Atomistic Thin Film Growth – EpiGrow Simulator
Case Studies

1. **A detailed real lattice based epitaxial growth of GaAs using MOCVD reactor's input conditions**

Gas-phase reactions:

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

Surface reaction

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

Reactions included in the gas-phase and surface-phase model. Note: Rate constants have been adopted from Ref. [20].

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

Various energy values used.

Parameters	Values	Units
Substrate surface energy (E_s)	1.75	eV
Schwoebel barrier energy (E_{shw})	0.02	eV
Incorporation barrier energy (E_i)	0.05	eV

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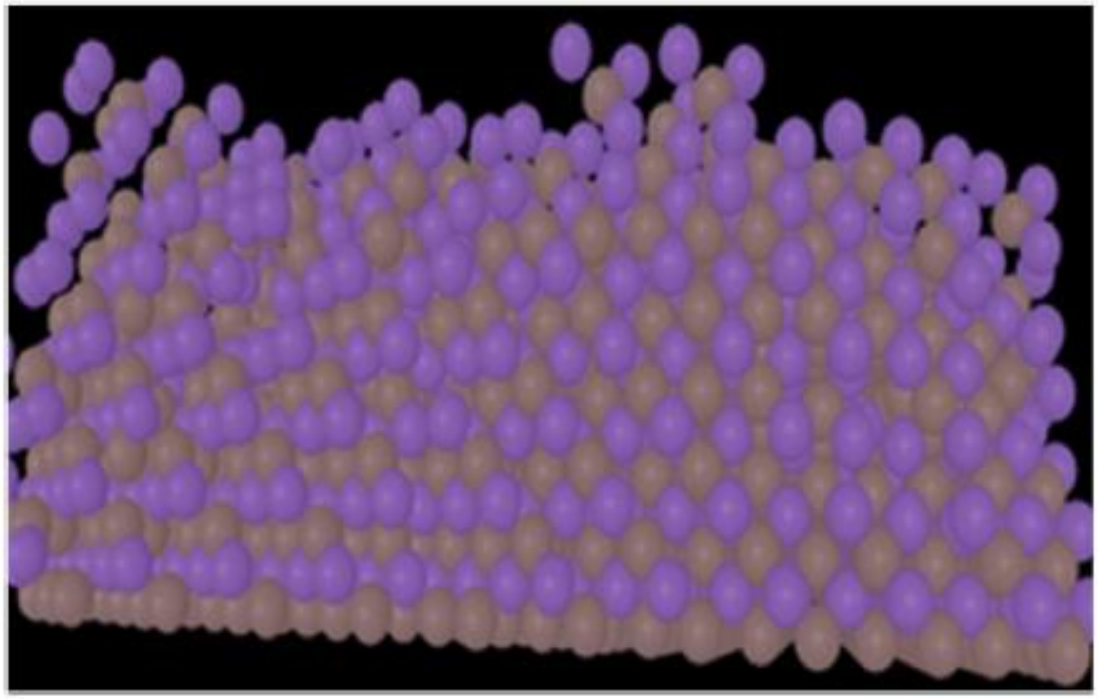

Fig. 2. The layered structure of GaAs thin film over GaAs crystal is clearly visible (Bottom first and second layer atoms are Ga and As which belong to substrate layer).

