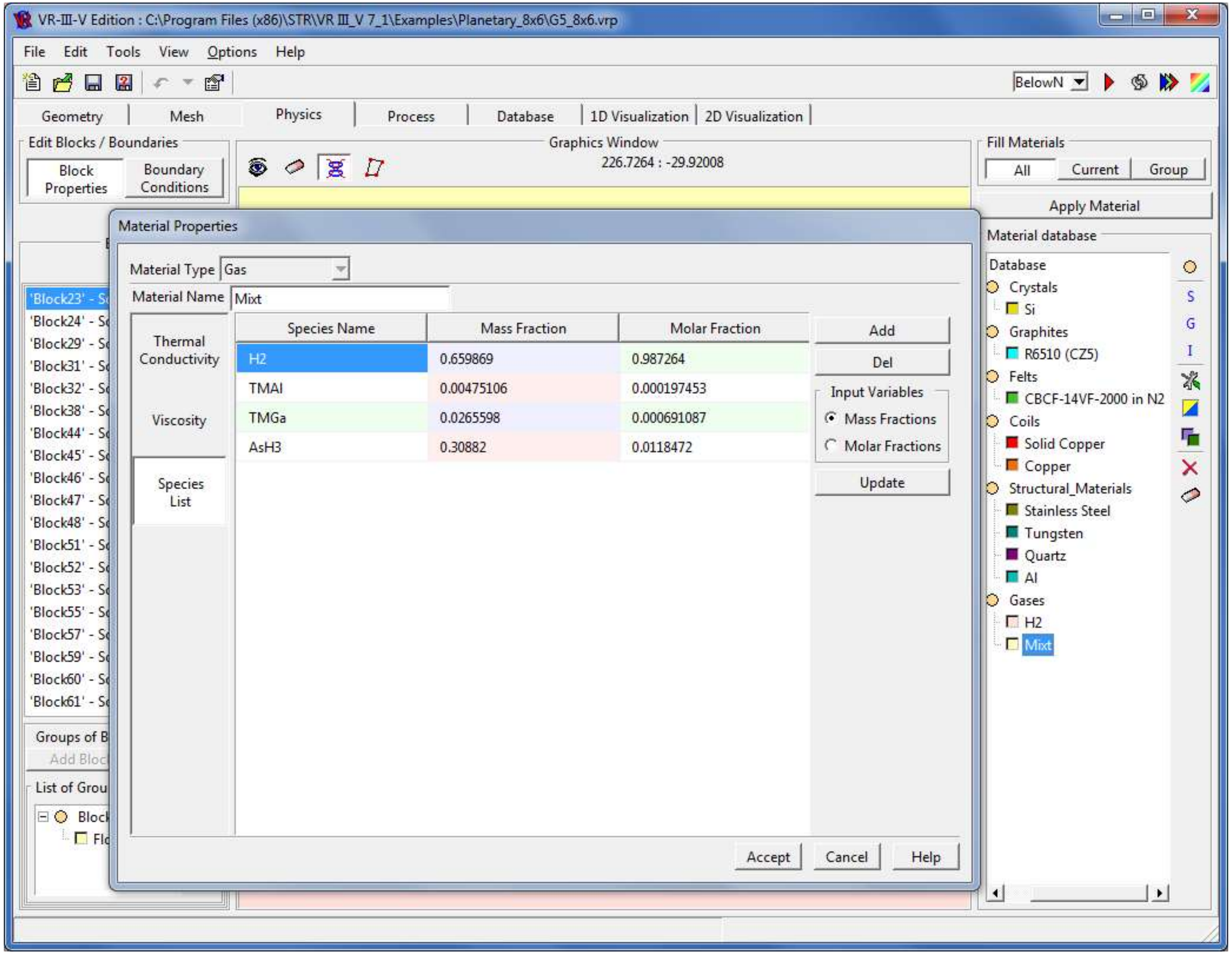
Thermal Conductivity $\lambda\left[\frac{W}{m\cdot K}\right]$ Dependence: Porous Graphite

Porosity: 0.1

T_0: 300

λ_0: 100

Specification of the Gas Mixture



VR-III-V Edition : C:\Program Files (x86)\STR\VR III_V 7_1\Examples\Planetary_8x6\G5_8x6.vrp

