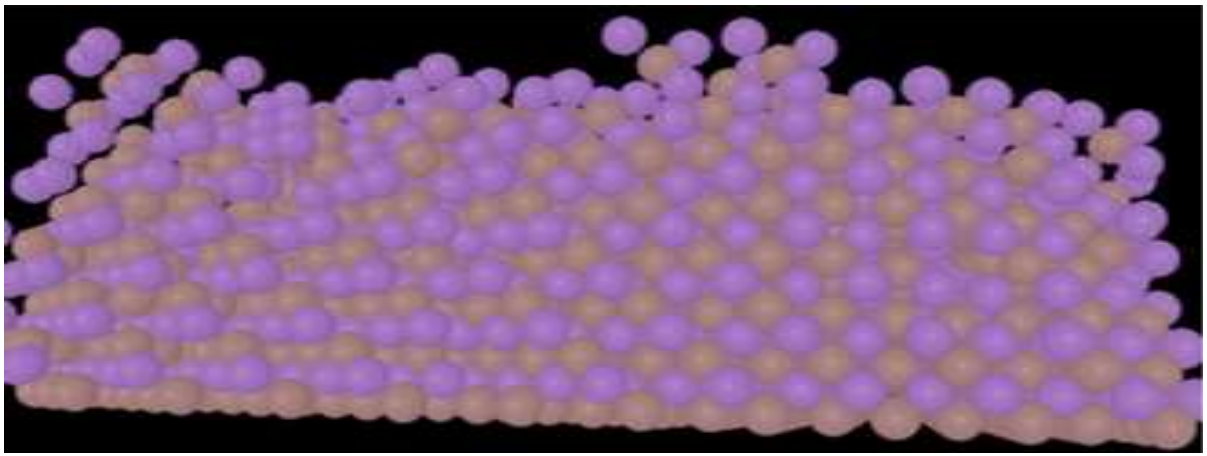
EpiGrow Simulator

An Unmatched Atomistic Epitaxial Growth Solution

Technology of Next Level driven through innovation



Bulk Crystal Growth

- Semiconductors in state of the art device technologies depends critically on:

  Purity & Perfection of the crystals

- Requires growth of bulk crystals, then sliced and polished
- Single crystal, ingots with large diameter and with few defects
- Limited to Si and GaAs (to some extent for InP)>

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Bulk Crystal Growth

- The elemental semiconductors have a well-defined melting point
- Solidification of GaAs, as an example, from its liquid does not happen at the stoichiometric composition
- A slightly As-rich liquid composition leading to inherently non-stoichiometric crystals.
- Perhaps subtle differences from the elemental semiconductors

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Bulk Crystal Growth

Silicon

- Available in up to >30 cm diameter
- Quite inexpensive and high quality
- Can be obtained *n*-type, *p*-type, or with high resistivity
- Used for Si and SiGe technologies
- Intense reserach to develop Si-based "pseudo-substrates" for GaAs, InP, CdTe...technologies

GaAs

- Available in up to >12 cm diameter
- High quality, more expensive than Si, but affordable
- Used for GaAs and AlGaAs, and strained InGaAs technologies
- Can be used for electronic and optoelectronic applications

InP

- 10 cm diameter available, but expensive
- InP and InGaAsP technologies can be grown
- Very important for optoelectronics and high performance electronics

SiC

- Small, very expensive substrates
- Very important for high power, large gap technologies
- Used for nitride technology

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Bulk Crystal Growth

- Other semiconductors, difficult to obtain high quality, large area substrates.
- Several semiconductor technologies dependent on non ideal substrates.
- III-Group Nitride materials process on Si, SiC or sapphire substrates
- No availability of reliable GaN substrate.
- II-VI materials having epitaxial growth problems, for the low & high bandgap semiconductors.

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Epitaxial Crystal Growth

LPE

- Very high quality material
- Near equilibrium growth for precise alloy compositions
- Relatively inexpensive
- Difficult to grow abrupt heterostructures
- Unable to grow immiscible alloys

VPE

- Extremely high purity material
- Not well suited for heterostructures

(MBE) (MOCVD) (MOMBE)

- High quality material
- Atomically abrupt interfaces
- Techniques can grow far from equilibrium systems reliably

Expensive growth technology ????

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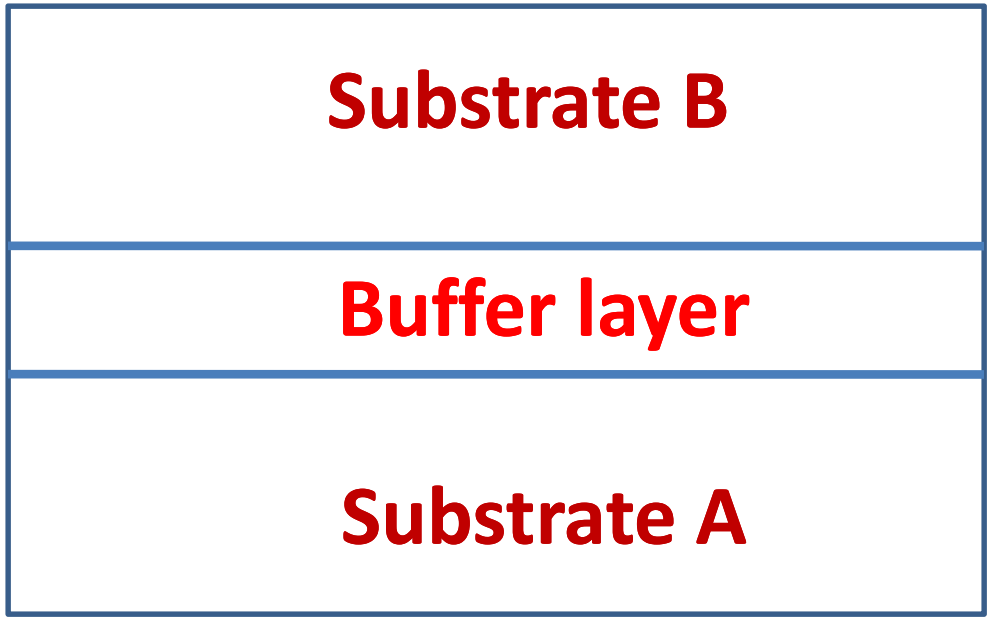
Crystal Growth Challenges

Development of psuedo - substrates to satisfy need for different semiconductors and hetero-structures



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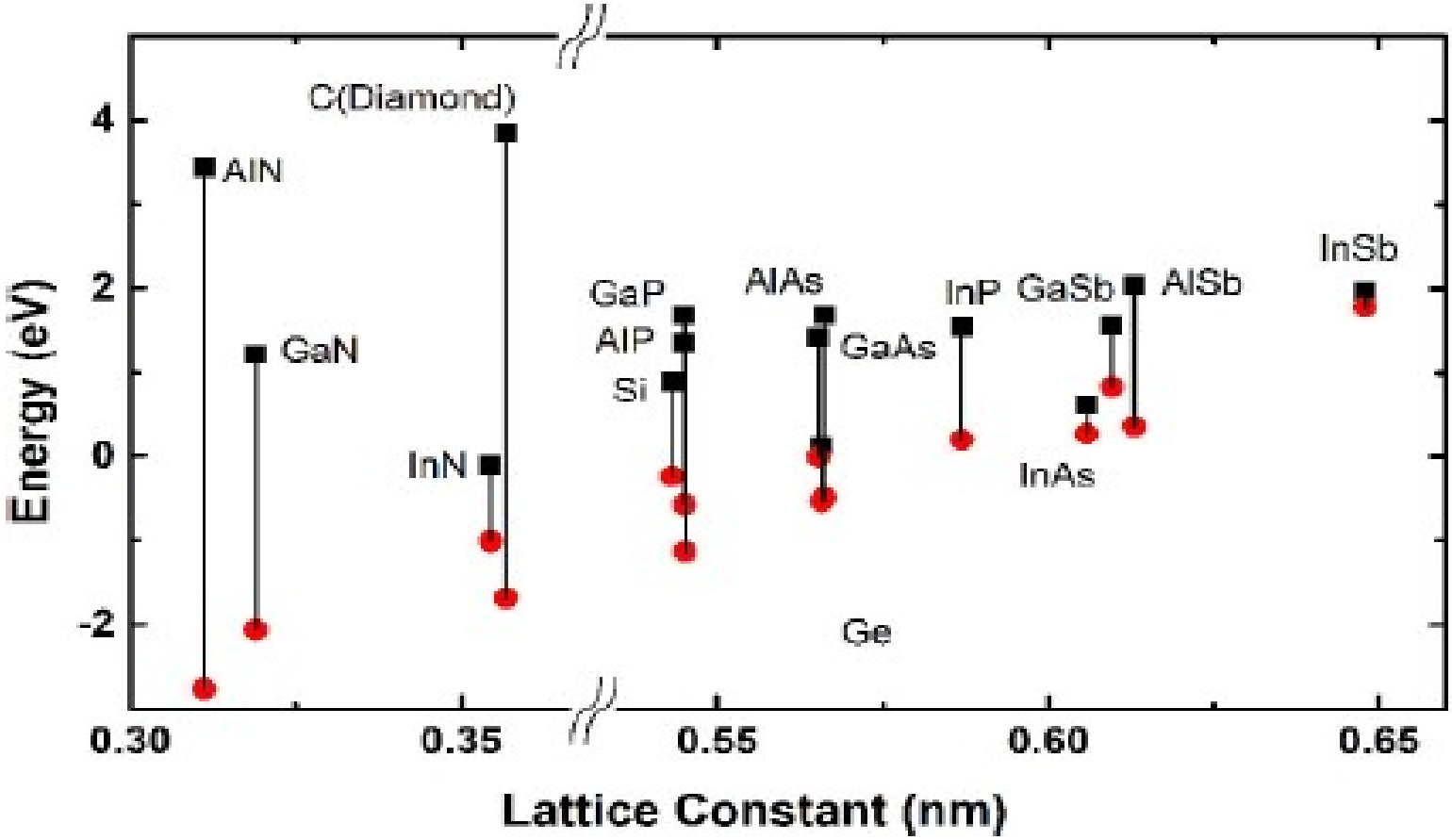
Crystal Growth Challenges



