Atomistic Level Process to Device Simulation of GaNFET Using TNL TCAD Tools

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Abstract An atomistic level process to device simulation tools developed by Tech Next Lab (TNL) is reported. Modeling of the deposition of high-quality ultrathin AlGaN epitaxial films grown on GaN substrates by molecular beam epitaxy (MBE) has been performed. The surface morphology, crystalline quality, and interfacial property of as-grown AlGaN epitaxial films on GaN substrates are studied using simulation. The epitaxial layer characterization for extract of exact carrier mobility and use of epitaxially grown material for GaN-FET device application has been demonstrated. Results obtained on the basis of process to device simulation have been calibrated with reported results.

Keywords GaN-FET · Epi-growth · Full band simulation · TNL

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1 Introduction

Transistors based on GaN significantly extend the capabilities of power electronics and microwave devices [1, 2]. GaN being a wide-gap semiconductor material is normally used for constructing the base material of a blue light emitting diode [3]. Furthermore, material properties such as high withstand voltage and low conducting resistance are well known [4]. It is a semiconductor material that is strongly expected to be applied to the next-generation power devices by taking advantage of these characteristics. In particular, the AlGaN/GaN-HEMT (high-electron-mobility transistor) structure based on GaN is expected as a high-speed switching element with high gain due to downsizing of device size and reduction of parasitic capacitance [5–8]. A high electron density in the region of the two-dimensional electron gas in combination with acceptable electron mobility makes it possible to implement high current densities in the transistor-channel cross section and high gains. However, experimental optimization of heterostructure transistors still remains a complicated and expensive procedure [9, 10].

The atomistic simulation suite developed at Tech Next Lab (TNL) consists of the following modules [11–13]:

- EpiGrow Simulator
- Full Energy Band Simulator
- Electron Mobility Simulator
- Monte Carlo Particle Device Simulator.

Based on the reactor process conditions such as partial pressures of elements of which thin film has to be grown, substrate orientation, and temperature, process simulation of the film deposition is performed. Extraction of the physical parameters of the deposited films such as lattice parameter, strain, deformation, and surface roughness of films is calculated. Full Energy Band Simulator provides various parameters for carrier's transportation on full band structure associated with epi-grown AlGaN monolayers.

Electron Mobility Simulator is capable to simulate carrier's mobility under the influence of external electric field and effect of same on the carrier transport on full energy band structure, and lastly the Monte Carlo Particle Device Simulator module [13] is used for particle-based device simulation.

2 Atomistic Process Simulation

A thin film of $Ga_{1\text{-}x}Al_xN$ (where $x = 0$, 0.15, 0.3, and 0.39) is grown on 3C-SiC substrate by EpiGrow simulator. The input parameters needed to grow thin film by EpiGrow simulator are energy values such as surface energy, film energy, and Schwoebel energies and reactor conditions as partial pressure substrate temperature. Surface diffusion energy barrier, E_s, is also called activation energy. The calculation of it is based on the assumption that bonds only exist between nearest neighboring atoms. E_n is nearest binding energy on the horizontal plane. If n is the number of nearest neighbors on the surface, the total activation energy is given as

$$E = E_s + nE_n \tag{1}$$

Epi-growth has been done with the following process parameters:

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 during simulation are

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

Figure 1 depicts the atomic lattice structure. On the lattice structure, the lattice constant, roughness, strain, and defects can be mapped and traced. Figure 2 represents the variation of lattice constant with respect to Al contents in the AlGaN material. One can establish a conclusion from Fig. 2 that increasing the Al contents, the lattice constant will be decreased, i.e., showing inversely dependence of lattice constant on the Al contents in the AlGaN alloy during epi-growth. Figure 3 shows different structure roughness at different operating temperature conditions. Roughness in the epi-growth layer increases with the rise in temperature due to dominance of diffusion process of atoms on the substrate.