Graphics Window 226.7264 : -29.92008

Material Properties

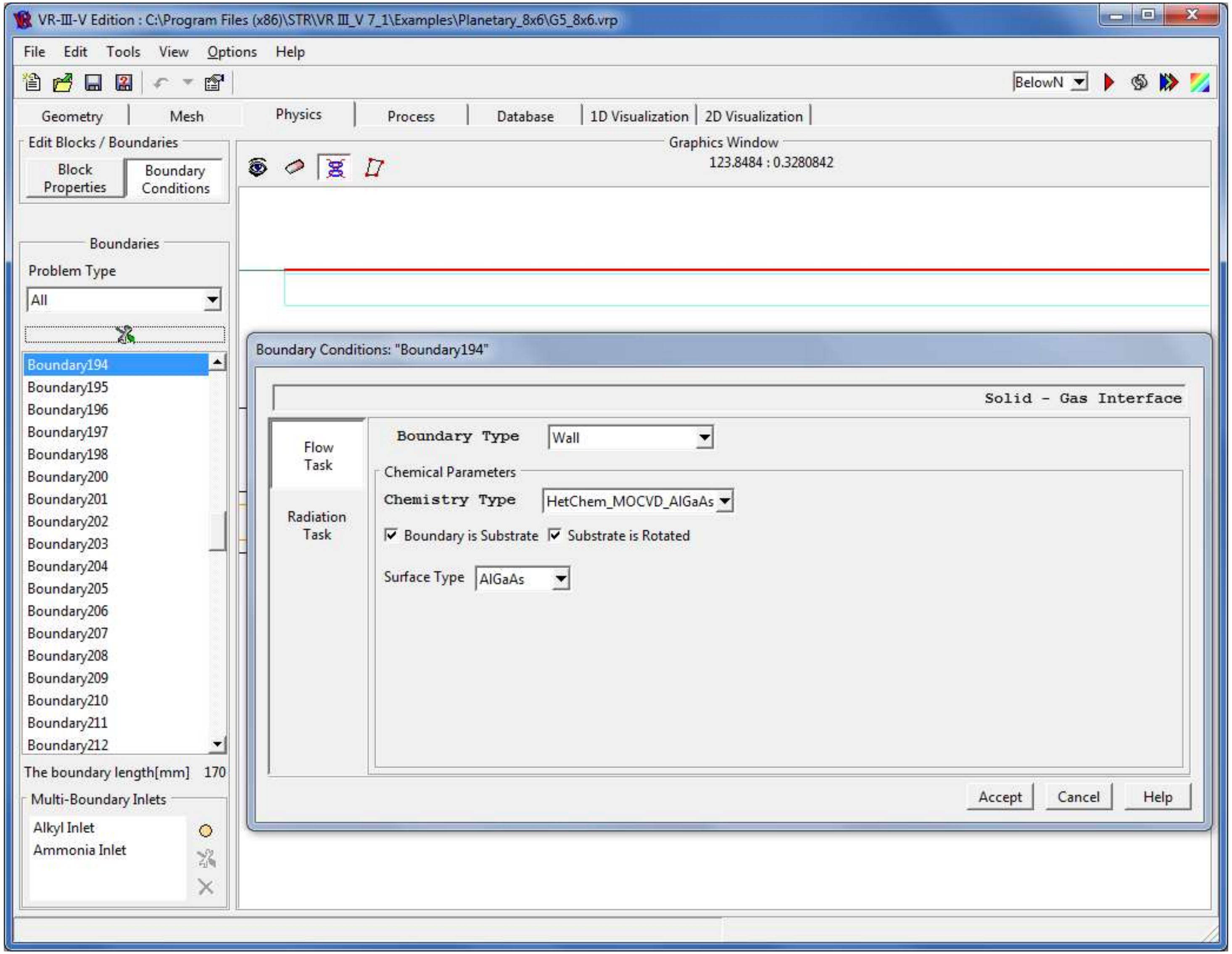
Material Type: Gas

Material Name: Mixt

Species Name	Mass Fraction	Molar Fraction
H2	0.659869	0.987264
TMAl	0.00475106	0.000197453
TMGa	0.0265598	0.000691087
AsH3	0.30882	0.0118472

Input Variables
● Mass Fractions
○ Molar Fractions

Specification of the Boundary Conditions – AlGaAs Surface


VR-III-V Edition : C:\Program Files (x86)\STR\VR III_V 7_1\Examples\Planetary_8x6\G5_8x6.vrp

Graphics Window 123.8484 : 0.3280842

Problem Type: All

The boundary length[mm] 170

Boundary Conditions: "Boundary194"