- E.T. Yu, J.O. McCaldin, T.C. McGill, Band offsets in semiconductor heterojunctions, in: E. Henry, T. David (Eds.), Solid State Physics, Academic Press, 1992, pp. 1–146

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Crystal Growth Challenges

- The lattice-matched composition checked by a line between the GaAs & InAs CB & VB leading to composition of $In_{0.53}Ga_{0.47}As$ lattice-matched to InP
- $In_xGa_{1-x}As_yP_{1-y}$ based lasers epitaxially grown on InP substrates
- The formation of multinary alloys presents additional technological challenges

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Crystal Growth Challenges

- III-V growth due to multi components of the growth system
- Point defects, e.g. vacancies, interstitial atoms, impact on the performance of the device
- Extended defects within the film are generally dislocations and stacking faults
- Dislocations can reduce or relax strain introduced through lattice mismatch or thermal expansion differences.

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Epitaxial Growth Challenges

Substrate	Si	Al_2O_3	SiC	Bulk GaN	AlN
Lattice Mismatch (%)	17	16	3.4	-	2.5
Thermal Conductivity (W/mm-k)	150	35	490	260	319
Resistivity (ohm-cm)	10^4	10^{14}	~10^{12}	-	>10^{14}

High thermal conductivity of the substrate require for HEMT structures to relax self-heating effect

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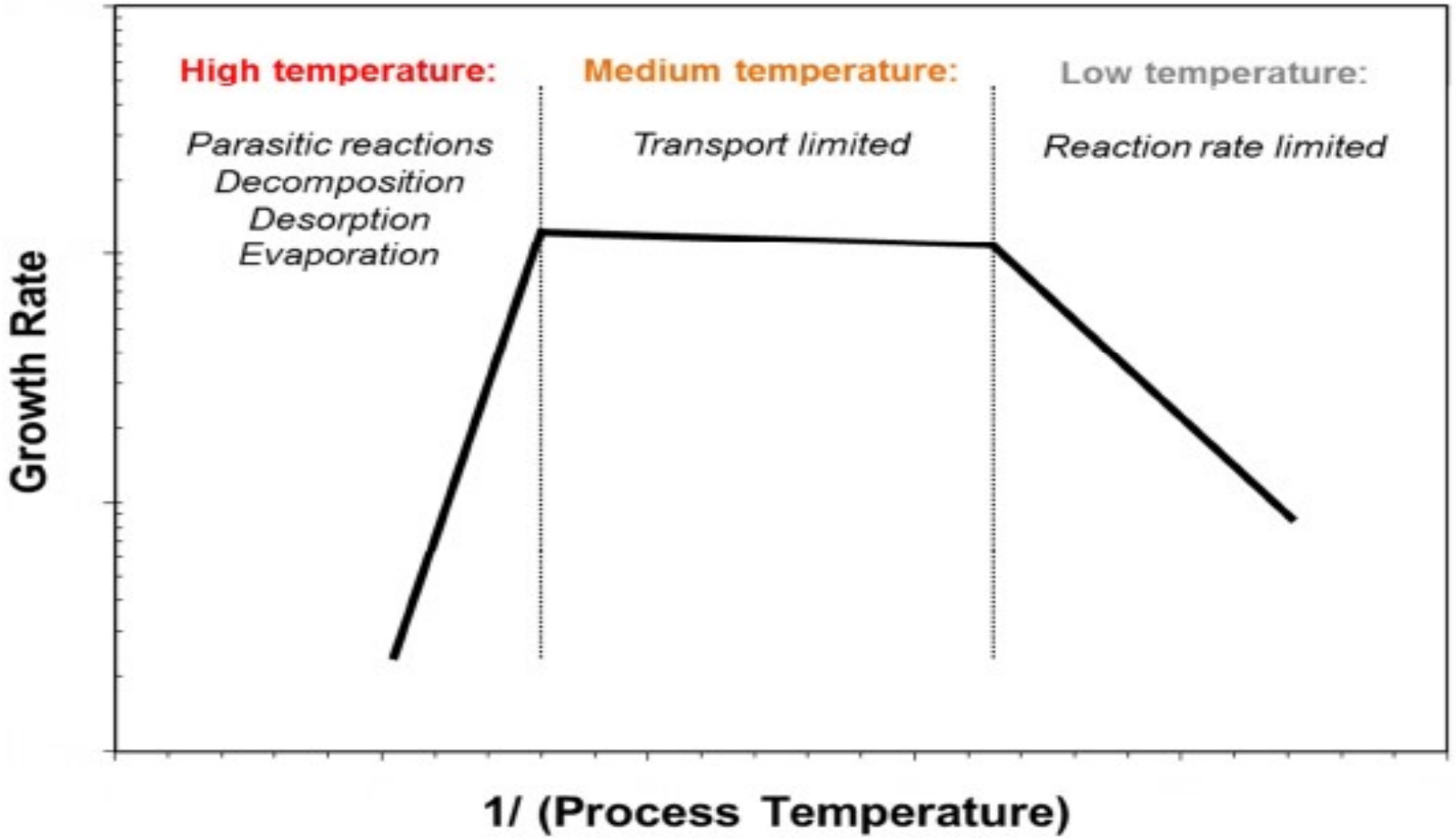
Epitaxial Growth Challenges



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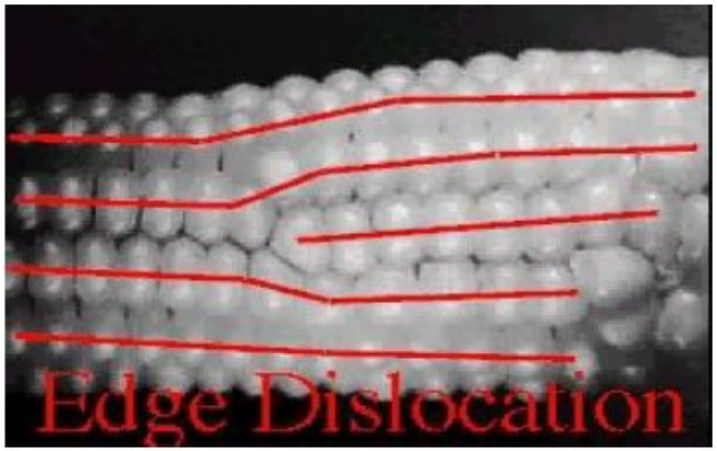
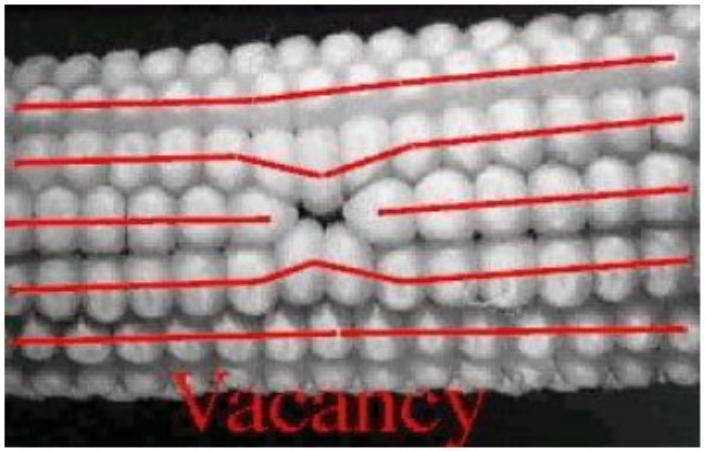
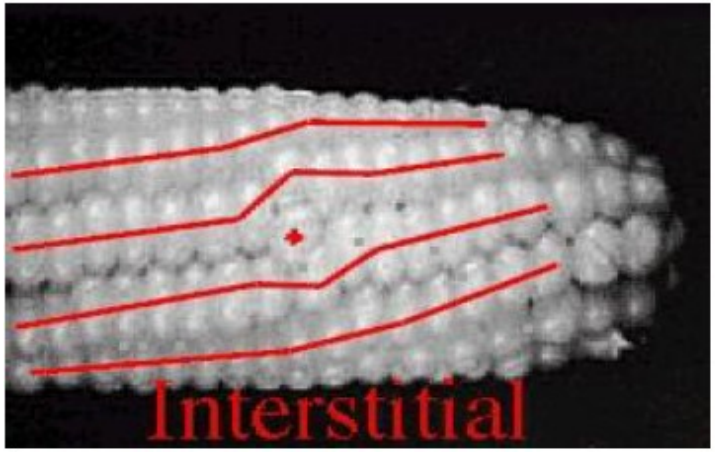
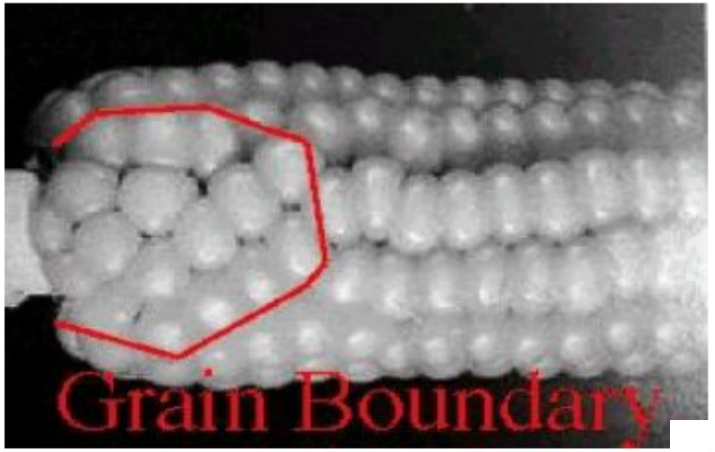
Defects - Epi Growth Challenges