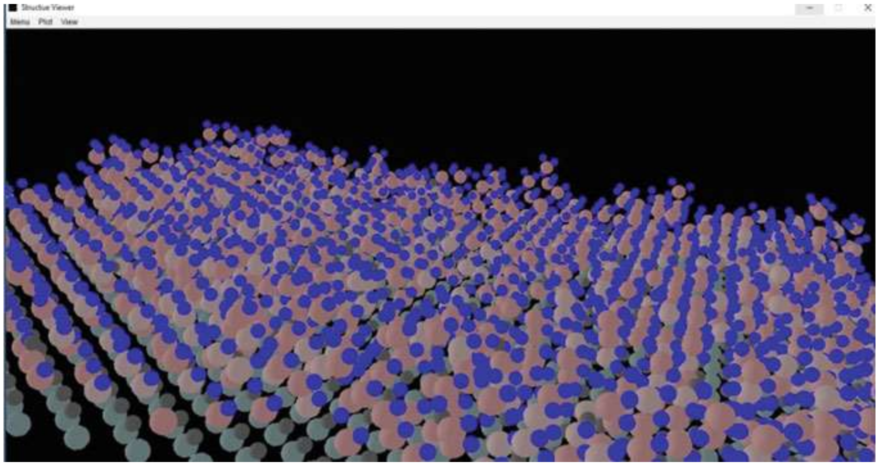


Fig. 1 Epitaxial growth of AlGaN over GaN using TNL EpiGrow simulator

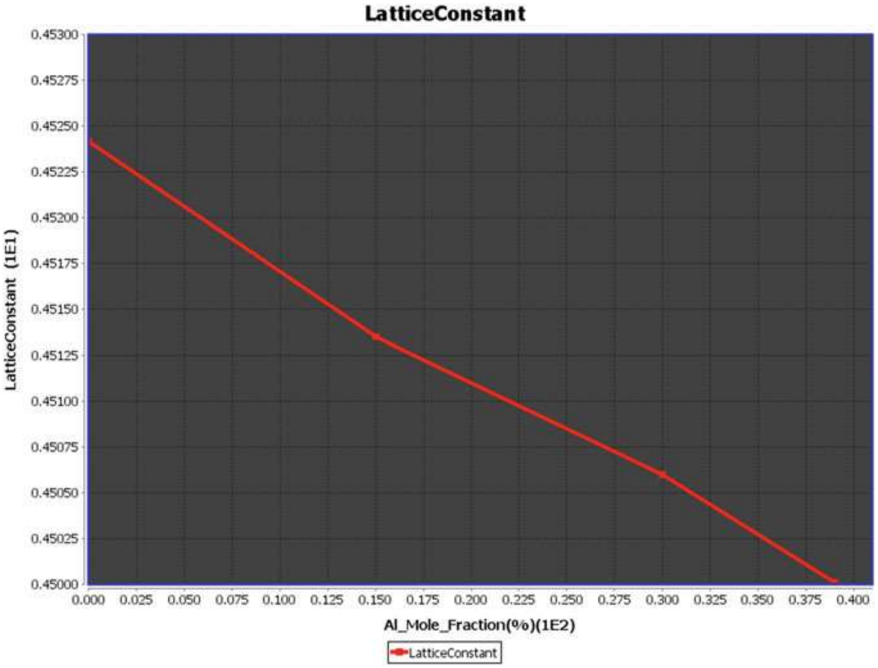