Solid - Gas Interface

Boundary Type: Wall

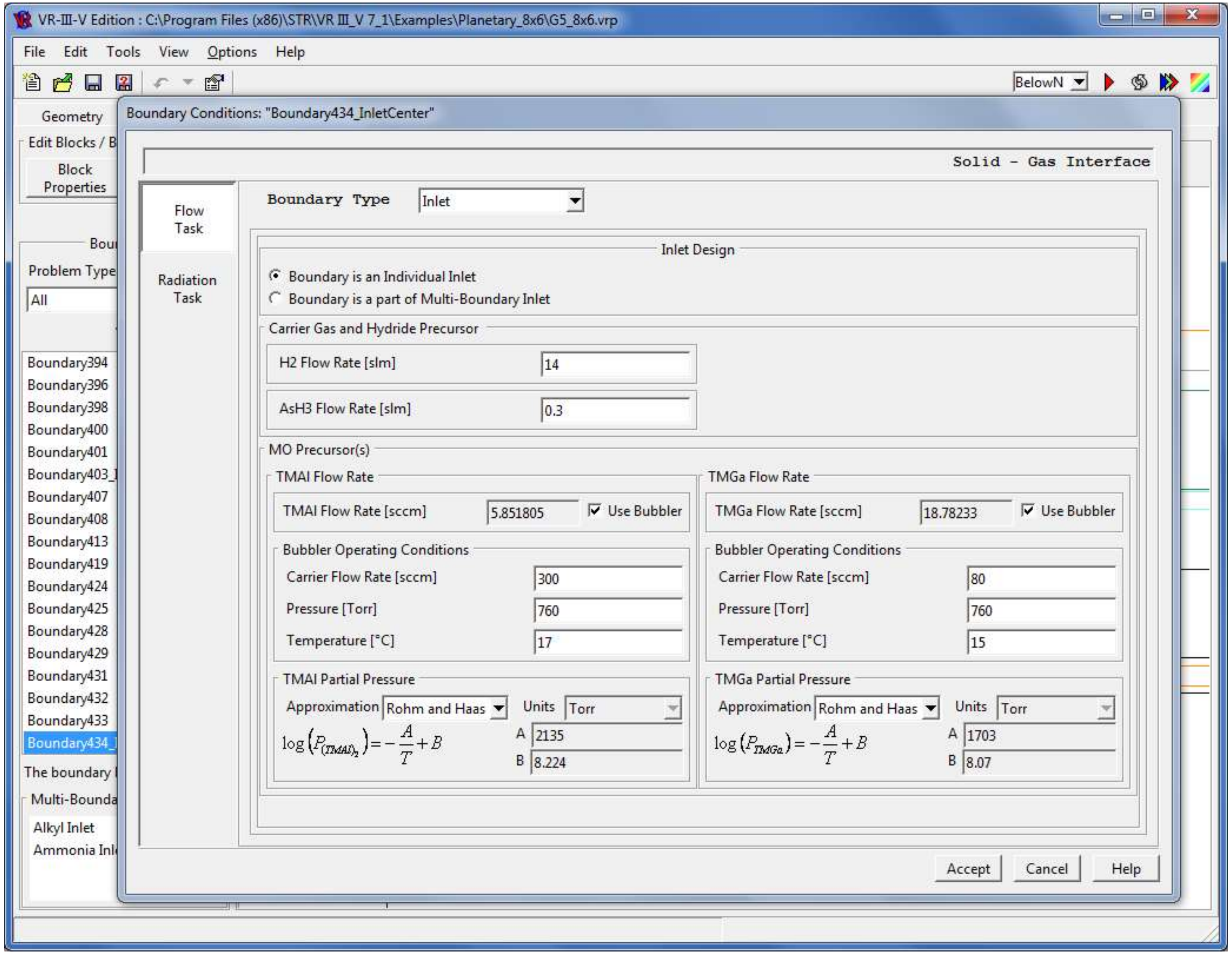
Chemical Parameters

Chemistry Type: HetChem_MOCVD_AlGaAs

☑ Boundary is Substrate ☑ Substrate is Rotated

Surface Type: AlGaAs

Specification of the Boundary Conditions – Inlets



Problem Type: All

Boundary Conditions: "Boundary434_InletCenter"

Solid - Gas Interface

Boundary Type: Inlet

Inlet Design

● Boundary is an Individual Inlet
○ Boundary is a part of Multi-Boundary Inlet

Carrier Gas and Hydride Precursor

H2 Flow Rate [slm]: 14
AsH3 Flow Rate [slm]: 0.3

MO Precursor(s)

TMAl Flow Rate

TMAl Flow Rate [sccm]: 5.851805 ☑ Use Bubbler

Bubbler Operating Conditions
Carrier Flow Rate [sccm]: 300
Pressure [Torr]: 760
Temperature [°C]: 17

TMAl Partial Pressure
Approximation: Rohm and Haas Units: Torr

$$\log\left(P_{(TMAl)_2}\right) = -\frac{A}{T} + B$$

A: 2135
B: 8.224

TMGa Flow Rate

TMGa Flow Rate [sccm]: 18.78233 ☑ Use Bubbler

Bubbler Operating Conditions
Carrier Flow Rate [sccm]: 80
Pressure [Torr]: 760
Temperature [°C]: 15