Current Scenario

- Design & optimization of CVD processes to fulfill the increasing demand in the semiconductor industry are very difficult and time-consuming tasks
- Lack of detailed fundamental models has forced industrial CVD practitioners to rely on methods of trial and error
- Statistical methods create purely empirical models of reactor behavior

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Current Scenario

- Empirical relations produced procedures, difficult to use if the reactants or the reactor geometry is changed
- Mathematical modeling and simulation provide an excellent economic alternative to trial and error-based experimental techniques.
- No RANDOMNESS based atomistic Epigrowth simulator in the market place

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EpiGrow Simulator

- Tech Next Lab (P) Ltd, presenting first innovative atomistic simulator for Stochastic Modeling of epi-growth process based on MOCVD/ MBE/ MOVPE/ GasMBE (under development) Reactors
- EpiGrow Simulator is based on RANDOMNESS phenomenon for growth
- No Statistical/thermodynamically assumptions
- Based on purely real rates

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EpiGrow Simulator

Benefits can be realized

- Users growth conditions
- Surface profiles Extracting Roughness
- Defects Extraction (point/clusters)
- Extraction of dislocations & Stress/Strain
- Fewer experiments for optimization
- Reduction in waste during experimentation
- Ability to deal with different reactive species and reactor geometries
- On-line process control

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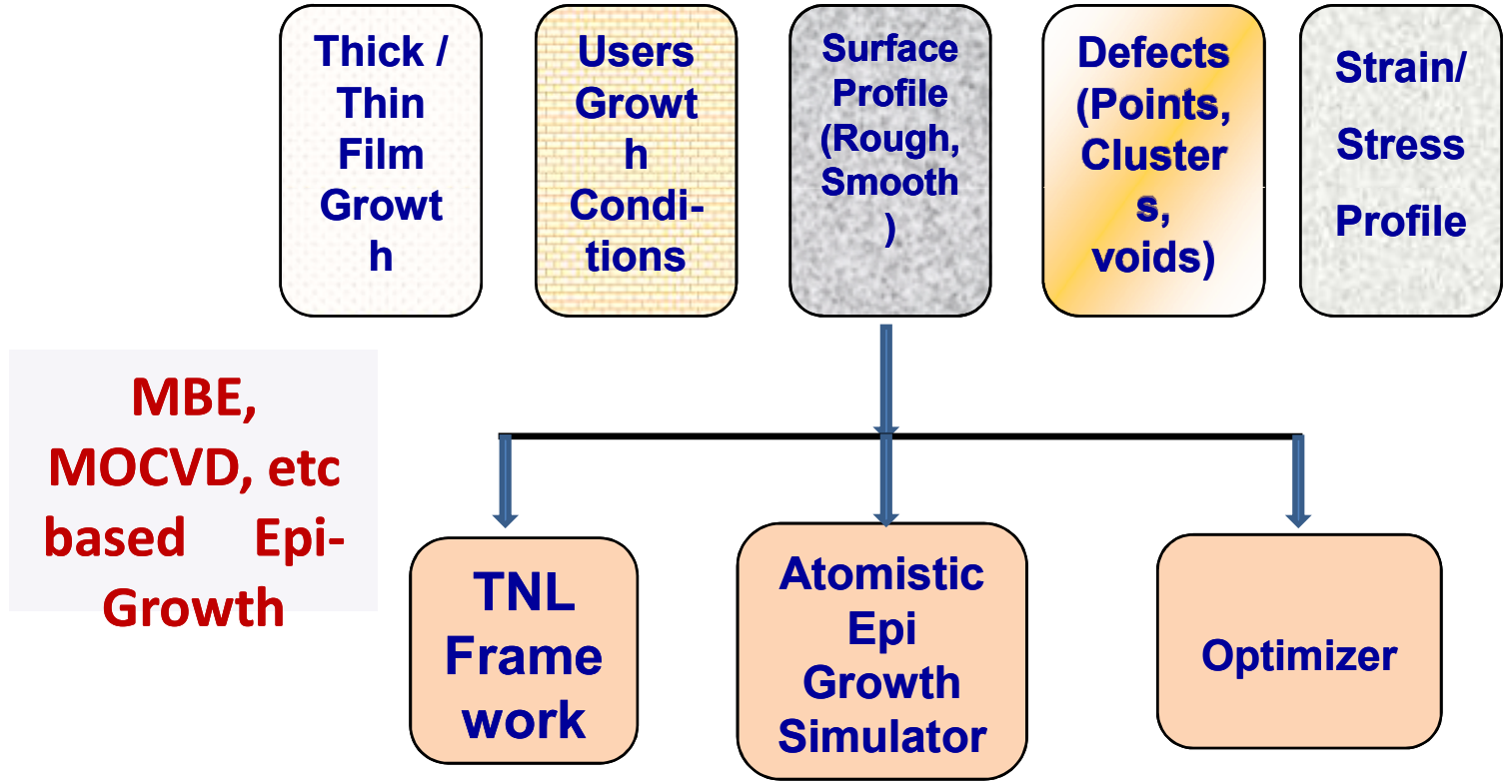
EpiGrowSimulator

Innovative Atomistic Reactor Simulation



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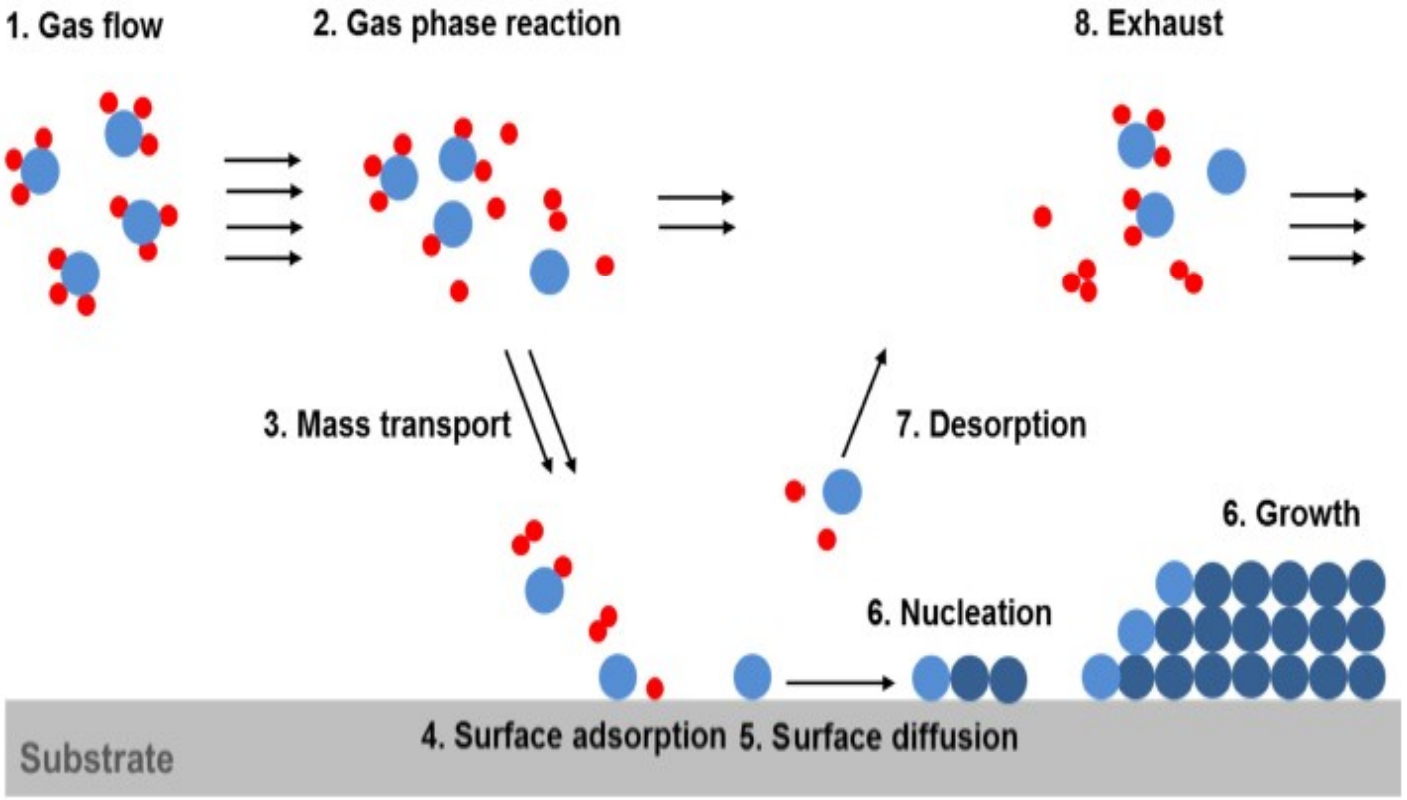
EpiGrow Simulator

