CVDSim™ – Nitride Edition

Chemical Vapor Deposition Simulator

Add-on for ANSYS Fluent

Simulation Tool for Modeling of CVD Processes
in Industrial Reactors

Release Notes

October 2012

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Abstract

1. We have developed a chemical model that is suitable for the modeling of **GaN growth in K465i** vertical high-speed rotating-disc reactors. The model is implemented into ANSYS Fluent and available through CVDSim menu. The corresponding example has been added in the **Examples** folder.

2. New **Boundary Conditions Editor** design has been developed and available in CVDSim menu. **Probe surface** option will help to select boundary with mouse right click from now on.

Modeling of GaN MOVPE in K465i Reactors

We have developed a chemical model that is suitable for the modeling of GaN growth in K465i vertical high-speed rotating-disc reactors. The most important aspects of the model include:

- quasi-equilibrium formation of adduct from TMGa and ammonia;
- low-activated irreversible formation of amide ($DMGaNH_2$) from adduct $TMGa:NH_3$;
- highly activated irreversible formation of GaN vapor form amide followed by generation of particles.

The model is able to reproduce the experimental dependencies of the GaN growth rate as a function of the flange temperature, pressure, TMGa flow rate, and other process parameters. Some modeling results in comparison with experimental data from [1] are shown below.

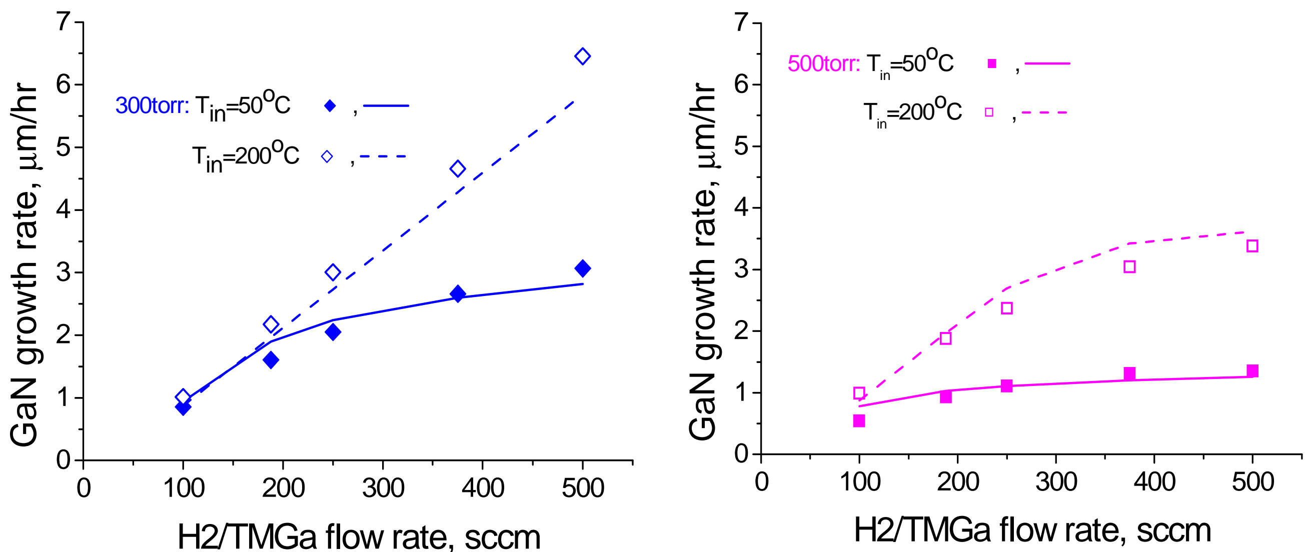


Fig. 1. GaN growth rate as a function of the bubbler TMGa flow rate for the flow flange temperatures of 50 °C (solid lines) and 200 °C (dashed lines) at the reactor pressure 300 torr (left) and 500 torr (right).