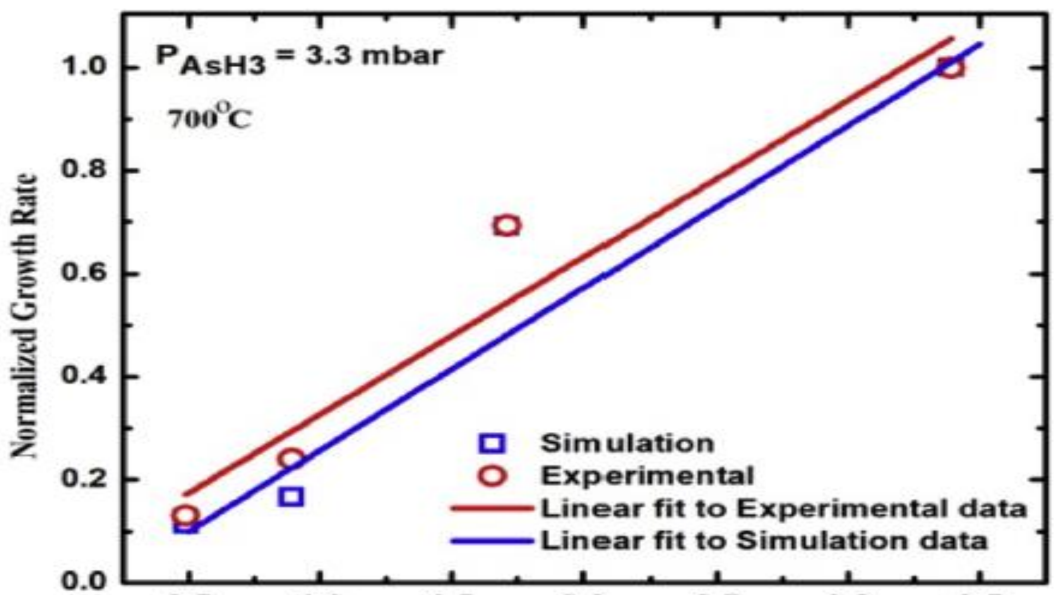

Fig. 4. The experimental data of growth rates vs partial pressure of TMG is retrieved and its normalized values are plotted here (Red circles). For comparison normalized data of simulation result is also plotted (Blue Squares). It is clear that both slopes are almost equal. (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

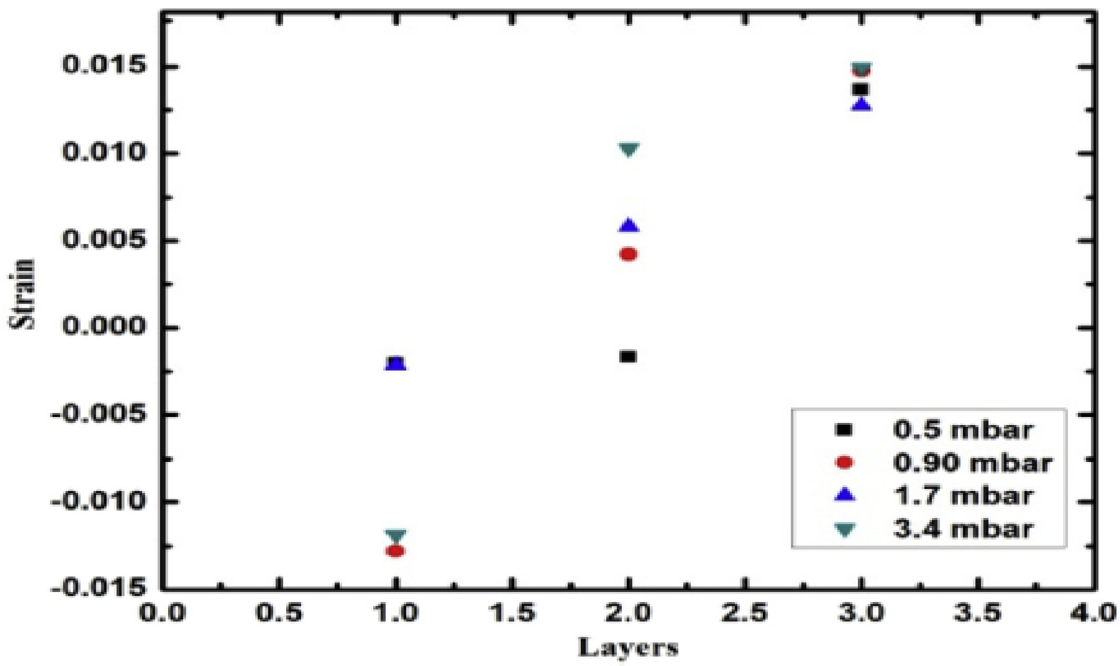

Fig. 6. Strain is extracted for every layer EpiGrow simulator and strain for first three layers is shown here. The average strain in the epi-grown sample including compressible and tensile is almost zero.