- **In-house Developed Simulator Core**



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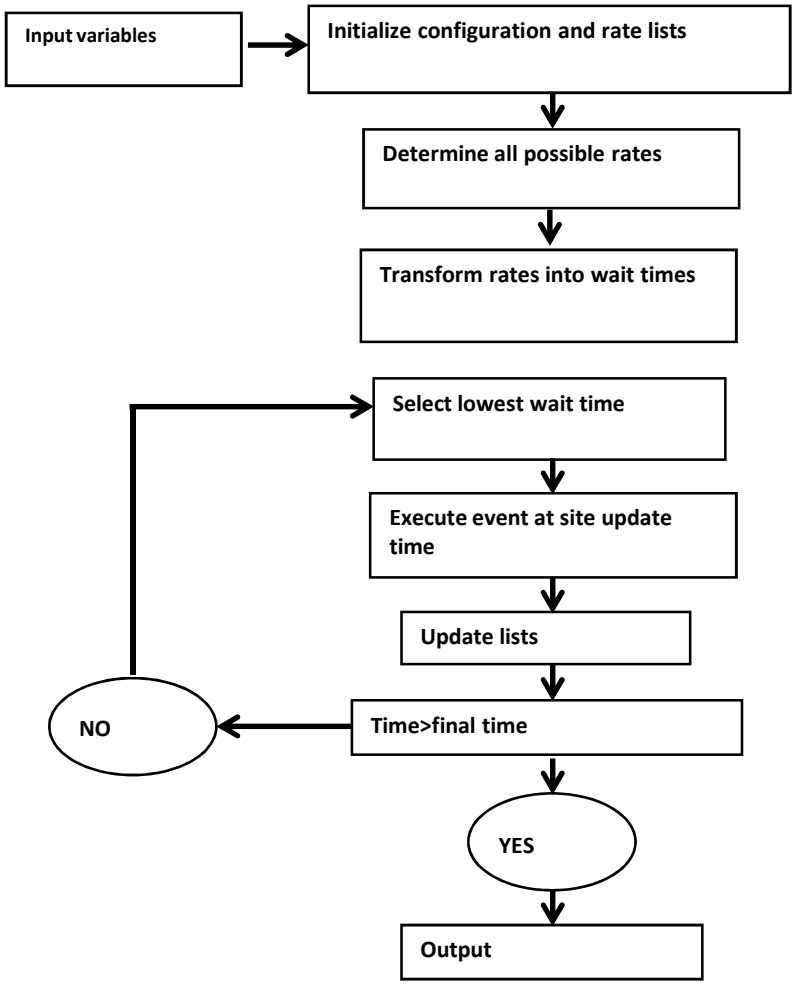
EpiGrow Simulator

The structure of EpiGrow Simulator is defined by flowchart



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Deposition

The absorption rate, which may also be called deposition rate, arriving rate, deposition flux, etc., is measured as number of absorbed atoms per unit site per unit time. Since this rate is identical at every site on the surface, the total absorption rate is thus the number of simulation cells multiplying deposition flux of each cell:

$$A = F \,.l\,.w$$

Here A denotes the total absorption rate, F denotes flux, and l and w denote length and width of substrate respectively.

Diffusion

The diffusion rate, also called hopping rate, is to measure the likelihood of an atom moving to its neighboring site. This is described as Arrhenius relation

$$h_j = D_0 e^{\frac{-E_j}{k_B T}}$$

Here h_j is the hopping rate of the j^{th} atom, E_j is the activation energy of the j^{th} atom, and T is the substrate temperature (K). The pre-factor D_0 corresponds to a vibration frequency which can be obtained by application of the equal-partition theorem. The characteristic vibration frequency (D_0) is described as:

$$D_0 = \frac{2k_B T}{h}$$

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The activation energy can be obtained using surface diffusion energy barrier (E_s) and nearest binding energy (E_n) by:

$$E = E_s + n.E_n$$

Where n as the number of nearest neighbors on the surface.

Including other effects on the surface diffusion, such as step-edge barriers from both descending steps (Schwoebel barrier) and ascending steps (incorporation barrier), the activation energy of an atom should be rewritten as:

$$E = E_s + n.E_n + E_b$$

or

$$E = E_s + n.E_n + E_i$$

where E_b denotes the Schwoebel barrier and E_i denotes the incorporation barrier.

As the activation energies are generally different for each atom, the hopping rates are naturally different. As a result, the total hopping rate can only be calculated by summation rather than multiplication:

$$H = \sum_j h_j$$

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Since A is the total absorption rate and H is the total hopping rate, the total transition rate is simply:

$$R = A + H$$

This R is to describe the rate of transition, or the times of events per unit time, and this event can be either a deposition or a diffusion.
The time interval of an event, on one hand, is statistically inversely proportional to the total transition rate; on the other hand, is exponentially distributed. Thus we construct the time interval formula according to our statistics knowledge:

$$\tau = -\frac{\log \xi}{R}$$

where τ denotes the time interval of an even, and ξ is a random number uniformly distributed between 0 and 1.

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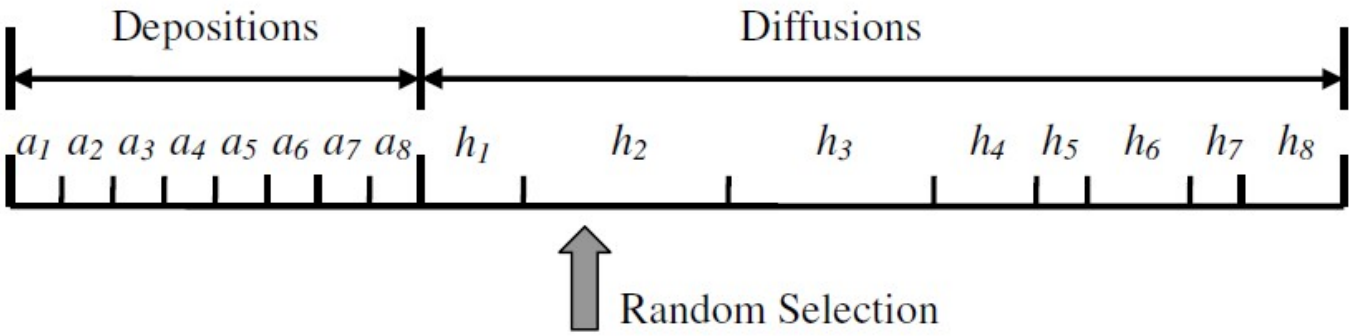
Event Selection

As described before, the KMC simulation model is built on a stochastic basis. To realize this model, we must determine the sequence of transitions, which is also randomly arranged. Each event selection is thereby illustrated in Figure.



As shown, the position of the arrow is controlled by a uniformly distributed random number ξ. If the total transition rate R multiplying ξ is smaller than the total deposition
rate A, i.e.,

$$\xi . R < A$$

the event is a deposition. If the product is not smaller than A, the event is a diffusion. In case of deposition, since the flux is the same for all sites, we may easily find the deposition site by:

EpiGrow Simulator

$$j = \left(\frac{lw\xi R}{A} \right)$$

where the lateral size of simulation surface l and w are measured by unit cell. And j means the deposition site is the jth one of the lw sites.