The mechanism of gas-phase reactions is named ***GaN_kinetic_DMGa_DMGaNH2***, the corresponding model of particle formation is available via section

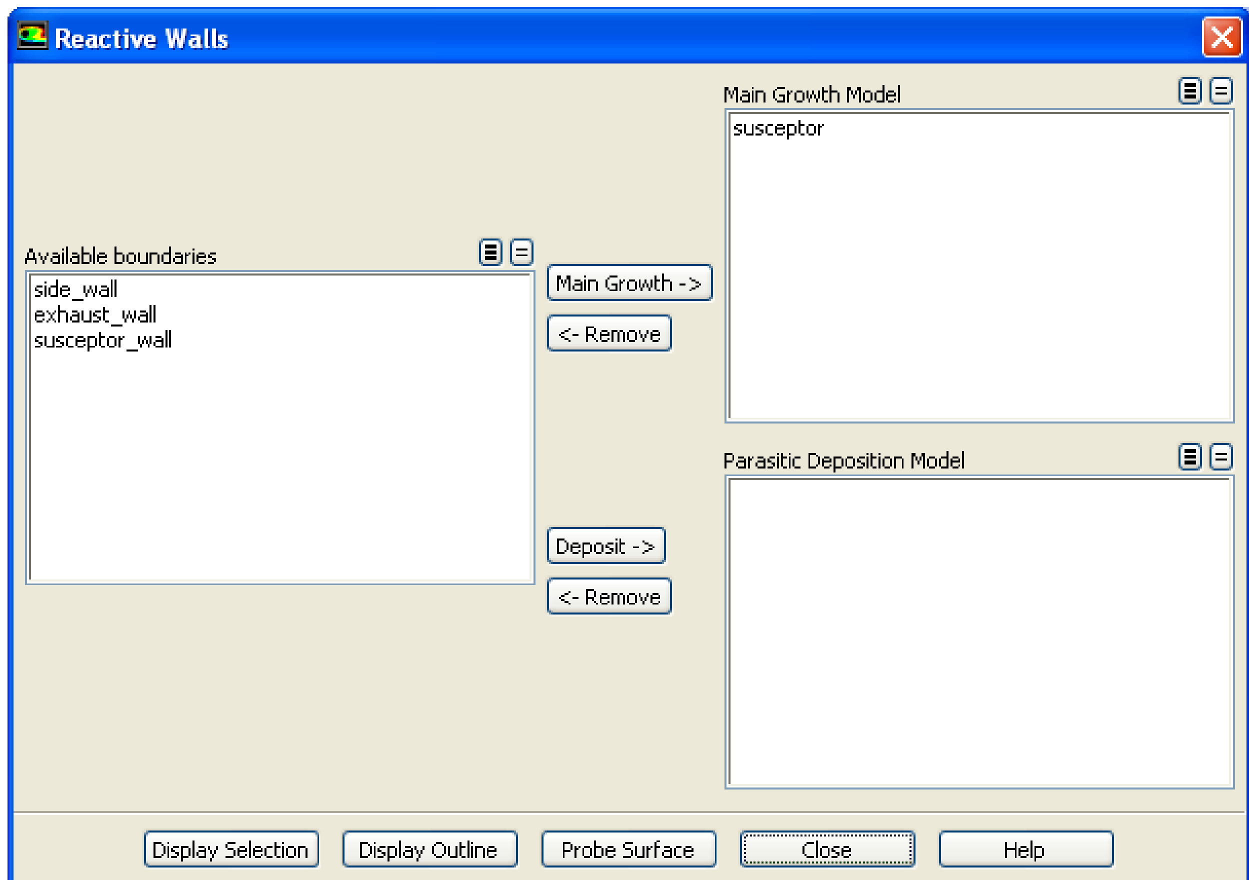
Condensation: GAN_201205

in the ***hetero.set file***.

Note also that *a6* coefficient of the polynomial approximation for $TMGa:NH_3$ properties has been corrected. This correction allows better agreement with experimental data on the TMGa-adduct equilibrium.

[1] J. Montgomery, presented at 2011 DOE Solid-State Lighting Manufacturing R&D Workshop, Boston, MA, April 12–13, 2011 (http://www1.eere.energy.gov/buildings/ssl/boston2011_materials.html).

BC editor



New **Boundary Conditions Editor** design has been developed. The style has become more Fluent-like. **Probe Surface** button has appeared. Pressing this button user can right-click in the display window, and the nearest boundary will be selected in the **Available boundaries** list.