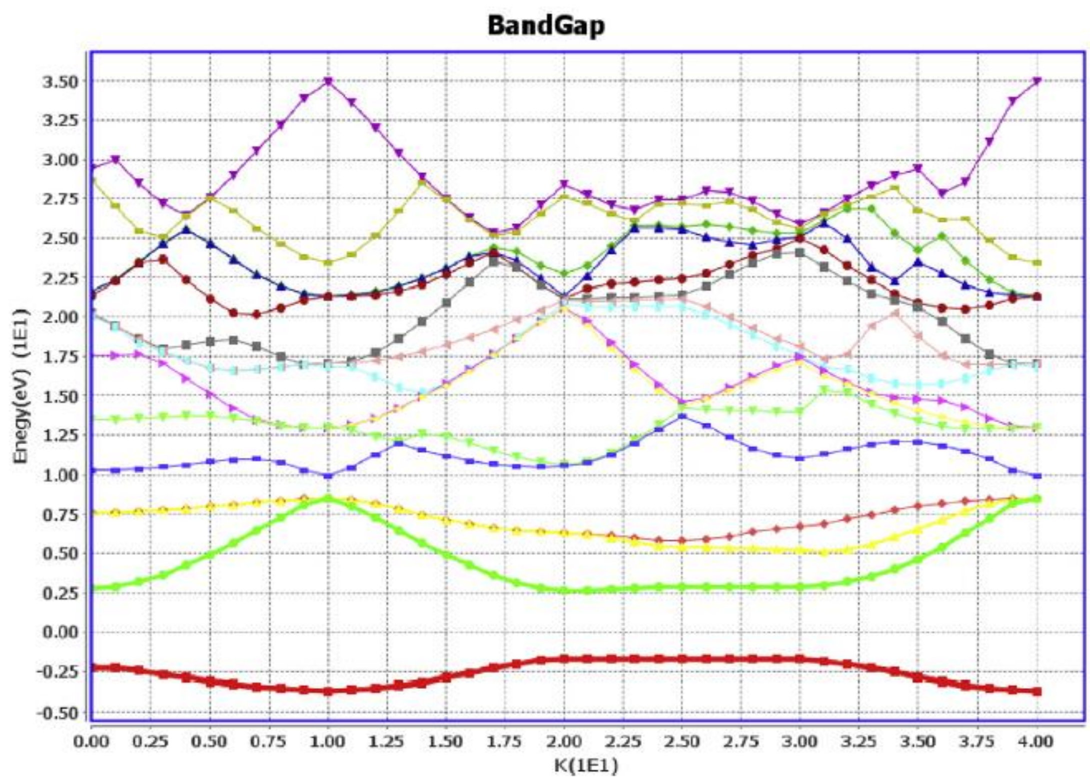

Fig. 7. Full energy band structure is shown for GaAs. Lower four lines depict Valence band while upper lines are showing Conduction band. Gamma point is at K (1E1) point value 10.0.

2. A detailed real lattice based epitaxial growth of GaN using MOCVD reactor's input conditions:

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

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

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			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

					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)	$NH_3 \cdot MMG(S)$
COMPM2(S)	$Ga \cdot NH_2 \cdot MMG(S)$
COMPM3(S)	$NH_3 \cdot Ga \cdot NH_2 \cdot MMG(S)$
COMPM4(S)	$Ga \cdot NH_2 \cdot Ga \cdot NH_2 \cdot MMG(S)$
COMPM5(S)	$NH_3 \cdot Ga \cdot NH_2 \cdot Ga \cdot NH_2 \cdot MMG(S)$
RINGM1(S)	$NH_2 \cdot Ga \cdot NH_2 \cdot Ga \cdot NH_2 \cdot Ga(S)$
RINGM2(S)	$(S)NH_2 \cdot Ga \cdot NH_2 \cdot Ga \cdot NH_2 \cdot Ga(S)$
COMPMM1(S)	$MMG \cdot GaNH_2(S)$
COMPMM2(S)	$NH_3 \cdot MMG \cdot GaNH_2 \cdot Ga(S)$
COMPMM3(S)	$NH_2 \cdot Ga \cdot NH_2 \cdot Ga(S)$
COMPMM4(S)	$MMG \cdot NH_2 \cdot Ga \cdot NH_2 \cdot Ga(S)$
COMPMM5(S)	$NH_3 \cdot MMG \cdot NH_2 \cdot Ga \cdot NH_2 \cdot Ga(S)$
TCOM1(S)	$NH_3 \cdot TMG(S)$
TCOM2(S)	$NH_2 \cdot DMG(S)$
TCOM3(3)	$(S)NH_2 \cdot DMG(S)$
COM1(S)	$RINGM2(S) \cdot CH_3$ complex

Process Parameters Used

Parameters	Values	Unit
Time	30	s
Temperature	800	°C
Surface energy	2	eV
Desorption barrier energy	4	eV
Schwoebel barrier	0.002	eV
Incorporation barrier	0.05	eV
Nearest neighbor attraction	0.05	eV

