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RAREFIED GAS DYNAMICS MODELLING IN INDUSTRIAL APPLICATIONS

TNO | Knowledge for business
TNO is active in five core areas

- Quality of Life
- Defence, Security & Safety
- Science & Industry
- Built Environment & Geosciences
- Information & Communication Technology
Playing field of IMC

Key expertise in:

- Mass and heat flow
- Process technology
- Control Engineering
ADDED VALUE in High-Tech Instrumentation

High-Tech Equipment
- Semi-conductor eq.
- Medical equipment
- Printing equipment

Space & Science
- Earth observation
- Astrophysics
- Nuclear fusion
Main message

Modeling rarefied gas dynamics adds value to the system engineering process

• Examples:
  • EUV lithography
  • Design and improvement of vacuum pumps
  • CVD & ALD optimization
  • MEMS design
  • Contamination control
  • Accelerators
  • Detector design and life time improvement
  • Etc.
  • Etc.
Example 1: CVD/ALD trench fill optimization using X-Stream/CVD-X for ASM International

1. Transient ALD simulations for a multi-wafer reactor with trenched wafers
   A.M. Lankhorst, B.D. Paarhuis, H.J.C.M. Terhorst, P.J.P.M. Simons
   & C.R. Kleijn, EURO-CVD 2007
<table>
<thead>
<tr>
<th>Name</th>
<th>X-Stream</th>
<th>GTM-X</th>
<th>CVD-X</th>
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</thead>
<tbody>
<tr>
<td>Application</td>
<td>General purpose CFD</td>
<td>Glass-dedicated</td>
<td>CVD-dedicated</td>
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</tbody>
</table>
| Functionality                      | • Time transient  
                              | • Steady state  
                              | • Batch  
                              | • Gas phase reactions  
                              | • Steady state  
                              | • Boosting  
                              | • Surface reactions  
                              | • Body-fitted  
                              | • Bubbling  
                              | • Sticking / ALD sticking  
                              | • Multi-domain  
                              | • Foam  
                              | • Trench Models  
                              | • Structured/collocated  
                              | • Redox  
                              | • Rarefied flow (DSMC)  
                              | • Parallel  
                              | • Volatilization  
                              | • CHEMKIN interface  
                              | • State-of-the-art solvers  
                              | • Corrosion  
                              | • Multi-component  
                              | • Turbulence  
                              | • Quality indices  
                              | • Plasma  
                              | • Combustion, soot, NOₓ  
                              | • Drawdown  
                              | • Rarefied flow (DSMC)  
                              | • Radiation  
                              | • Thermal homogeneity  
                              | • 3D & 1D walls  
                              | • Refractory wear  
                              | • Particle trace  
                              | • Stiff systems solvers  
                              | • Boundary conditions  

Problem description

• 3 dimensional, transient ALD/CVD simulations on a multi-wafer reactor with TEMAH-HfO₂ deposition on *trenched wafers*

• Trenches can easily multiply the effective area by a factor of 10

*Multi-scale physical problem in terms of flow regimes and time scales involved*
Problem description

- **Flow regimes**
  - Compressible flow at gas injectors
  - Laminar incompressible flow in corridor
  - Transitional regime in between wafers
  - Molecular in trenches
Problem solution

- **CFD model**
  - Compressible flow model
- **Slip flow boundary conditions in between wafers**
- **Knudsen-diffusion model in trenches**
  - Bi-directional coupling between CFD domain and molecular domain
  - Mass flow, pressure, temperature, trench area are all dynamically determined
- **Trench model validated with DSMC**
Trench model

- Different trench models available
  - Effective area
  - Gordon
  - Knudsen-Diffusion

Only for ALD, high $f_s$ and narrow trenches
CVD deposition in shallow trenches
Physical background

Trench

- CVD process

gas: $M_g$, $P_g$, $T$
Physical background

Trench

- CVD process
  - Cross section trench-entrance
  - Penetration depth molecules
  - Surface reaction probability

\[ \text{gas: } M_g, P_g, T \]
Physical background

Trench

- CVD process
  - Cross section trench-entrance
  - Penetration depth molecules
  - Surface reaction probability
  - Diffusion time
  - Layer thickness

\[ \text{gas: } M_g, P_g, T \]
Physical background

Trench

- CVD process
  - Cross section trench-entrance
  - Penetration depth molecules
  - Surface reaction probability
  - Diffusion time
  - Layer thickness
  - Step coverage
  - Enclosures (process stops)

gas: $M_g$, $P_g$, $T$
Physical background

Trench

\textit{gas: } M_g, P_g, T

• ALD process
Physical background

Trench

gas: $M, P, T$

- ALD process
  - Only one monolayer
Physical background

Trench

- ALD process
  - Only one monolayer
  - Site coverage increases

\( \text{gas: } M_g, P_g, T \)
Physical background

Trench

gas: $M_g$, $P_g$, $T$

- **ALD process**
  - Only one monolayer
  - Site coverage increases
  - As coverage proceeds, $K$ becomes smaller and less molecules will enter
Physical background

Trench

- ALD process
  - Only one monolayer
  - Site coverage increases
  - As coverage proceeds, less molecules will enter
  - 100% coverage, process stops