In **case of diffusion**, due to the different hopping rates for different atoms, we can only describe the hopping site by:

$$A + \sum_{k=1}^{j-1} h_k < \xi . R < A + \sum_{k=1}^{j} h_k$$

where j means the diffusing atom is the j^{th} one.

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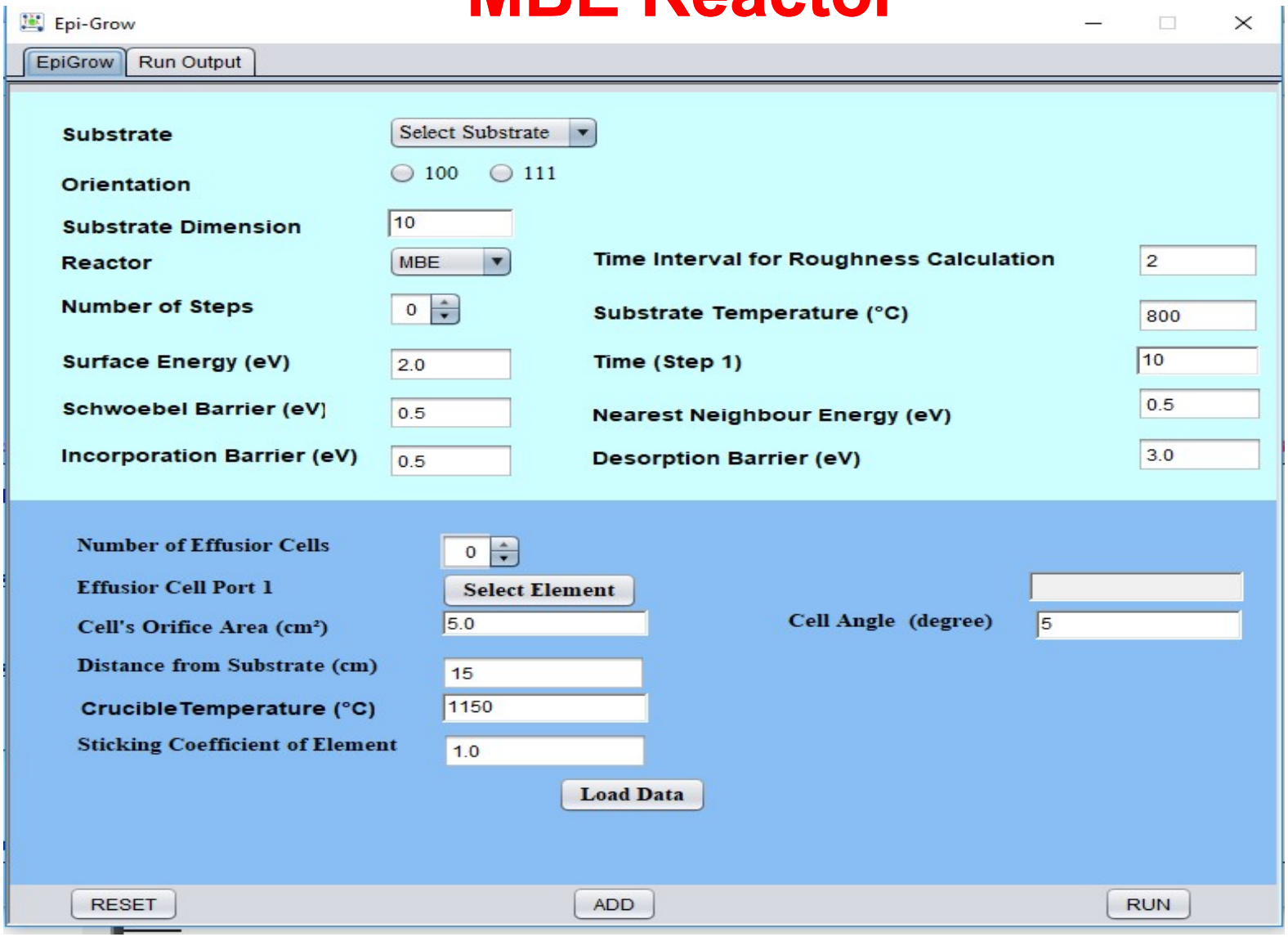
MBE Reactor



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MBE Reactor

Both the film constituent and the dopant atom arrival rates at the substrate may be calculated from the vapor pressure data. Dopants having a lower vapor pressure than the film materials generally have unity sticking coefficients. If we assume the vapor in the effusion cell is near equilibrium condition and the aperture of the cell has an area A. the total number of atoms escaping through the aperture per second is

$$\Gamma = \frac{pAN}{\sqrt{(2\pi MRT)}}$$

where p is the pressure in the cell, N is Avogardro's number, M is the molecular weight, R is the gas constant, and T (K) is the temperature of the cell, if p is expressed in Torr and A in cm^2, the effusion rate is then

$$\Gamma = 3.51 \times 10^{22} \frac{pA}{\sqrt{(MT)}} \quad \text{molecules } s^{-1}$$

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MBE Reactor

If the substrate is positioned at a distance l from the aperture and is directly in line with the aperture, the expression for the number of molecules per second striking the substrate of unit area (Viz., "flux") is

$$\Gamma = 1.118 \times 10^{22} \frac{pA}{l^2\sqrt{(MT)}} \quad \text{molecules cm}^{-2}\,\text{s}^{-1}$$

The general equation which is employed for vapor pressure calculation is a polynomial in temperature

$$\text{Log P (atm)} = A + B.T^{-1} + \text{C.log}T + D.T.10^{-3}$$

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MOCVD Reactor

Epi-Grow

EpiGrow | Run Output

Substrate	Select Substrate		
Orientation	100 111		
Substrate Dimension	10		
Reactor	MOCVD	Time Interval for Roughness Calculation	2
Number of Steps	0	Substrate Temperature (°C)	800
Surface Energy (eV)	2.0	Time (Step 1)	10
Schwoebel Barrier (eV)	0.5	Nearest Neighbour Energy (eV)	0.5
Incorporation Barrier (eV)	0.5	Desorption Barrier (eV)	3.0

Precursor source | MOCVD Parameter

Number of Port	0	
Precursor 1	Select Precursor	
Flow Rate		atm cc/s
Celing Temperature (°C)	100	
Sticking Coefficient of Element	1.0	

Load Data

RESET ADD RUN

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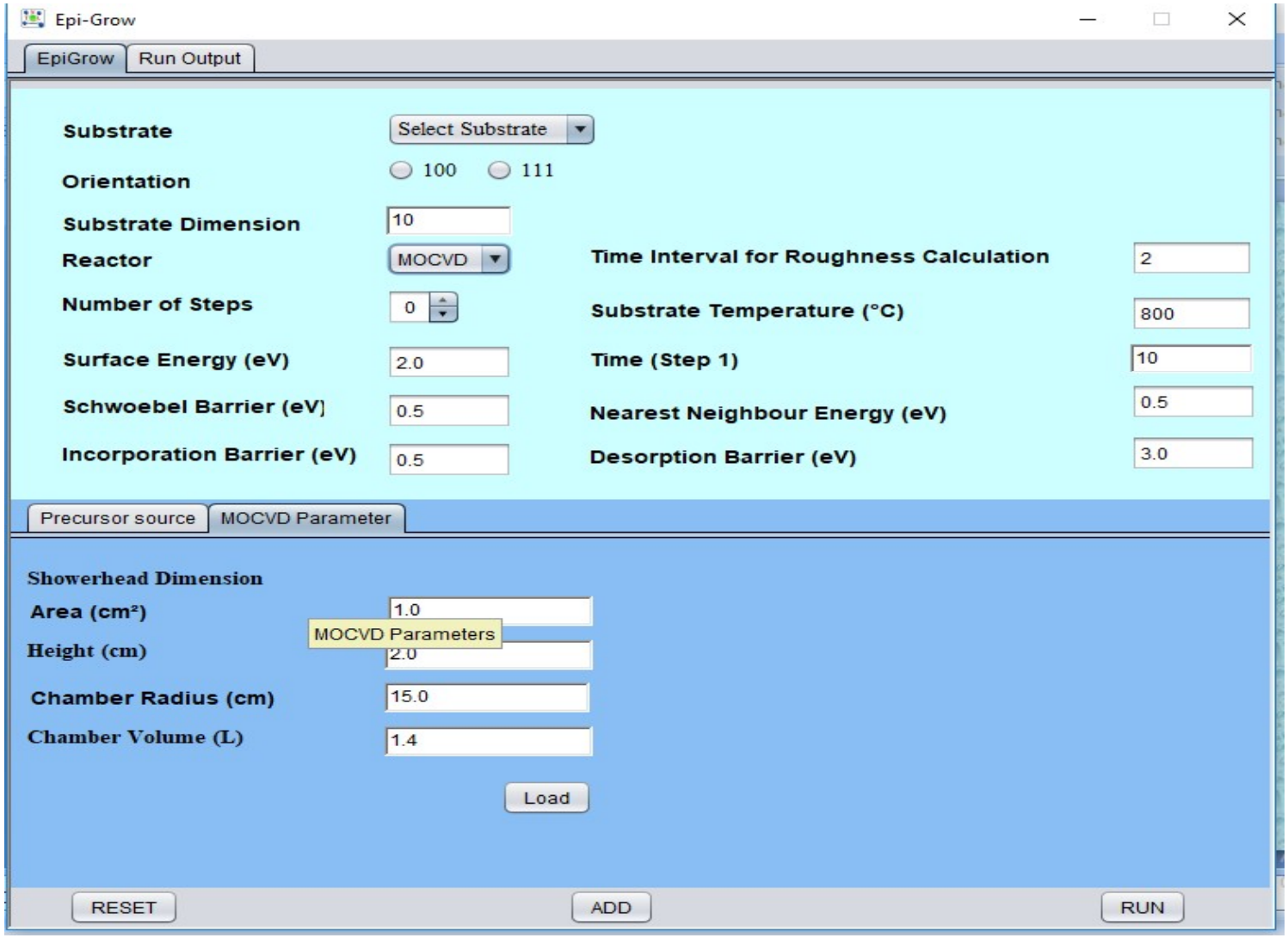
MOCVD Reactor



