Virtual Reactor

VR™ Nitride Edition

Software for Modeling of Epitaxial Growth of Group-III Nitrides by Metal-Organic Chemical Vapor Deposition

Version 7.2

Code Description

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Software Overview

Virtual Reactor (**VR™**) is a family of two-dimensional software tools designed for the simulation of growth of bulk crystals and thin films from the vapor phase. **VR™ Nitride Edition** is designed for modeling of epitaxy of thin films of Group-III Nitrides.

Virtual Reactor provides comprehensive information about numerous physical processes responsible for crystal growth and film epitaxy. This includes information on the distribution of temperature and gas species concentrations, heat fluxes, deposition rate and other parameters in the overall reactor and along all walls of the reactor units. This, in turn, provides wide possibilities for profound investigations of the phenomena underlying the growth, which allows optimization of the reactor geometry and growth conditions.

The problem is considered in axisymmetric or plane 2D approximation. The growth simulation includes modeling of the heat transfer, gas mixture flow and reactive species mass transport, in particular, multi-component diffusion and chemical reactions in the gas domain. The software employs a homogeneous chemistry model involving precursor decomposition, model of the particle nucleation and original heterogeneous chemistry models.

The **Virtual Reactor** is designed with a friendly user interface (GUI) which is aimed at minimization of the user efforts needed for the problem specification. The user needs to prescribe reactor geometry and specify the growth conditions.

Unstructured triangular and quadrilateral non-matched computational grids are used in numerical simulation. The grid generation is carried out for each geometry block providing the required grid density.

Series computations of the heat- and mass transport at a set of computation stages with user-specified values of the precursor flow rates, reference temperature, coil position and total gas pressure allow parametric study of the epitaxial growth dependence on the operating conditions.

Run-time and post-processing visualization is available within the GUI, presenting the two-dimensional and one-dimensional distributions of temperature and other variables. In addition, **Virtual Reactor** is supplied with external visualization tool **View 2D**. The computational results are also stored in plain text files allowing a post-processing analysis using Tecplot and other commercial graphical packages.

Key Features

VR™ Nitride Edition software tool includes the following modes:

- MOCVD-GaN: GaN epitaxy from TMGa and NH_3 with H_2 and N_2 as carriers
- MOCVD-AlN: AlN epitaxy from TMAl and NH_3 with H_2 and N_2 as carriers
- MOCVD-InGaN_TMGa: $In_xGa_{1-x}N$ epitaxy from TMGa, TMIn, and NH_3 with N_2 as carrier
- MOCVD-InGaN_TEGa: $In_xGa_{1-x}N$ epitaxy from TEGa, TMIn, and NH_3 with N_2 as carrier
- MOCVD-AlGaN: $Al_xGa_{1-x}N$ epitaxy from TMAl, TMGa, and NH_3 with H_2 and N_2 as carriers
- MOCVD-AlInN: $Al_xIn_{1-x}N$ epitaxy from TMAl, TMIn, and NH_3 with N_2 as carrier

The mass transport and chemistry models incorporated into **VR™ Nitride Edition** can be applied to the following types of MOVPE reactors:

- Planetary reactors
- High-speed rotation Turbodisc reactors
- Horizontal reactors
- Close-coupled showerhead reactors
- Home-made reactors that can be simulated within a 2D plane or axisymmetric model

The following options are incorporated in the **VR™ Nitride Edition** software tool:

- Modeling of the global heat transfer problem in a MOCVD reactor, including
  - ✓ Inductive heating (for axisymmetric problems only). The computation of the Joule heat sources due to inductive heating is carried out by solving the Maxwell equations.
  - ✓ Resistive heating. The resistive heating is modeled by assigning a uniform heat release distribution in the heater. The user can split the heater block into several units and specify either the global heat release in the heater or the power density in each unit.
  - ✓ Temperature fitting. The program predicts power needed to maintain the desired temperature in a reference point.
  - ✓ Conductive heat transfer in solid materials. The thermal conductivity of the materials used in the growth system can be prescribed by the user as a function of temperature. Anisotropic thermal conductivity can be assigned
  - ✓ Convective and radiative heat transfer in transparent gas blocks. The view-factor technique is used to model the radiation heat exchange. The surface emissivities are assigned as constant values.

- Modeling of the mass transport in the reactor includes
  - ✓ Non-isothermal flow of gas mixture. Heat conductivity and viscosity of the mixture are calculated in terms of molecular kinetic theory.
  - ✓ Multi-component diffusion of reactive species.
  - ✓ Homogeneous chemistry.
  - ✓ Gas-phase nucleation and transport of nanoparticles.
  - ✓ Instantaneous values of the growth rate and compound composition and the averaged values calculated accounting for the substrate rotation.
- Turbulent flow considered using an algebraic turbulence model
- Database of Material Properties, User Manual, Context Help, and files with examples of computations.
- Modeling of surface chemistry on chemically reactive surfaces of the substrate and parasitic deposition on the reactor side walls accounting for the kinetic limitations, which are calculated by the program as a function of temperature and local gas mixture composition.
- Visualization of the obtained results.

More Info

More detailed information about the **VR™ Nitride Edition** can be requested by the e-mail address VR-support@str-soft.com.

Support

Hot-line support is provided on request. The support includes supply of updated versions released during the license period and technical consulting on the **VR™ Nitride Edition** operation.