$\text{gas: } M_g, P_g, T$
CVD, Knudsen Diffusion, transient

CVD-X simulation of a CVD process
Duct, U = 0.1
Knudsen diffusion model

CVD-X simulation of a CVD process
Duct, U = 1.0
Knudsen diffusion model

CVD-X simulation of a CVD process
Duct, U = 10
Knudsen diffusion model

Duct, U = 0.1
\( t = 10.000 \text{ s} \)

Duct, U = 1.0
\( t = 9.000 \text{ s} \)

Duct, U = 10
\( t = 100 \text{ s} \)
Geometry and grid

- 66 wafers
- Two top-dump injectors
- One outlet at bottom
- Complete reactor
- Double pitch

- **Number of grid cells:**
  - 500,000
- **Building time:**
  - 1 day
- **Steady-state flow simulation:**
  - 3 hr
- **Transient simulation for 120 s, timestep 0.1 s:**
  - 16 hr)
Process settings and model input

**TEMAH-HfO\(_2\):** Hf \([\text{N(C}_2\text{H}_5)\text{(CH}_3)\text{]}_4 + 2 \text{O}_3 \leftrightarrow \text{HfO}_2\)

- **T** = 220 °C
- **P\(_\text{mix}\)** = 700 mtorr
- **flow\(_\text{mix}\)** = 1.3 slm
- **\(\rho\text{mix}\)** = 6.918 \(\cdot\) \(10^{-4}\) kg/m\(^3\)
- **\(\eta\text{N}_2\)** = 2.504 \(\cdot\) \(10^{-5}\) Pas
- **ID\(_\text{TEMAH}\)** = 0.0196 m\(^2\)/s
- **\(\omega\text{TEMAH}\)** = 0.085 kg/kg\(_\text{mix}\)

- **M\(_\text{TEMAH}\)** = 410.9 g/mol
- **M\(_\text{HfO}_2\)** = 210.5 g/mol
- **\(\rho\text{HfO}_2\)** = 9700.0 kg/m\(^3\)
- **sticking coeff** = 0.1
- **site density** = 8.3 \(\cdot\) \(10^{-6}\) mol/m\(^2\)
- **d\(_\text{monolayer}\)** = 0.18 nm
- **N\(_\text{wafers}\)** = 66
- **pitch** = 14.0 mm

Trenched cases: Upper side of all wafers trenched

Lower side of all wafers, reactor walls, top/bottom plates not trenched
Multi wafer reactor

- Rarefied gas transport trench models have been developed and incorporated in CVD-X
- Validation of trench models with DSMC
- Multi-scale physical simulations for complete wafer reactor with short calculation times
- Added value for customer
  - Much better insight in process parameters
  - Better control over throughput (speed!)
  - Better control over expensive precursor flow – Flow out of reactor should be avoided, but enough precursor should be present to account for the presence of trenches
Example 2: Mirror contamination control in EUV lithography
EUV lithography
Problem description

- EUV Lithography uses 13.5 nm radiation
- Is absorbed by all materials and most gases even at moderate pressures (<1 mbar)
- Gaseous (carbon hydroxides) contamination is fatal for mirror reflectivity (one monolayer)
- Control/mitigation of contamination is a key issue
Problem description

- Lenses use multilayer coatings
- 100 layers
- Some are only a few atoms thick
- $R \approx 0.65$
- $9 \text{ reflections: } (0.65)^9 \approx 0.02$
- Reflection loss (EUV stimulated)
- Oxidation
- Carbonization
- $0.60^9 \approx 0.01$
Problem description

• How to prevent gaseous contamination to reach the mirror surfaces from various sources?
  • Outgassing/desorption
  • Sensors
  • Robot bearings
  • Valves
  • Wafer (!)
  • Etc.
Problem solution

- Combination of different solutions
  - Minimization of contaminations
  - Suppression of contamination
  - Mirror cleaning systems
  - Etc..

- Example: Suppression of diffusion (calculations)
DSMC Example

Contamination source

Purge flow

Clean area

What is the contamination pressure (or suppression)??
DSMC calculation of suppression ratio

- Suppression of diffusive flux by convective flux
- Suppression of diffusion ratio of diffusion ratio (only at transitional or continuum flow)
- PE ~ e^P (continuum)
- Spec: R > 300
- \( P_e = \frac{L/A}{c_o \cdot D \cdot P} \)
- Issues
  - Highly sensitive to parameters
  - Formula above only for continuum flow
  - Exact mass flux and speed unknown
  - Analytical and network calculation showed R = 23 · · · 5000
- Highly sensitive to parameters

- DSMC calculation of suppression ratio
DSMC case

- Species suppression with DSMC

- Geometry
- Purge pressure
- Purge velocity
- Temperature
- Species density
- Species suppression
EUV contamination

- Quick and accurate calculation of mass flow
- At transitional flow conditions
- Added value for customer
  - Quick answer on problem which is difficult to solve with engineering/analytical calculations
  - Easy to vary parameters such as purge species, contamination species
  - Validation of specifications by simulation
  - Insight in experimental conditions for experimental qualification !! (absolute pressures, partial pressures, etc…)

Take home message

- Modelling of rarefied gas dynamics results in added value for the international industry
  - Problem solving
  - Product performance
  - Product quality (lifetime, contamination control)
  - Accuracy (thermal stability, dynamical stability, …)
  - Overall: innovative, cheaper, faster, more stable systems and solutions
Word of thanks

Thank you for your attention!

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