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GaAs - MOCVD Reactor

The growth of GaAs film from TMGa (trimethyl-gallium, group III) and TBAs, (tertiary-butylarsine) using hydrogen as the carrier gas in a reactor can be described by the gas-phase reactions and the surface reaction as follows[1]:

Gas-phase reactions:

(G1) $TMGa + H_2 = MMGa + 2CH_4$

(G2) $TBAs = AsH + C_4H_8 + H_2$

Surface reaction:

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

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GaAs - MOCVD Reactor

In the above expressions, the rate constant (k) obeys the Arrhenius law given[2]

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

where A is the pre-exponential factor, n is the temperature exponent, E_a is the activation energy for the reaction and R is the universal gas constant.

Reference:

1. Journal of the Taiwan Institute of Chemical Engineers 45 (2014) 254–267
2. Coatings 2017, 7, 43

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GaAs - MOCVD Reactor

For GaAs epitaxial Growth case : n=0

Reactions included in the gas-phase and surface-phase model.

Kinetic Parameter	Value	Unit
A_{G1}	1.2×10^{15}	S^{-1}
A_{G2}	5.32×10^{15}	S^{-1}
A_{S1}	1.23×10^{9}	m/s
E_{G1}	196	kJ/mol
E_{G2}	203	kJ/mol
E_{S1}	130	kJ/mol

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GaN - MOCVD Reactor

- The growth of GaN film from TMG, DMG, MMG, & NH_3
- Hydrogen as the carrier gas
- Gas-phase reactions & the surface reaction dictated by *Arrhenius* Eqn:

$$k = AT^n \exp(-E_a/RT)$$

where A is the pre-exponential factor, n is the temperature exponent, E_a is the activation energy for the reaction and R is the universal gas constant.

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GaN - MOCVD Reactor

Gas-phase Mechanisms:

										A	n	E_a
				$k = AT^n e^{-Ea/RT}$								
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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GaN - MOCVD Reactor

Surface phase Mechanisms: PATH 1

	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

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GaN - MOCVD Reactor

Surface phase Mechanisms: PATH 2

	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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GaN - MOCVD Reactor

Surface phase Mechanisms: PATH 3

	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

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GaN - MOCVD Reactor

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

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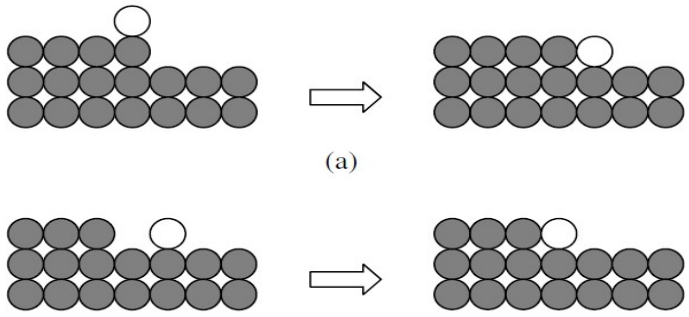
Barriers

Schwoebel barrier: The atom diffuses from the site exactly above the edge atom to the site immediately next to the edge atom,

Incorporation barrier: The atom incorporates into the edge on the same surface level.

These two barriers are destination dependent, so the activation energy for the same atom is also dependent on diffusion destination.



Side view for the case of Schwoebel barrier (a) and that of incorporation barrier (b), where the white atom is the diffusing one.

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EpiGrow Simulator

- s_c is the local sticking coefficient play significant role in deciding the adsorption of atom on appropriate position available.

$$s_c = P_{ads}(1-m)\sum_{n=0}^{\infty} P_{hop}^{n}$$

P_{ads} & P_{hop} are adsorption & hopping probability, m is site occupancy factor.

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EpiGrow Simulator

Total Rates

$$R_T = R_{ads} + R_{hop} + R_{des}$$

Here ads ~ adsorption Rate on substrate

Hop ~ hopping rate on substrate

Des ~ desorption rate

All rates define competitive processes and RANDOM in nature dependent on positions available

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EpiGrow Simulator

- The wait time contains two parts, the current system (elapsed) time and an additional time that represents the time it will take for the next event to take place.
- The system time is the sum of the times for each previously executed event.
- The wait time is described by the equation:

$$wait\_time = \tau + \frac{-\ln(u)}{r}$$

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EpiGrow Simulator

- Focus on the evolution of surface microstructure from nano to micrometer length scales
- Nitride alloys grown via MOCVD most commonly use
  - Hydride Ammonia (NH_3)
  - MO Alkyl Sources (TMGa, TMIn, TMAl…)
  - Dopant sources (Silane SiH_4, Si_2H_6, $MOCp_2Mg$)

Users may add different reactions inside reactor and its kinetic parameters values.

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EpiGrow Simulator

- Process largely dictated by use of Ammonia
- Low cracking efficiency of NH_3
- Volatility of N → N_2
- High growth temperatures required to obtain good crystal quality
- Low growth temperatures preferred for N bonding
- High temperature can liberate N from lattice
- Weak bond of N in nitride solid

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Outputs - EpiGrow Simulator

1. Lattice constant :

- User may extract layer by layer lattice constant.
- Averaging layer by layer lattice constant may produce overall lattice constant of film.
- The lattice constant can be calibrated with lattice constant with XRD studies.
- Lattice constant includes all the strain, defects etc effects.

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Outputs - EpiGrow Simulator

2. Strain:

- **User may extract strain through the eqn:**

$$\text{strain} = (a - a_0) / a_0$$

where a is the lattice constant of upper monolayer and a_0 is beneath monolayer.

- **Averaging layer by layer strain will produce overall strain in the film.**
- **The strain can be calibrated with experimental strain.**

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Outputs - EpiGrow Simulator

3. Surface Roughness:

- **User may extract surface roughness w.r.t time, included through the eqn:**

$$r = \sqrt{\frac{\sum_{i=1}^{N}\sum_{j=1}^{N}[h_{ij}-\bar{h}]^2}{NxN}}$$

Here N is the total number of lattice points, h_{ij} is the height at a given lattice point located at position *i* and *j*, on the lattice and h_{avg} is the average height of all lattice points.

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Outputs - EpiGrow Simulator

4. Mole fraction:

- User may extract number of atoms of different constituents layer by layer.
- With the number of group III and group V atoms, molefraction can be produced.

