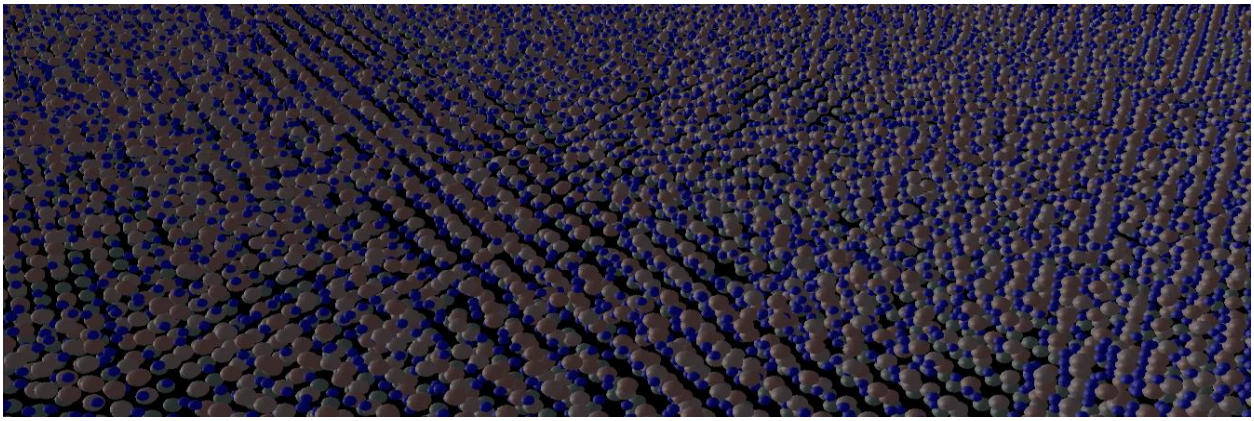
Atomistic Thin Film Growth – EpiGrow Simulator

Metalorganic Chemical Vapor Deposition (MOCVD)



Introduction

EpiGrow Simulator, **MOCVD Reactor algorithms include precursors which are used in their gaseous form. Ultra-pure gases are introduced in the reaction chamber. This gas is carefully dosed with the precursor material in over to deposit an extremely fine layer of atoms on the surface of the wafer/substrate.**

Crystal growth is favoured by the surface reactions dominated by their reaction rates taking place on the substrate surface. These reactions involve organic compounds or metalorganics and hydrides (which contain the required chemical elements for producing final end product) as the reactants. The thin films of the required material or compound semiconductor are epitaxially grown on the substrate surface.

Features

- **In EpiGrow MOCVD Simulator, crystalline layers to create complex semiconductor multilayer structures**
- **Growth of crystals are through chemical reactions and not physical deposition, incorporating thermodynamically metastable alloys**

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- **Ultra-pure precursor gases are injected into a reactor, usually with a non-reactive carrier gas.**
- **EpiGrow MOCVD reactors simulator typically operate under mass-transport-limited growth regime.**
- **Required pyrolysis temperature increases with increasing chemical bond strength of the precursor**
- **EpiGrow MOCVD reactors simulator can be used to optimize Ideal processes to minimize the production of waste products**

Chemical Reactions Inbuilt

Few Examples

Gas-phase reactions:

(G1) $TMGa + H_2 = MMGa + 2CH_4$
(G2) $TBAs = AsH + C_4H_8 + H_2$

Surface reaction

(S1) $MMGa + AsH = GaAs(s) + CH_4$

Gas-phase Mechanisms:

										$k = AT^n e^{-Ea/RT}$	A	n	E_a
G1	TMG	=	DMG	+	CH_3						1.00×10^{47}	−9.18	76,996
G2	DMG	=	MMG	+	CH_3						7.67×10^{43}	−9.8	34,017
G3	MMG	=	Ga	+	CH_3						1.68×10^{30}	−5.07	84,030
G4	TMG	+	NH_3	→	TMG:NH_3						2.28×10^{34}	−8.31	3115
G5	TMG	+	NH_3	→	DMG:NH_2	+	CH_4				1.70×10^{4}	2	19,969
G6	DMG	+	NH_3	→	DMG:NH_3						4.08×10^{31}	−7.03	3234
G7	DMG	+	NH_3	→	MMG:NH_2	+	CH_4				5.30×10^{5}	1.56	20,744
G8	MMG	+	NH_3	→	MMG:NH_3						7.95×10^{24}	−5.21	2094
G9	MMG	+	NH_3	→	$GaNH_2$	+	CH_4				8.10×10^{5}	1.3	17,722
G10	NH_3	+	CH_3	→	NH_2	+	CH_4				3.31×10^{3}	2.51	9859
G11	CH_3	+	H_2	→	CH_4	+	H				1.20×10^{12}	0	12,518
G12	TMG	+	H	→	DMG	+	CH_4				5.00×10^{13}	0	10,036
G13	DMG	+	H	→	MMG	+	CH_4				5.00×10^{13}	0	10,036
G14	TMG:NH_3	→	MMG	+	$2CH_3$	+	NH_3				1.33×10^{44}	−8.24	77,791
G15	CH_3	+	H	+	M	→	CH_4	+	NH_3		2.40×10^{22}	−1	0
G16	$2CH_3$	=	C_2H_6								2.00×10^{13}	0	0
G17	2H	+	M	=	H_2	+	M				2.00×10^{16}	0	0