Precursors and Gas ambience Used

Materials	Partial pressure		
	Ga (mbar)	Al (mbar)	N2 (mbar)
GaN	0.3	0.0	3.0
$Ga_{0.85}Al_{0.15}N$	0.3	0.03	3.0
$Ga_{0.7}Al_{0.3}N$	0.28	0.05	3.0
$Ga_{0.61}Al_{0.39}N$	0.25	0.10	3.0

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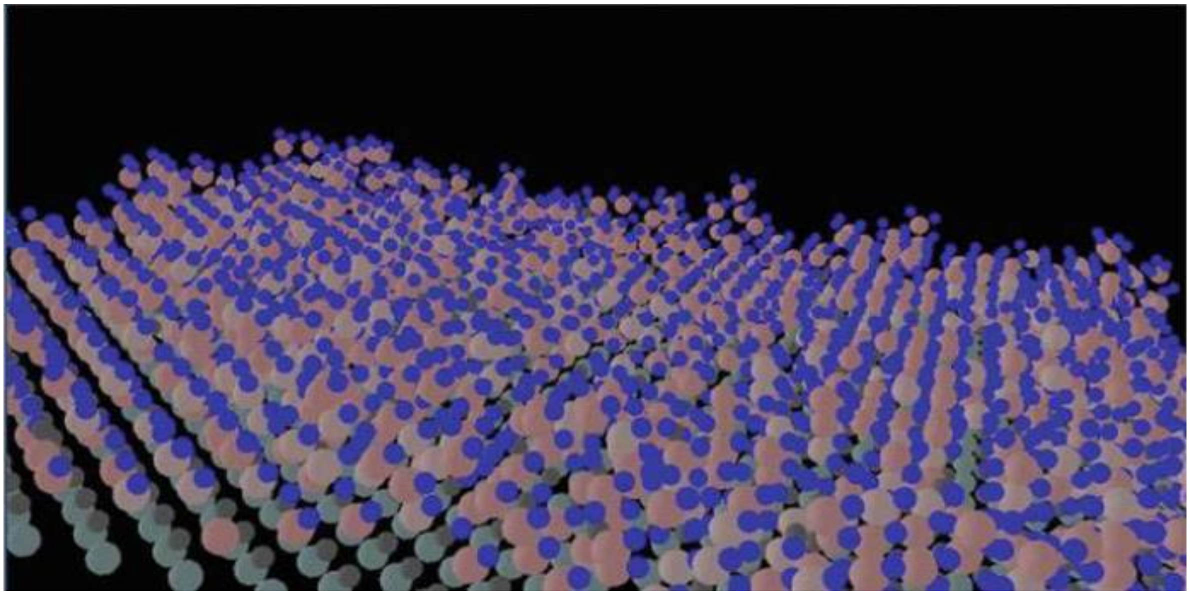

