Thin-film manufacturing process technology

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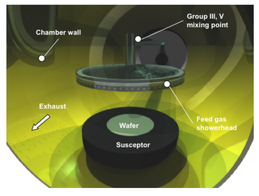
THIRTY YEARS OF SYSTEMS RESEARCH EXCELLENCE

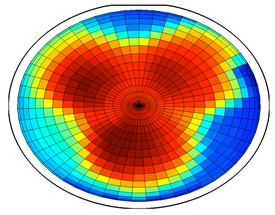
INSTITUTE FOR SYSTEMS RESEARCH
A. JAMES CLARK SCHOOL OF ENGINEERING

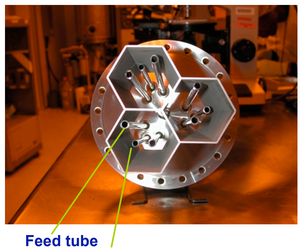
Historical context: Chemical vapor deposition process model-based design and optimization

- Modeling, design, and experimental evaluation of spatially programmable CVD processes
- GaN MOVCVD modeling and process optimization with Northrop Grumman

Extensive collaboration with Prof. Gary Rubloff

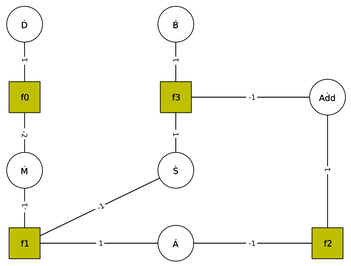


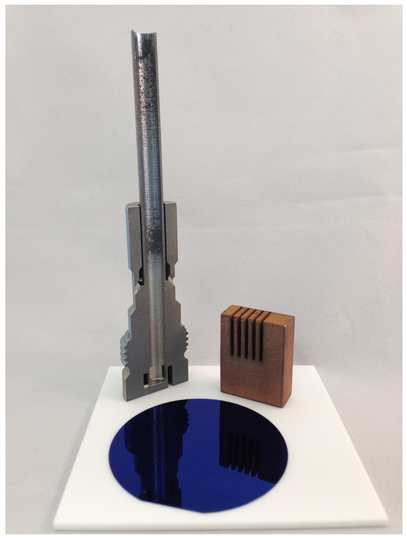




Future directions

- Atomic Layer Deposition simulation for aerospace applications in collaboration with NASA
- Exploring the connection between graph theory and deposition reaction networks





Dynamic dimension reduction of deposition mechanisms

$$2M \Leftrightarrow D \qquad G_0 = \frac{1}{\epsilon_0}\left(K_0[M]^2 - [D]\right) \qquad \text{mol s}^{-1}\text{m}^{-3}$$

$$M \Leftrightarrow A \qquad G_1 = \frac{1}{\epsilon_1}\left(K_1[M] - [A]\right) \qquad \text{mol s}^{-1}\text{m}^{-2}$$

$$A \rightarrow B \qquad F_0 = k_0[A] \qquad \text{mol s}^{-1}\text{m}^{-2}$$

Modeling equations for the heterogeneous tubular CVD system

$$\frac{\partial}{\partial t}\begin{bmatrix}[D]\\ [M]\\ [A]\\ \text{L}\\ [B]\end{bmatrix} = \begin{bmatrix}\partial J_D/\partial\zeta\\ \partial J_M/\partial\zeta\\ 0\\ 0\\ 0\end{bmatrix} + \begin{bmatrix}1 & 0 & 0 & 0\\ -2 & -\sigma & 0 & 0\\ 0 & 1 & -1 & 0\\ 0 & 0 & 0 & 1\\ 0 & 0 & 1 & 0\end{bmatrix}\begin{bmatrix}G_0\\ G_1\\ F_0\\ F_1\end{bmatrix}$$

or

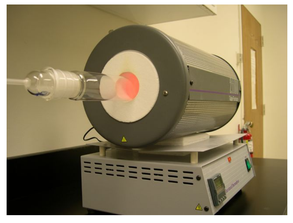
$$\frac{\partial \mathbf{c}}{\partial t} = \mathbf{j} + \mathbf{S}\begin{bmatrix}G_0\\ G_1\\ F_0\\ F_1\end{bmatrix}.$$

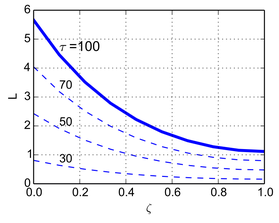
Factorization matrix

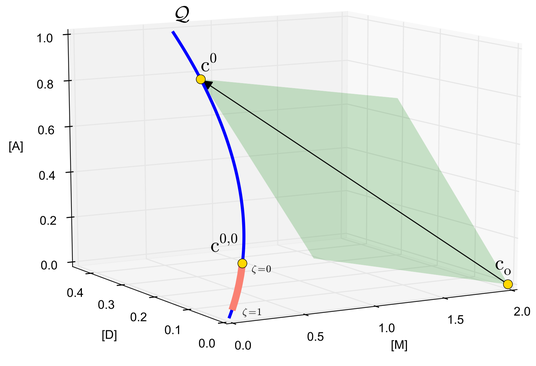
$$\mathbf{S}_F = \mathbf{U}\cdot\mathbf{S} = \begin{bmatrix}1 & 0 & 0 & 0 & 0\\ 2 & 1 & 0 & 0 & 0\\ 2 & 1 & \sigma & 0 & 0\\ 0 & 0 & 0 & 1 & 0\\ 2 & 1 & \sigma & 0 & \sigma\end{bmatrix}\cdot\begin{bmatrix}1 & 0 & 0 & 0\\ -2 & -\sigma & 0 & 0\\ 0 & 1 & -1 & 0\\ 0 & 0 & 0 & 1\\ 0 & 0 & 1 & 0\end{bmatrix} = \begin{bmatrix}1 & 0 & 0 & 0\\ 0 & -\sigma & 0 & 0\\ 0 & 0 & \sigma & 0\\ 0 & 0 & 0 & 1\\ 0 & 0 & 0 & 0\end{bmatrix}$$