5. Defects :

- User may extract number of interstitials, vacancy etc layer by layer

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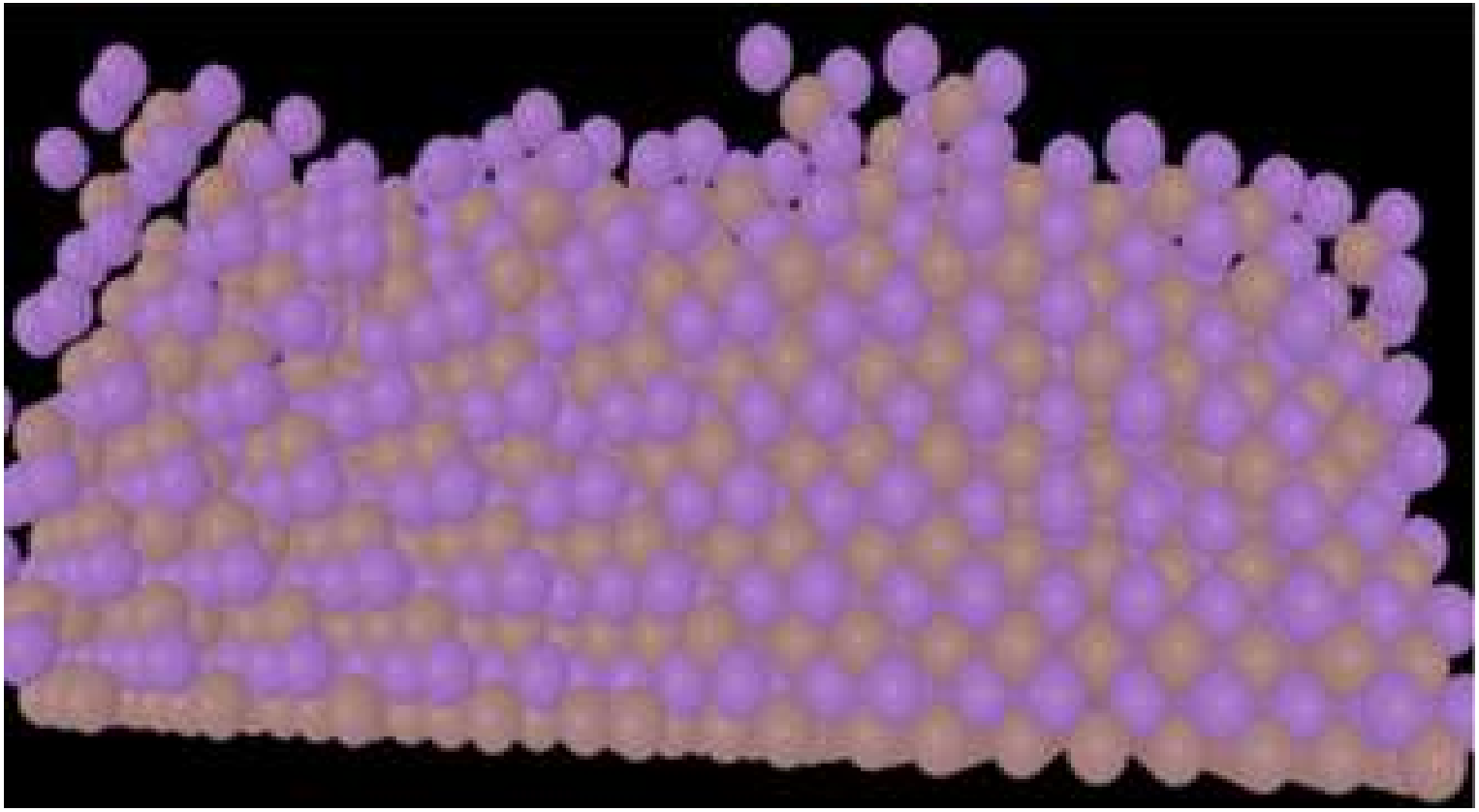
Outputs

GaAs monolayers growth over GaAs



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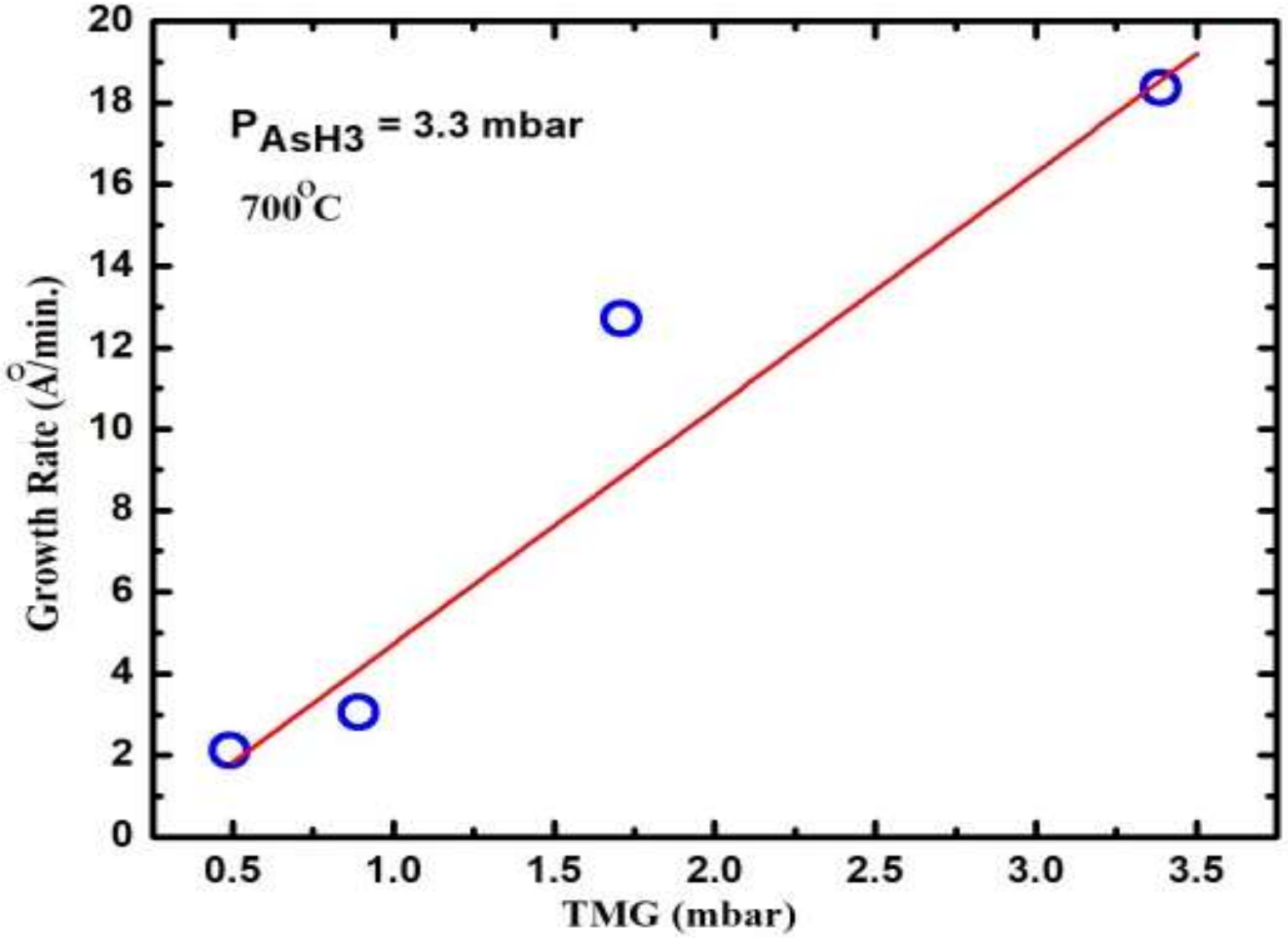

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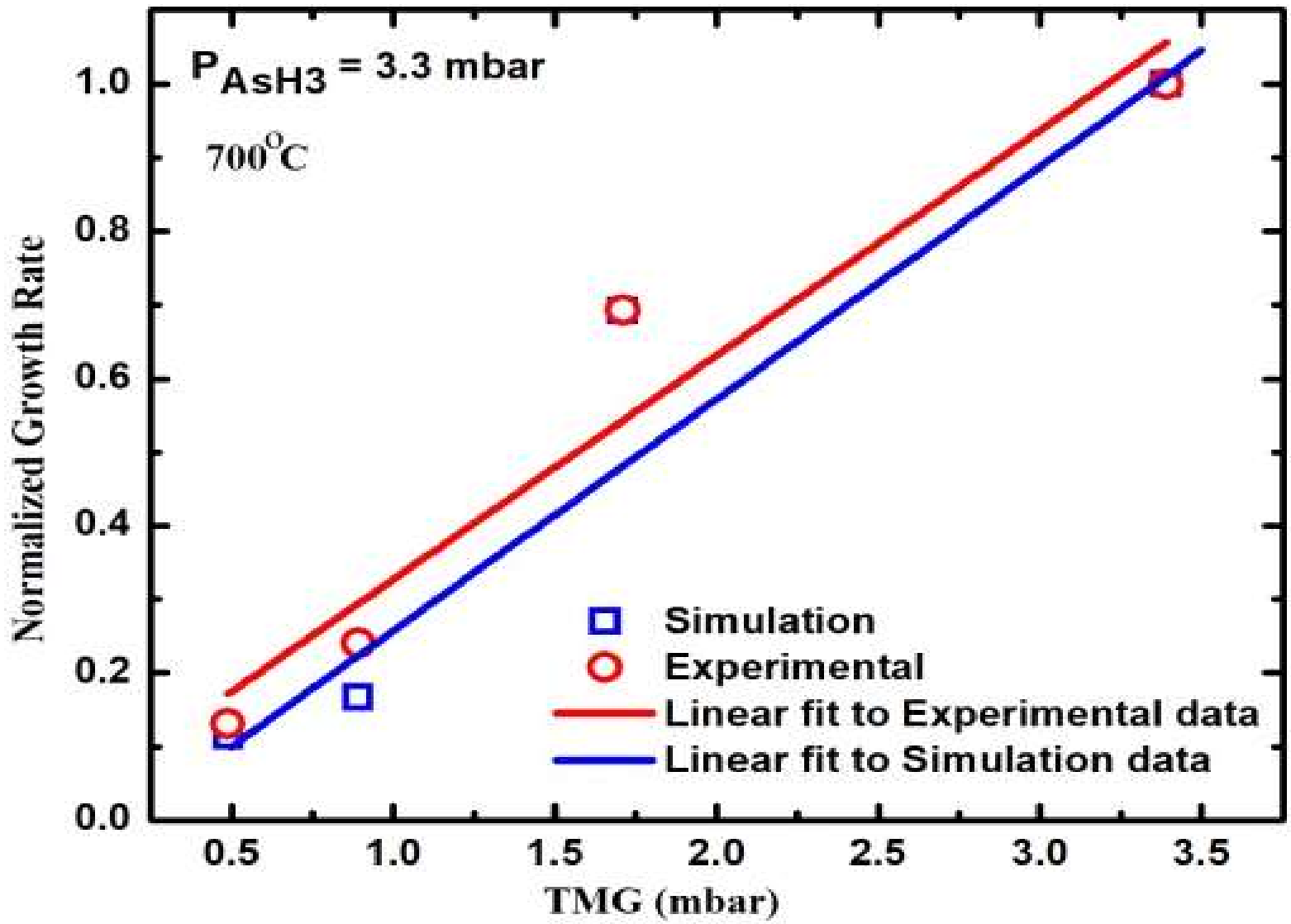