TMGa Partial Pressure
Approximation: Rohm and Haas Units: Torr

$$\log\left(P_{TMGa}\right) = -\frac{A}{T} + B$$

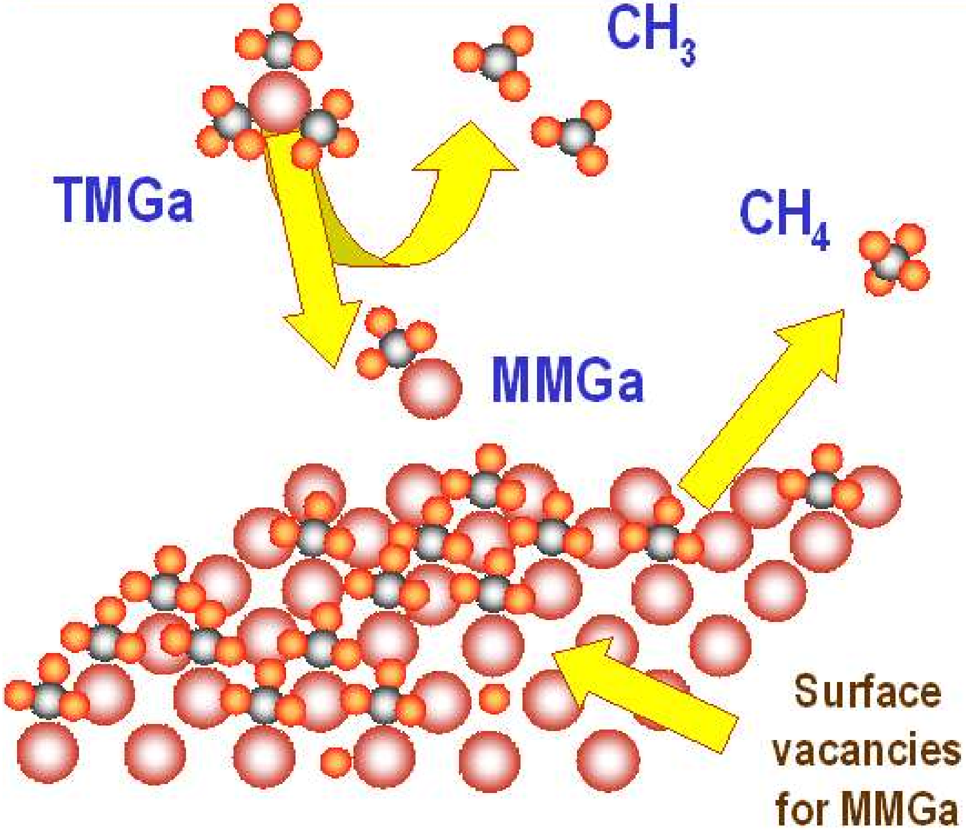
A: 1703
B: 8.07

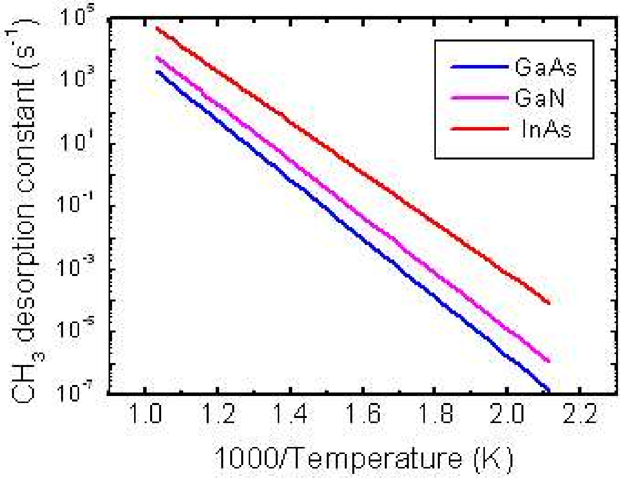
VR™-III-V Edition

Validation of the Chemical Models

Low-temperature kinetic effects in MOVPE of III-V compounds

Assumption: Hydrocarbon species block free adsorption sites for group-III species



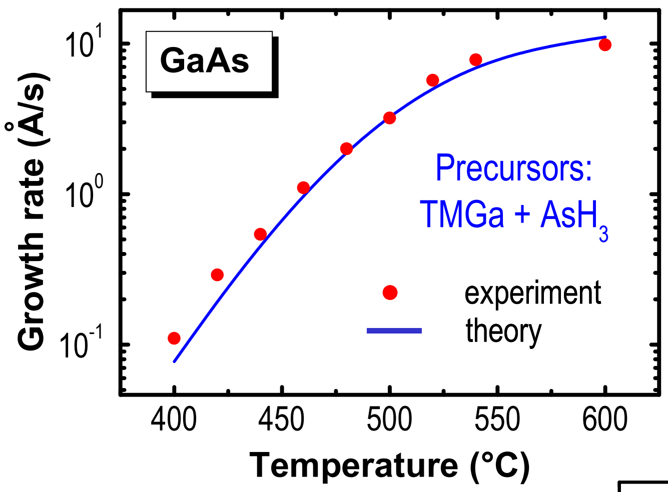


Data on desorption constants from TPD experiments:

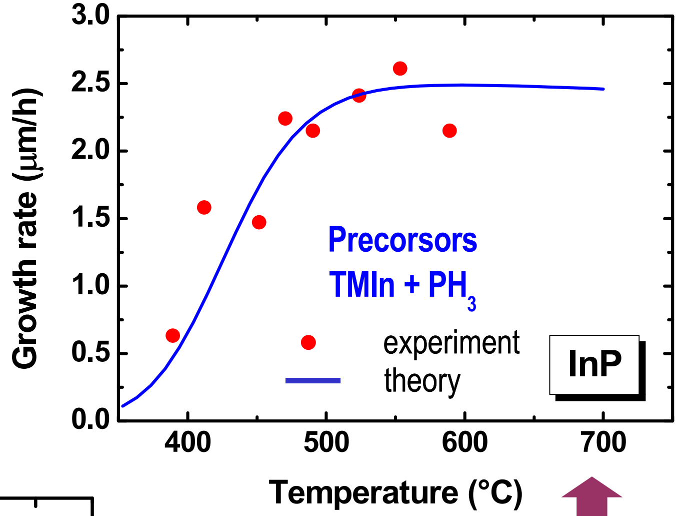
J.A.McCaulley et al., J.Vac. Sci.Technol. A 9 (1991) 2872

H.-T.Lam et al., Surf.Sci. 426 (1999) 199

Low-temperature growth of various III-V compounds

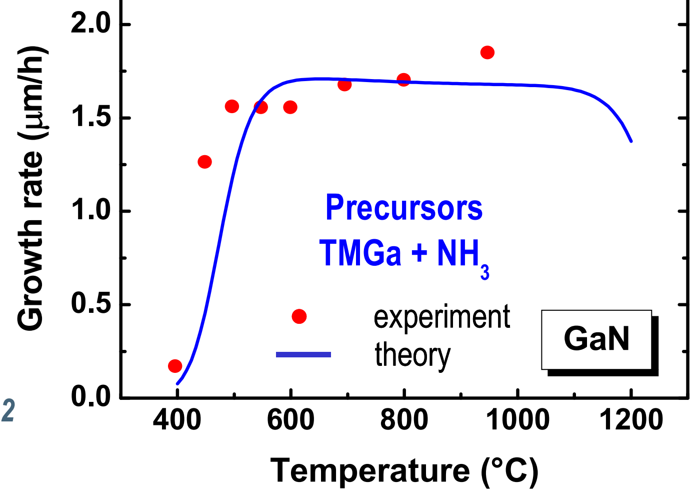


Data:
J.R. Creighton et al., Electrochem. Soc. Proc., 98-23, 75 (1999)