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Surface phase Mechanisms: Path 1, Path 2 and Path 3

	Path 1, $k = AT^n e^{-Ea/RT}$							A	n	E_a
1	MMG	+	N(S)	→	MMG(S)			1.16×10^5	2.98	0
2	MMG(S)	→	MMG	+	N(S)			1.12×10^{14}	0.55	107,673
3	NH_3	+	MMG(S)	→	COMPM1(S)			3.35×10^7	3.33	0
4	COMPM1(S)	→	NH_3	+	MMG(S)			5.70×10^{13}	−0.16	8146
5	MMG	+	COMPM1(S)	→	CH4	+	COMPM2(S)	1.23×10^{10}	3.22	23,446
6	NH_3	+	COMPM2(S)	→	COMPM3(S)			3.35×10^7	3.33	0
7	COMPM3(S)	→	NH_3	+	COMPM2(S)			5.70×10^{13}	−0.161	8146
8	MMG	+	COMPM3(S)	→	CH_4	+	COMPM4(S)	1.23×10^{10}	3.22	23,446
9	NH_3	+	COMPM4(S)	→	COMPM5(S)			3.35×10^7	3.33	0
10	COMPM5(S)	→	NH_3	+	COMPM4(S)			5.70×10^{13}	−0.161	8146
11	COMPM5(S)	→	CH4	+	RINGM1(S)			1.23×10^7	3.22	23,446
12	Ga(S)	+	RINGM1(S)	→	RINGM2(S)	+	N(S)	3.35×10^7	3.33	0
13	RINGM2(S)	→	$3H_2$	+	3GaN(B)	+	Ga(S)	3.68×10^9	2.05	59,610

	Path 2, $k = AT^n e^{-Ea/RT}$							A	n	E_a
14	CH_3	+	Ga(S)	→	MMG(S)			1.76×10^9	1.39	0
15	MMG(S)	→	CH_3	+	Ga(S)			4.54×10^{13}	0.0346	79,480
16	NH_2	+	Ga(S)	→	NH_2(S)			3.17×10^8	1.83	0
17	$GaNH_2$	+	N(S)	→	$GaNH_2$(s)			2.27×10^6	2.247	0
18	$GaNH_2$(S)	→	$GaNH_2$	+	N(S)			4.83×10^{13}	0.614	83,881
19	COMPMM1(S)	→	CH_4	+	$GaNH_2$(S)			1.49×10^{11}	0.609	25,950
20	MMG	+	$GaNH_2$(S)	→	COMPMM1(S)			1.16×10^5	2.98	0
21	NH_3	+	COMPMM1(S)	→	COMPMM2(S)			3.35×10^7	3.33	0
22	COMPMM2(S)	→	CH_4	+	COMPMM3(S)			1.49×10^{11}	0.609	25,950
23	MMG	+	COMPMM3(S)	→	COMPMM4(S)			1.16×10^5	2.98	0
24	NH_3	+	COMPMM4(S)	→	COMPMM5(S)			3.35×10^7	3.33	0
25	COMPMM5(S)	→	CH_4	+	RINGM1(S)			1.49×10^{11}	0.609	25,950
26	NH_2(S)	→	NH_2	+	Ga(S)			1.45×10^{14}	0.09	59,786
27	COMPMM1(S)	→	MMG	+	$GaNH_2$(S)			1.00×10^{14}	0.55	42,819
28	COMPMM2(S)	→	NH_3	+	COMPMM1(S)			5.70×10^{13}	−0.1	8146
29	COMPMM4(S)	→	MMG	+	COMPMM3(S)			1.00×10^{14}	0.55	42,819
30	COMPMM5(S)	→	NH_3	+	COMPMM4(S)			5.70×10^{13}	−0.1	8146
31	Ga	+	N(S)	→	Ga(S)			1.00×10^{11}	1.5	0
32	Ga(S)	+	NH_2(S)	→	$GaNH_2$	+	Ga(S)	1.00×10^{25}	0	0
33	Ga(S)	→	Ga	+	N(S)			1.00×10^{13}	0	45,168
34	$6CH_3$	+	RINGM2(S)	→	COM1(S)			7.55×10^7	2.31	0
35	COM1(S)	→	$6CH_3$	+	RINGM2(S)			1.00×10^{13}	0.71	45,506
36	COM1(S)	→	$6CH_4$	+	3GaN(B)	+	Ga(S)	4.00×10^{12}	0	49,675