Epitaxial growth of AlGaN over GaN using TNL EpiGrow simulator

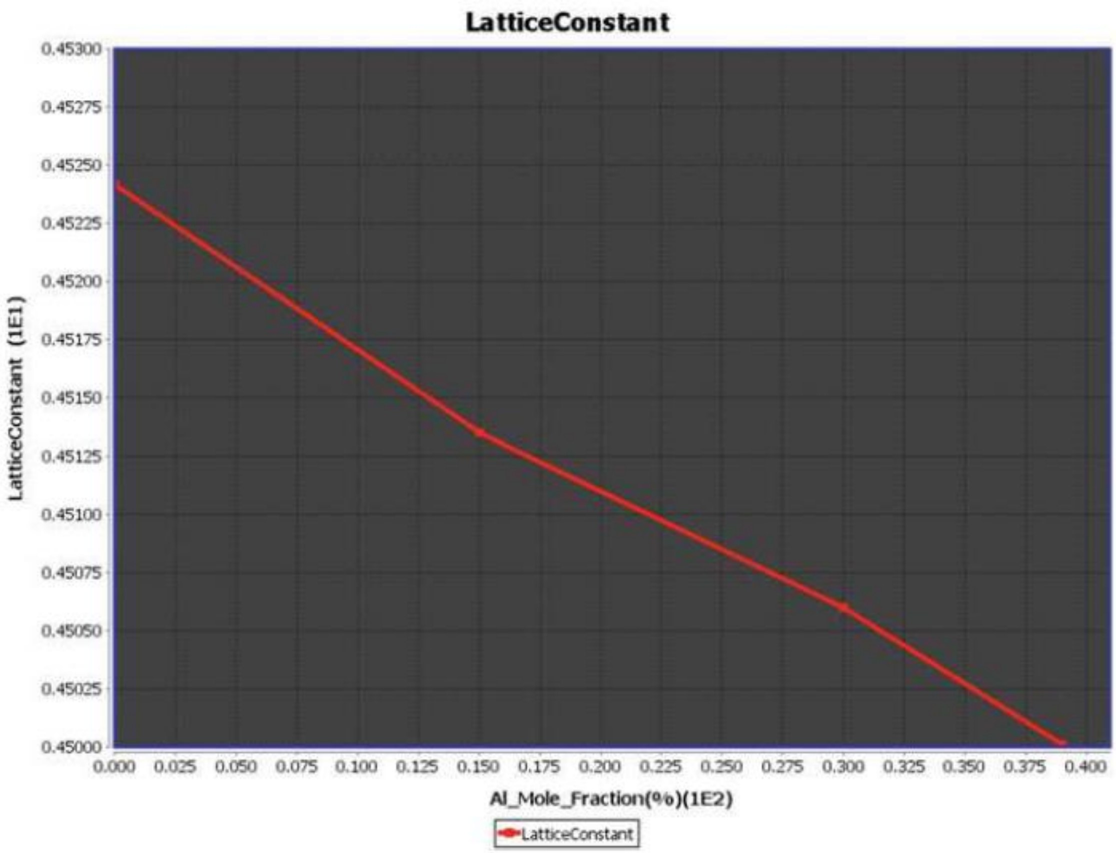

Fig. 2 Variation of lattice constant with Al mole fraction

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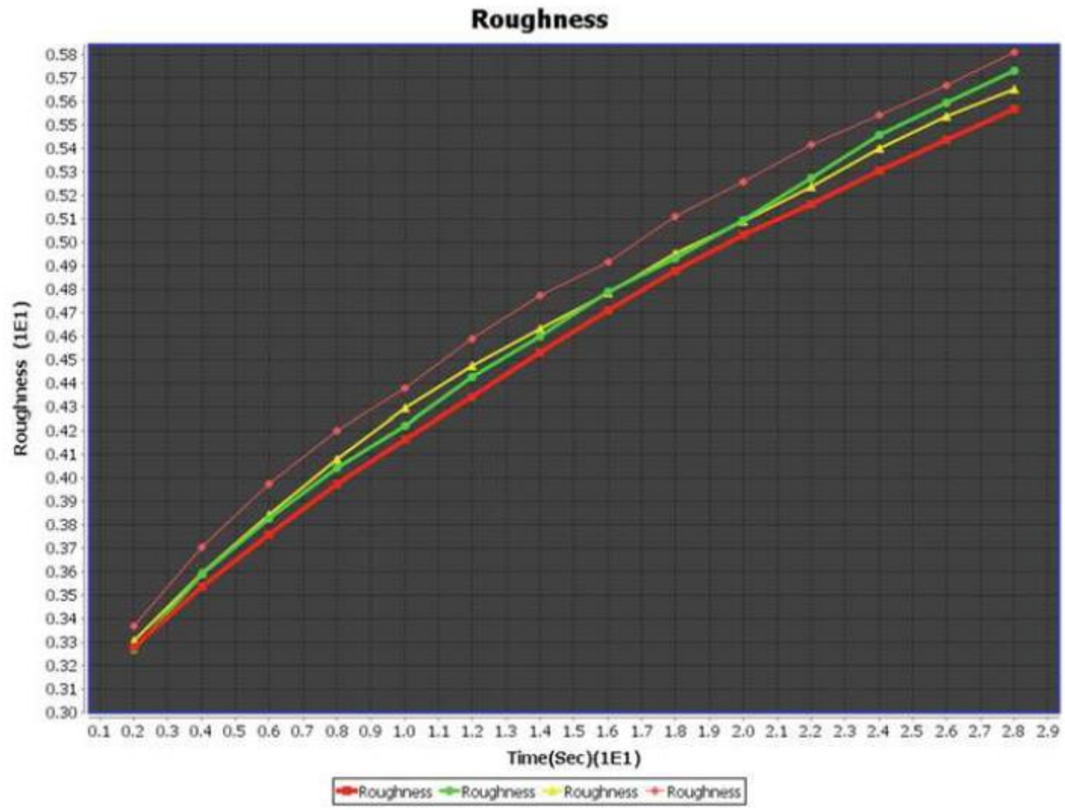

Fig. 3 Surface roughness at the interface of AlGaN/GaN