Data: C.Theodoropoulos et al., J.Electrochem. Soc. 142 (1995) 2086

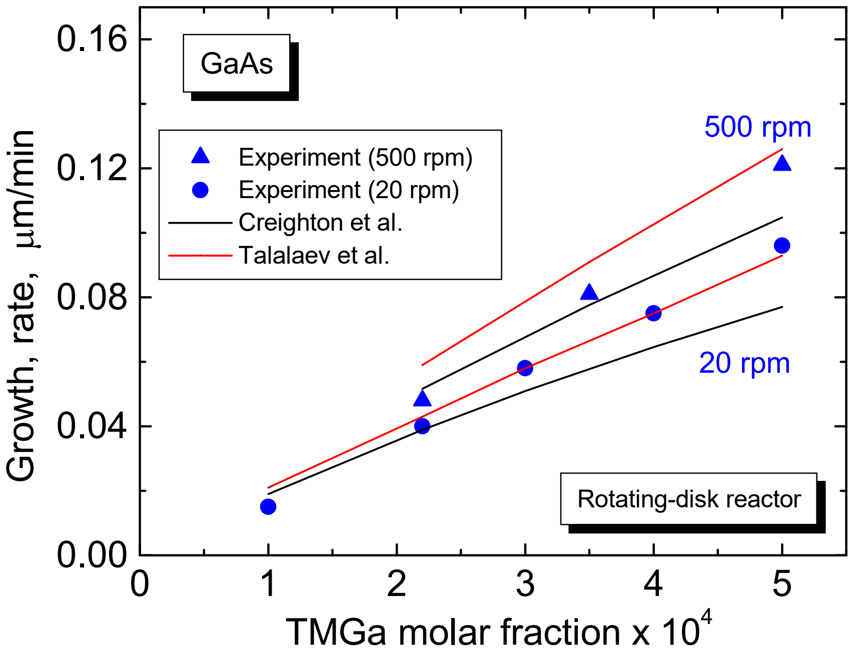
The model works well for various materials

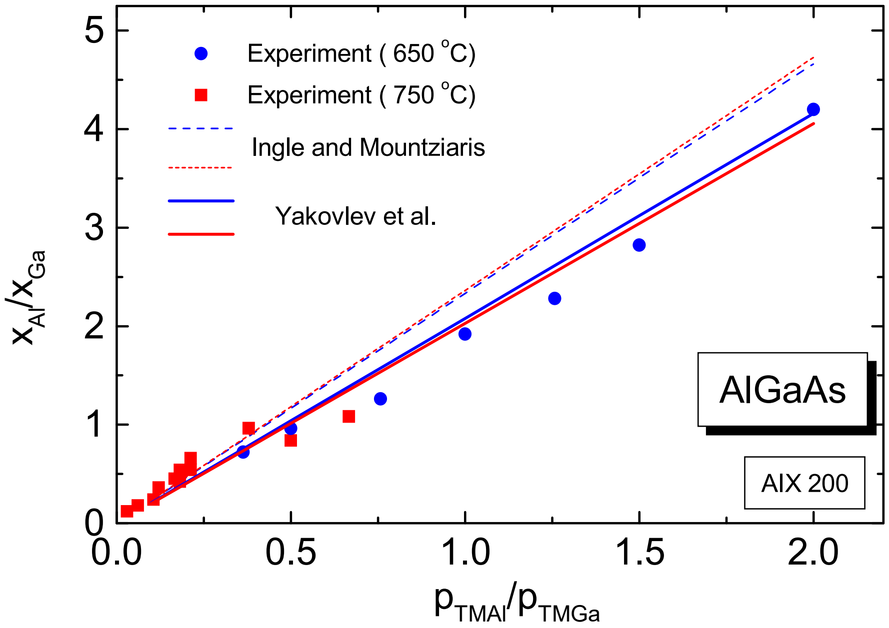


Data: C.H. Chen et al, J. Electron. Mat., 25, 1004 (1996)

