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



# **Virtual Reactor**



2018 STR Group, Inc.



**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<sup>™</sup>-PVT SiC
  - For growth of AIN: VR<sup>™</sup>-PVT AIN
- Hydride Vapor Phase Epitaxy: HEpiGaNS™
  - For growth of GaN
  - For growth of AIN and AIGaN
- Chemical Vapor Deposition
  - For growth of SiC: VR<sup>™</sup>-CVD SiC
- Metal-Organic Chemical Vapor Deposition
  - For growth of GaN, AIN, InGaN, AlGaN, and AlInN: VR™-Nitride Edition
  - For growth of AIAs, AIP, GaAs, GaP, InAs, InP, AIGaAs, InGaAs, InGaP and AlInGaP: VR™-III-V Edition



# **VR<sup>™</sup>-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**



- 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;

**Materials** 

- 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.



2D View

Stream Traces and Temperature Distribution



#### **Gas-Phase Chemistry**

- Gas-phase chemistry is relatively simple compared to VR Nitride Edition (lower temperatures);
- Ga/In/AI 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.



MMAI Partial Pressure

#### **TMAI** Partial Pressure



#### **Gas-Phase Chemistry**



#### **TMGa Partial Pressure**

MMGa Partial Pressure



AsH<sub>3</sub> Partial Pressure

CH<sub>3</sub> Partial Pressure



#### **Surface Chemistry**

- Ga/In/AI 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  $Al_xGa_{1-x}As$  (right) across the susceptor

**Graphical User Interface** 



## **VR<sup>™</sup>-III-V** Edition

### **Graphical User Interface**



#### **Specification of the Reactor Geometry**

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'Block74' - Solid			
'Block33' - Gas			
'Block34' - Gas			
'Block54' - Gas			
'Block73' - Gas			
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#### **Mesh Generation**





#### **Specification of the Materials Properties**

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#### **Specification of the Gas Mixture**

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#### **Specification of the Boundary Conditions – AlGaAs Surface**

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#### **Specification of the Boundary Conditions – Inlets**

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## **VR™-III-V Edition**

### **Validation of the Chemical Models**

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



#### Low-temperature growth of various III-V compounds



#### 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.



## AIGaAs growth rate distribution along the static and 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



## 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



✓ Consulting service & software support:

vr-support@str-soft.com

 ✓ Information on commercial software <u>www.str-soft.com</u>

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











