User Story

Application of *kinetics*™ to Chemical Vapor Deposition (CVD) Process

A Generic Reactor Network feature in *kinetics*™ was applied to model surface and gas phase chemistry involved in the CVD process

THE CHALLENGE

To accurately and rapidly simulate the gas and surface chemistry involved in a CVD process in order to account for deposition and growth of the material being deposited

To study the growth of species such as Carbon Nanotubes (CNT), Silicon (Si) and Silicon Nitride (Si_3N_4)

THE SOLUTION

- A detailed mechanism describing the surface and gas phase chemistry implemented in the Generic Reactor Network feature in *kinetics*™
- The chemistry is solved as a set of coupled ODEs for individual species and temperature with kinetic information as in terms of a Modified Arrhenius Equation parameters or the Sticking Equation parameters

THE RESULTS

- Quick simulation of detailed chemical kinetic models for deposition of materials on a surface and accounting for it's growth, using *kinetics*™
- Deposit thickness is calculated from the surface molar coverage of particle(s) of interest using mass density and molar mass
- Account for variation in CVD process conditions such as mass flow rates and deposition temperature

OVERVIEW

The Generic Reactor Network feature in CMCL Innovations' proprietary software *kinetics*™ enables the implementation of surface and gas phase chemistry used for the simulation and optimization of CVD processes for the deposition of a material on a surface.

Chemical Vapour Deposition (CVD) process involves the deposition of a solid material from gaseous pre-cursors (Figure 1). CVD is widely used in the semi-conductor industry for coating thin films onto substrates such as wafers. It allows for great control over the thickness and other physical aspects of the coated material.

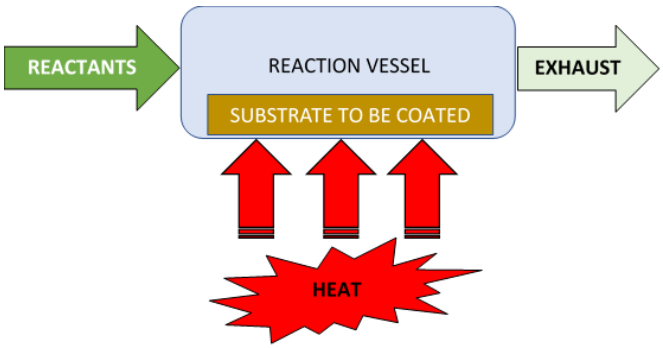

Figure 1: General Schematic of a CVD Process

Simulations of CVD involve handling the chemistry and the hydrodynamics of the process. *kinetics*™ allows for a quick, yet detailed representation and solution of the chemistry in a CVD process. It handles the chemistry in 3 parts – the gaseous, surface and the bulk phase (Figure 2), directed by the standardised input chemical mechanism file.

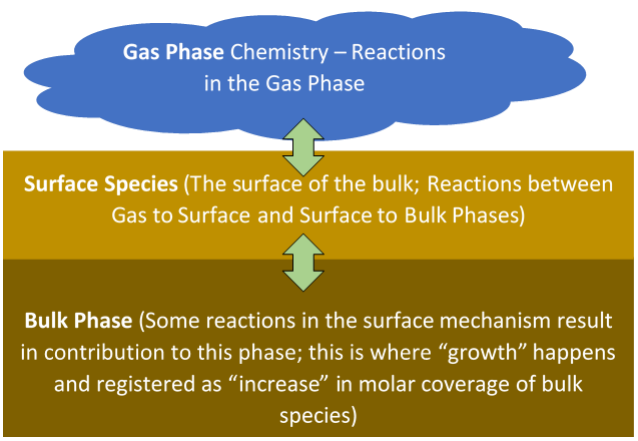

Figure 2: Chemistry description in *kinetics*™

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RESULTS

kinetics™ was applied to three different CVD processes – deposition of Si_3N_4[1], growth of Carbon Nanotubes (CNT)[2] and Silicon (Si) Epitaxy[3]. The processes were represented using either a single or network of perfectly stirred reactors (PSR) with a substrate present for deposition on the basis of the operating conditions presented in the publications.

The growth rate variation as a function of the operating temperature for the CNT case is shown in **Figure 3**. It demonstrates the role of the surge in temperature that increases the rates of gas phase and surface reactions, and hence the growth rate.

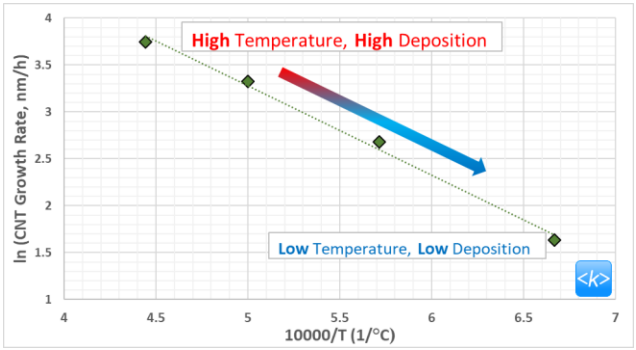

Figure 3: CNT Growth Rate Variation with Temperature

APPLICATION AREAS

- Modelling chemical kinetics in CVD reactors
- Study the effects of process variables such as temperature, flow rates, volumes and inlet compositions, on the key outputs such as growth and deposition

- *kinetics*™ toolkit offers:
  - A stand-alone test bed for chemical kinetics investigations
  - API to provide chemical source terms to 3rd party software including fast-response as well as 3D CFD models

PRODUCTS USED

- *kinetics*™

The variation of growth with mass flow rates for the Si_3N_4 process is shown in **Figure 4**. As the exit concentrations increase with the flow rates, which, in the case of a PSR, suggests a higher reaction rate and thus the deposition rate in the reactor.

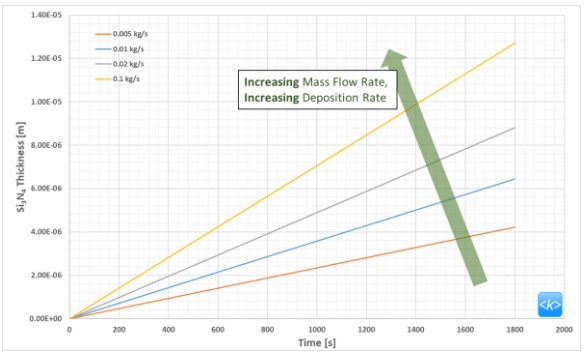

Figure 4: Si_3N_4 Growth variation with Mass Flow Rate

The growth of Si in a CVD reactor is shown in **Figure 5**. This growth rate is continual and does not reach a steady state. This is attributed to the fact that the site saturation is not accounted for in this study.

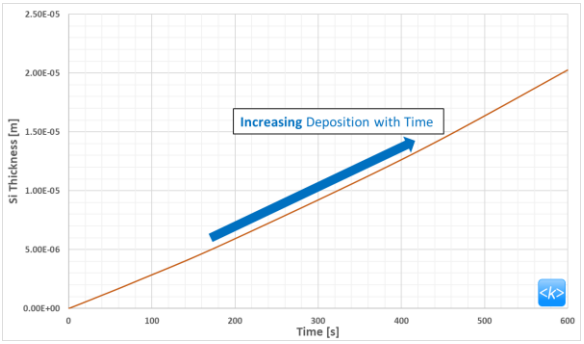

Figure 5: Si Growth with Time

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1. C. Gomez-Aleixandre et al., Journal of Materials Science, 1991
2. I. Hinkov et al., Journal of Surface Engineered Materials and Advanced Technology, 2014
3. P. Ho et al., Sandia National Laboratories, 1998

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