R.A. Talalaev et al., JCG 230 (2001) 232

Growth of arsenides in different reactors

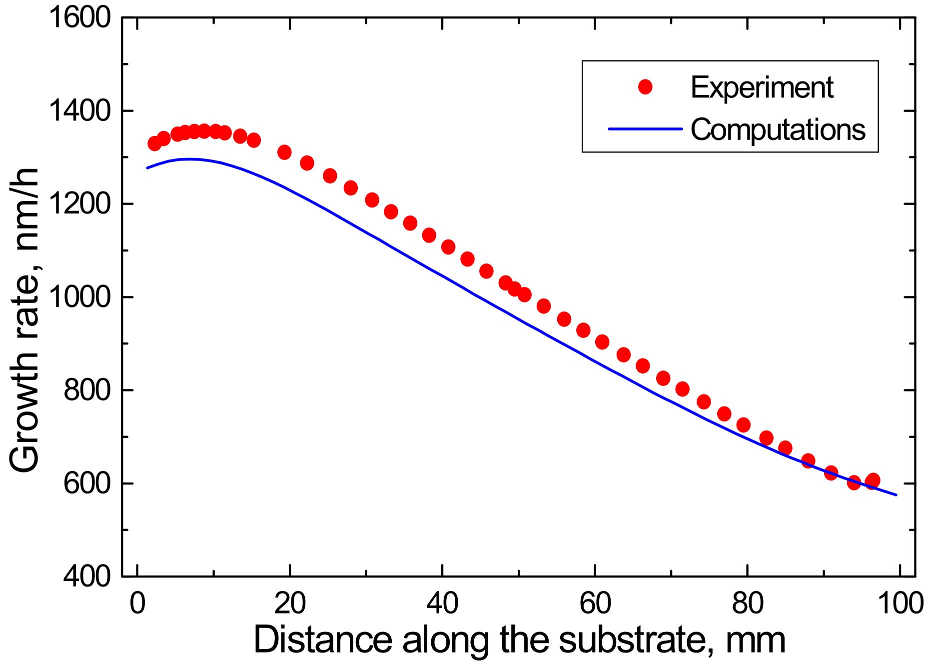




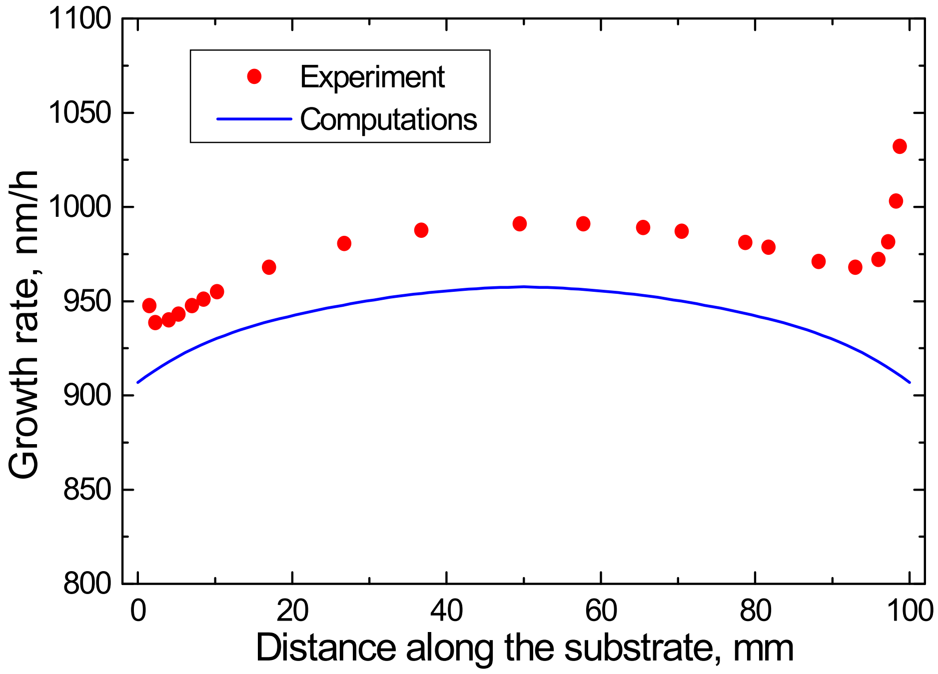
VR-III-V Edition predicts the growth rates and layer compositions without adjusting of any parameter with the accuracy comparable to (and higher than) best kinetic models.

AlGaAs growth rate distribution along the static and rotating wafer

static wafer



rotating wafer



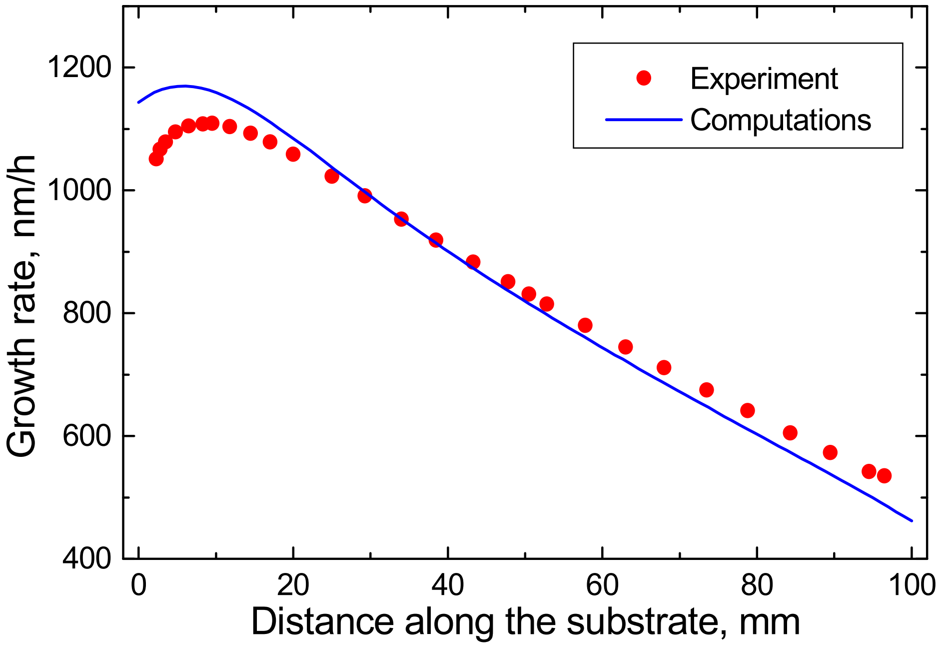
data: E.V. Yakovlev et al., *Electrochem. Soc. Proc.*, **2000-13** (2000) 723.