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	Path 3, $k = AT^n e^{-Ea/RT}$								A	n	E_a
37	TMG	+	N(S)	→	TMG(S)				1.16×10^5	2.98	0
38	NH_3	+	TMG(S)	→	TCOM1(S)				3.35×10^7	3.33	0
39	TCOM1(S)	→	CH_4	+	TCOM2(S)				1.49×10^{11}	0.609	32,785
40	Ga(S)	+	TCOM2(S)	→	TCOM3(S)	+	N(S)		3.35×10^7	3.33	0
41	TCOM3(S)	→	$2CH_4$	+	GaN(B)	+	Ga(S)		1.49×10^{11}	0.609	49,675
42	TMG(S)	→	TMG	+	N(S)				1.12×10^{14}	0.55	49,675
43	TCOM1(S)	→	NH_3	+	TMG(S)				5.70×10^{13}	−0.161	11,922
44	TMG:NH_3	+	N(S)	→	TCOM1(S)				1.16×10^5	2.98	0
45	TCOM1(S)	→	TMG:NH_3	+	N(S)				1.12×10^{14}	0.55	49,675
46	TCOM1(S)	→	$2CH_3$	+	MMG(S)	+	NH_3 +N(S)		1.12×10^{14}	0.55	10,7673
47	MMGNH_3	+	N(S)	→	COMPM1(S)				1.16×10^5	2.98	0
48	COMPM1(S)	→	MMG:NH_3	+	N(S)				1.12×10^{14}	0.55	107,673
49	MMG:NH_3	+	COMPM1(S)	→	CH_4	+	COMPM3(S)		1.23×10^{10}	3.22	23,446
50	MMG:NH_3	+	COMPM3(S)	→	CH_4	+	COMPM5(S)		1.23×10^{10}	3.22	23,446
51	MMG:NH_3	+	$GaNH_2$(S)	→	COMPMM2(S)				1.16×10^5	2.98	0
52	MMG:NH_3	+	COMPMM3(S)	→	COMPMM5(S)				1.16×10^5	2.98	0

Chemical Composition of compound on the surface

Compounds Names	Chemical Formula
COMPM1(S)	NH_3·MMG(S)
COMPM2(S)	Ga·NH_2·MMG(S)
COMPM3(S)	NH_3·Ga·NH_2·MMG(S)
COMPM4(S)	Ga·NH_2·Ga·NH_2·MMG(S)
COMPM5(S)	NH_3·Ga·NH_2·Ga·NH_2·MMG(S)
RINGM1(S)	NH_2·Ga·NH_2·Ga·NH_2·Ga(S)
RINGM2(S)	(S)NH_2·Ga·NH_2·Ga·NH_2·Ga(S)
COMPMM1(S)	MMG·$GaNH_2$(S)
COMPMM2(S)	NH_3·MMG·$GaNH_2$·Ga(S)
COMPMM3(S)	NH_2·Ga·NH_2·Ga(S)
COMPMM4(S)	MMG·NH_2·Ga·NH_2·Ga(S)
COMPMM5(S)	NH_3·MMG·NH_2·Ga·NH_2·Ga(S)
TCOM1(S)	NH_3·TMG(S)
TCOM2(S)	NH_2·DMG(S)
TCOM3(3)	(S)NH_2·DMG(S)
COM1(S)	RINGM2(S)·CH_3 complex

Physics

Reaction rates depend on the concentrations of the reactants involved in the reaction equation. A rate law is used to express the relation between the rate and these concentrations. Usually reactions have their rate laws in the following form-

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$$r = k[A]^x[B]^y \ldots\ldots$$

where '*k*' is rate constant, feature of a given reaction. The powers x, y ... are the numbers that must be determined experimentally. '*x*' is the order with respect to A, and '*y*' is the order of B.

- **Partial pressure is defined using flow rates of precursors:**

$$\boldsymbol{P = \frac{nRT}{V}}$$

Here,

n= Number of moles of reactants, R=Gas constant= 8.31446261815324 $JK^{-1}mol^{-1}$

T= Temperature and V=Chamber Volume (Litre)

- **The forward rate constant (growth rate) is found to have the relation with temperature as follows-**

$$K = AT^n exp((-\boldsymbol{E_a})/\boldsymbol{RT})$$

The activation energy E_a, which is the minimum amount of energy required to initiate a chemical reaction, is in unit of energy.mol^{-1} and T is temperature exponent. A is the pre-exponential factor and it is usually found to be independent of temperature. Besides it must have the same dimensions and units as k.

Benefits can be realized

- **Graphical User Interface (GUI) based Simulator**
- **Binary, ternary and quaternary compound semiconductor based epitaxial growth**
- **Users have flexibilities to accommodate by inputting their own chemical reactions as text file**
- **Surface profiles Extracting Roughness**
- **Defects Extraction (point/clusters)**
- **Extraction of dislocations & Stress/Strain**
- **Fewer experiments for optimization**
- **Reduction in waste during experimentation**

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- **Ability to deal with different reactive species and reactor geometries**
- **On-line process control**

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