New coordinates

$$\mathbf{y} = \mathbf{U}\cdot\mathbf{c} = \begin{bmatrix}1 & 0 & 0 & 0 & 0\\ 2 & 1 & 0 & 0 & 0\\ 2 & 1 & \sigma & 0 & 0\\ 0 & 0 & 0 & 1 & 0\\ 2 & 1 & \sigma & 0 & \sigma\end{bmatrix}\cdot\begin{bmatrix}[D]\\ [M]\\ [A]\\ \text{L}\\ [B]\end{bmatrix} = \begin{bmatrix}[D]\\ 2[D]+[M]\\ 2[D]+[M]+\sigma[A]\\ \text{L}\\ 2[D]+[M]+\sigma[A]+\sigma[B]\end{bmatrix}$$





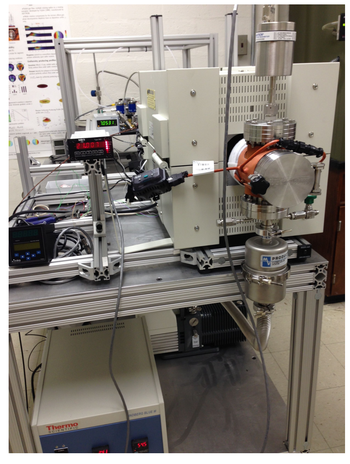


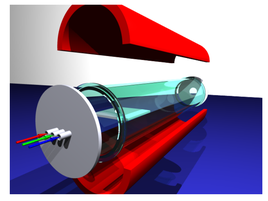
ALD reaction sequence during a TMA exposure

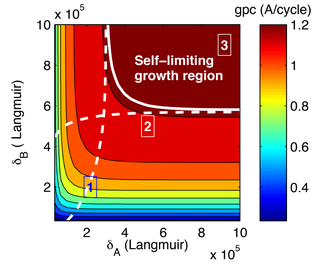
$AlMe_3$ + OH	$\xrightleftharpoons{E_0}$	$AlMe_3$ OH	$\xrightleftharpoons{E_1}$	Me Me Al H Al O Me	$\xrightarrow{I_0}$	Me Me Al O + CH_4
Me_3Al' + HO′ + 3S		Me_3AlHO		$Me_3AlHO^{\ddagger}$		Me_2Al' + Al′ + MeH + S
OH + Me Me Al O	$\xrightleftharpoons{E_2}$	Me Me Al HO O	$\xrightleftharpoons{E_3}$	Me Me Al H Al O O	$\xrightarrow{I_1}$	Me Al O O + CH_4
HO′ + Me_2Al'		Me_2AlHO		$Me_2AlHO^{\ddagger}$		MeAl′ + Al′ + MeH + S
Me Al O O + OH	$\xrightleftharpoons{E_4}$	Me Al O O OH	$\xrightleftharpoons{E_5}$	Me Al H O O O	$\xrightarrow{I_2}$	Al O O O + CH_4
MeAl′ + HO′		MeAlHO		$MeAlHO^{\ddagger}$		Al′ + MeH + S

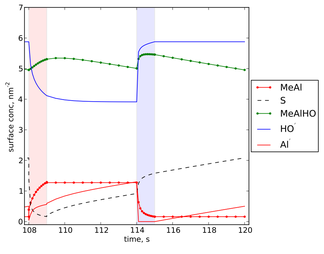
Reaction sequence for the subsequent water reactions

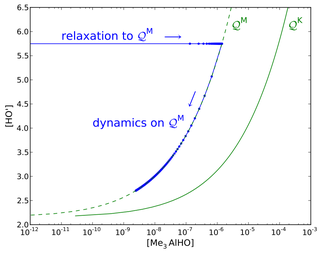
Al O O O + H_2O	$\xrightleftharpoons{E_6}$	OH_2 Al O O O				
Al′ + H_2O'		AlH_2O				
OH_2 Al O O O + Al O O O	$\xrightleftharpoons{E_7}$	H O Al H Al O O O O O	$\xrightarrow{I_3}$	2 OH Al O O O		
AlH_2O + Al′		$Al_2H_2O^{\ddagger}$		2HO′		

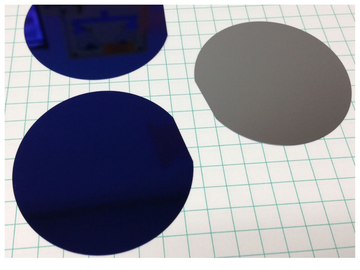












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