Computations predict the growth rate with the accuracy about 5 % for the static wafer and about 8 % for the rotating wafer

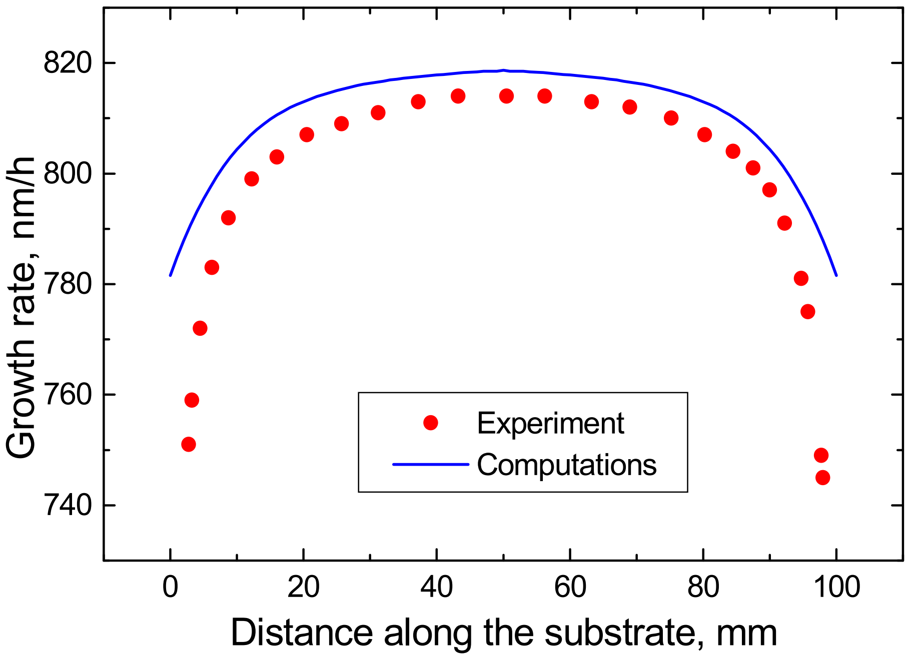
Model Validation

InGaP growth rate distribution along the static and rotating wafer

static wafer



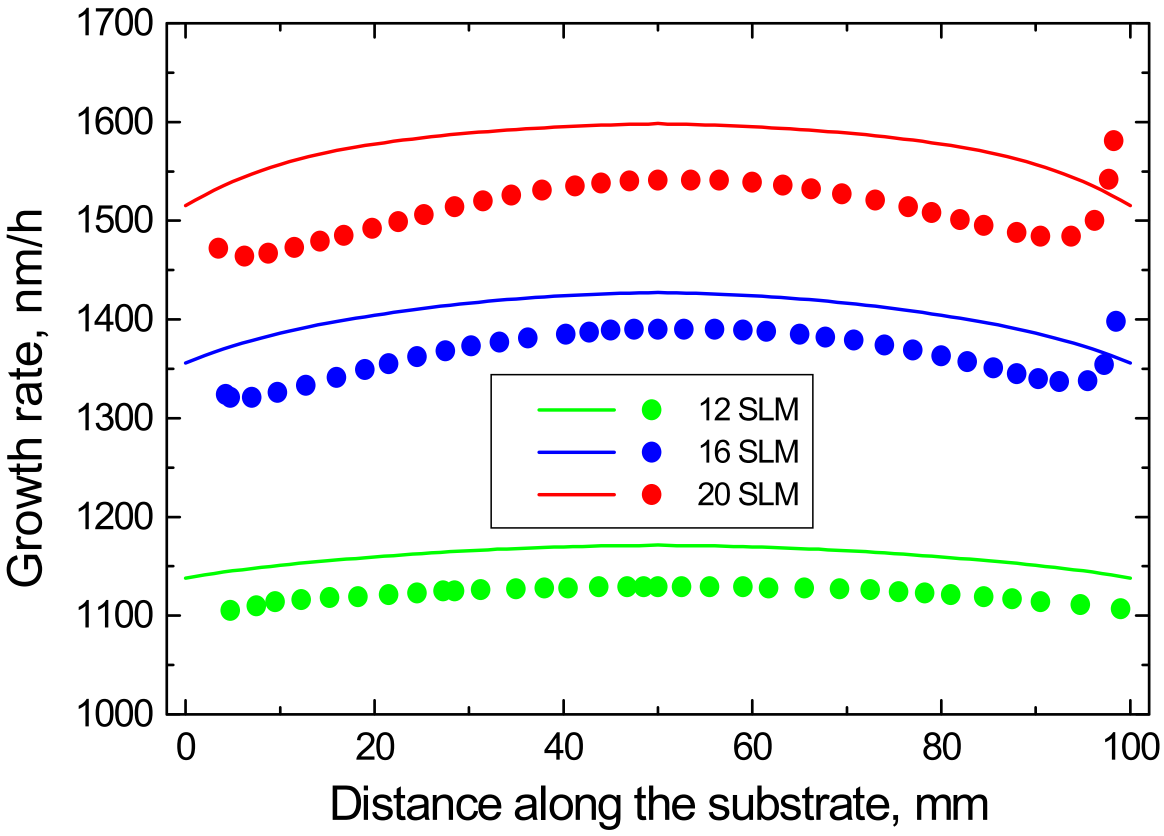
rotating wafer



data: E.V. Yakovlev et al., *Electrochem. Soc. Proc.*, **2000-13** (2000) 723.