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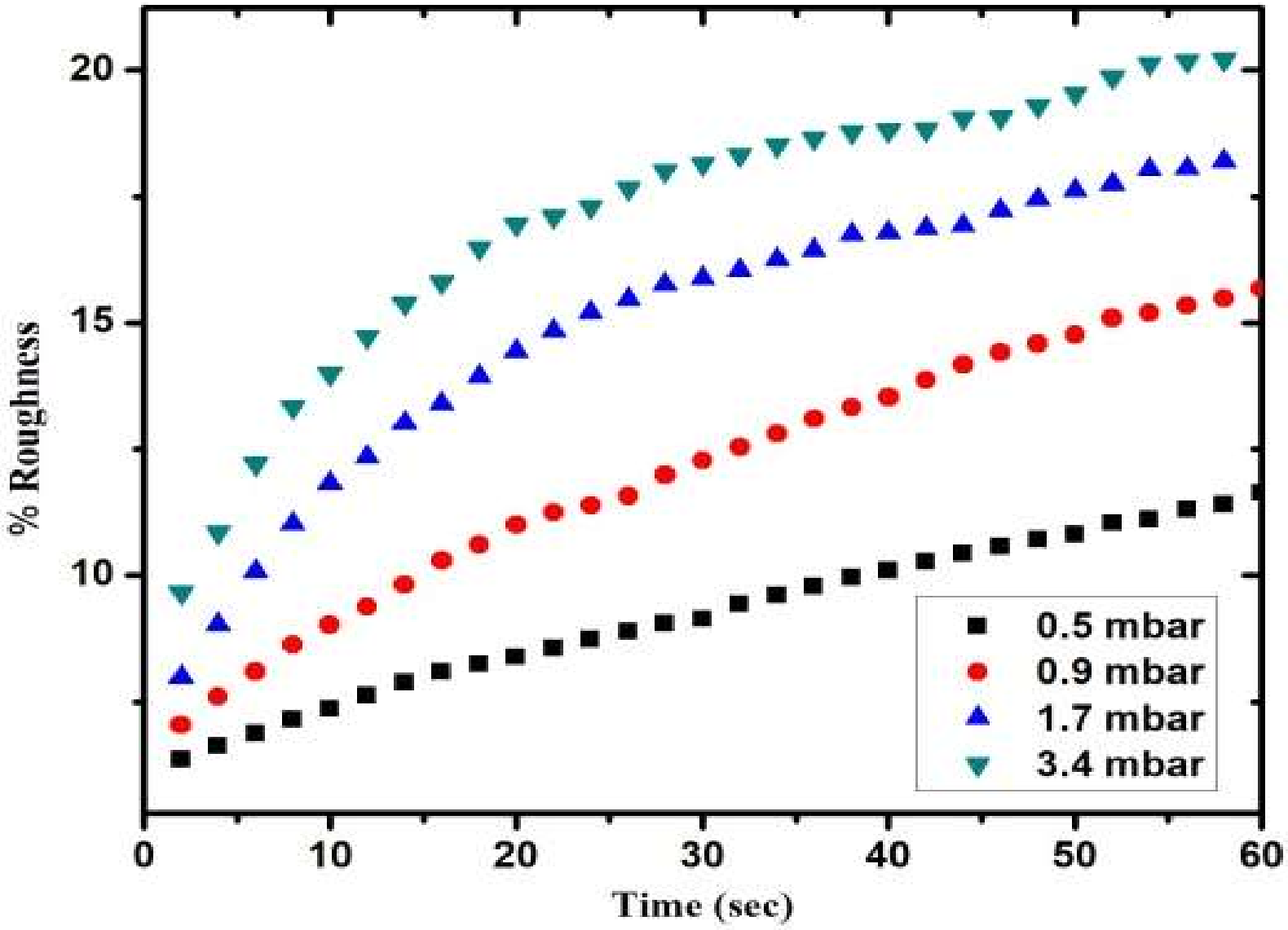

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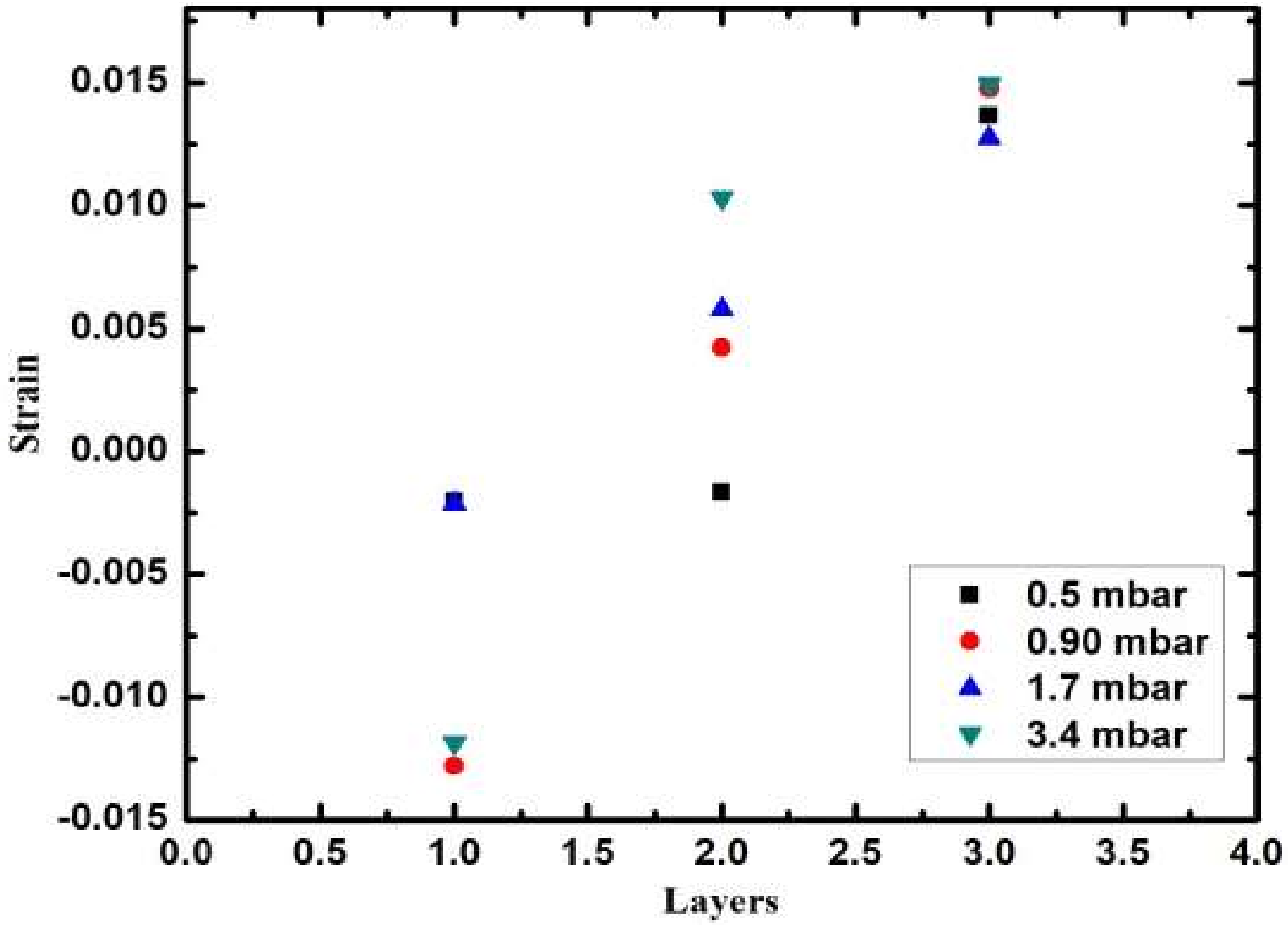

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Thank You

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