Computations predict the growth rate with the accuracy not exceeding 3 % for both static and rotating wafers

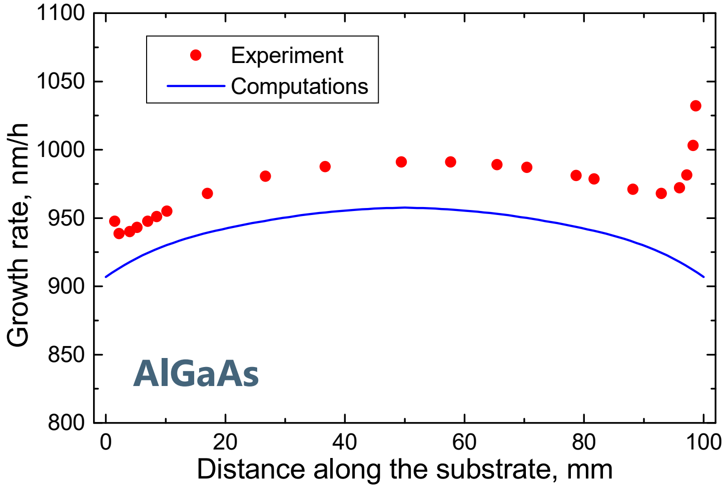
Effect of the total flow on the thickness uniformity

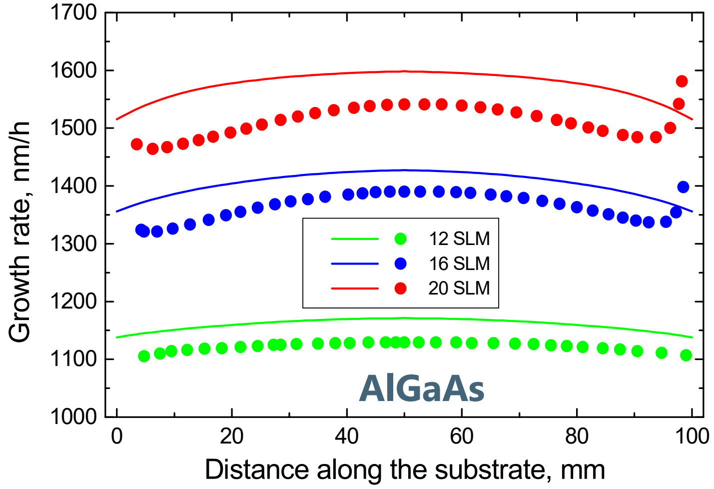


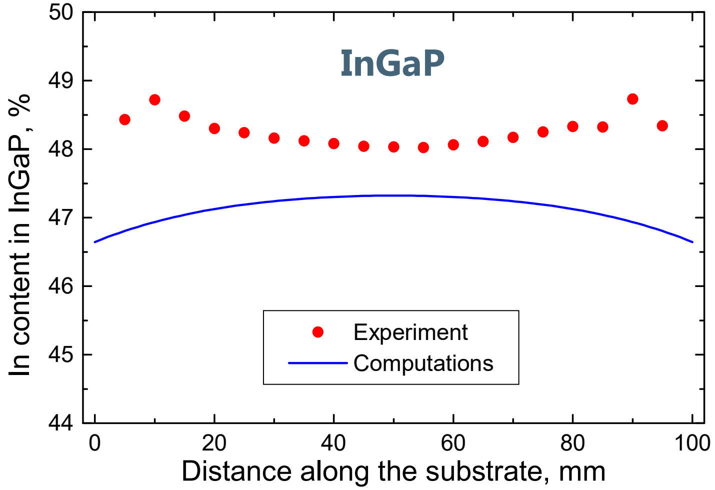
data: T. Bergunde et al., *Presented at EWMOVPE-IX* (2001).

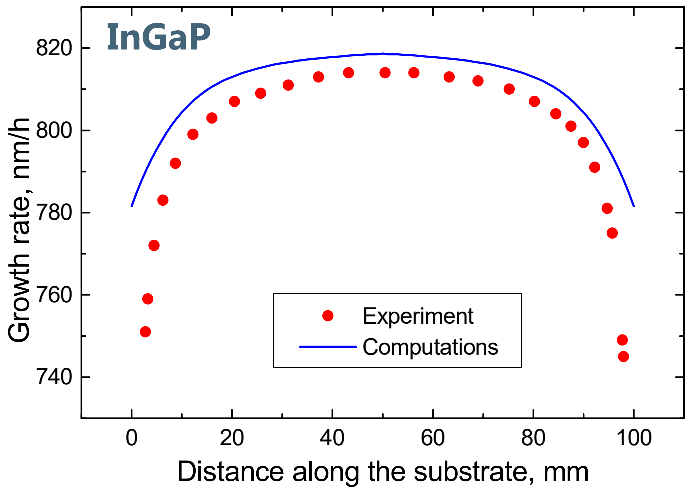
The effect of the total flow on the growth rate values and uniformity is captured well by the modeling

Model application to the AIX 2400 G3 reactor: summary









Modeling reproduces well both growth rate and layer composition distributions over 4” wafer in the Planetary reactor

Auxiliary materials

✓ Consulting service & software support:

vr-support@str-soft.com

✓ Information on commercial software

www.str-soft.com

Detailed info is supplied to VR customers and is available upon request:

- Demo version
- Physical summary
- Code description
- GUI manual
- VR tutorials

Some VR users in Europe

SiCrystal AG

НИТРИДНЫЕ КРИСТАЛЛЫ

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WARSAW UNIVERSITY OF TECHNOLOGY

LINKÖPINGS UNIVERSITET

Физико-технический институт им.А.Ф.Иоффе

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JOINT-STOCK COMPANY «RADIO ENGINEERING CORPORATION «VEGA»

Some VR users in South-East Asia

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SHOWA DENKO

KICET KOREA INSTITUTE OF CERAMIC ENGINEERING AND TECHNOLOGY

SUMITOMO ELECTRIC

CRIEPI Central Research Institute of Electric Power Industry

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