Fig. 2 Variation of lattice constant with Al mole fraction

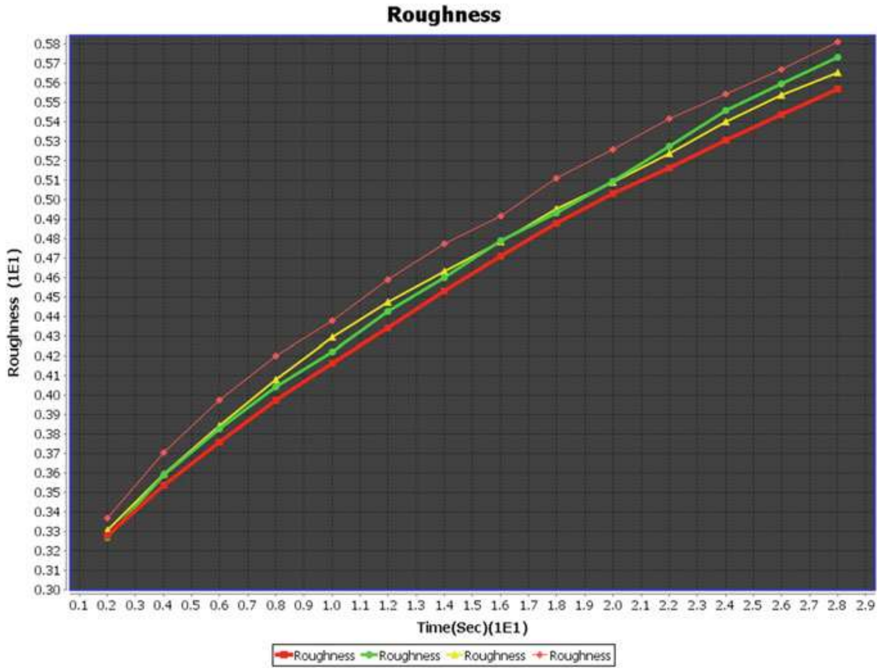
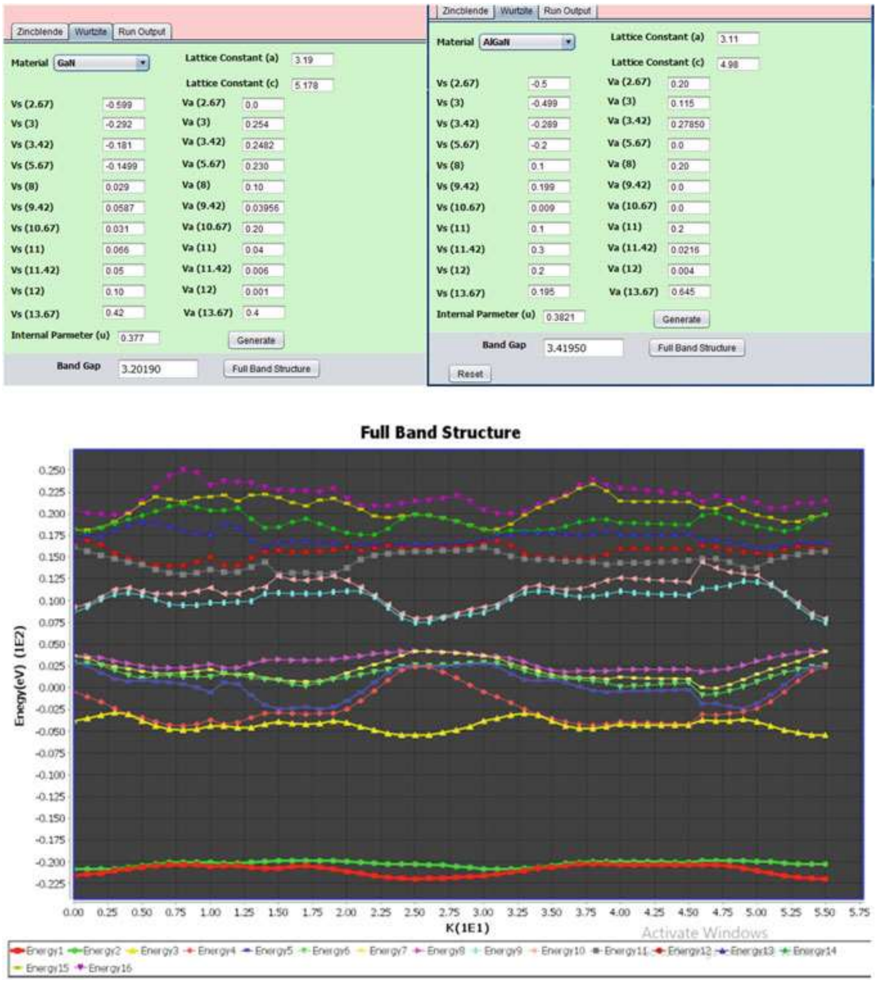


Fig. 3 Surface roughness at the interface of AlGaN/GaN

3 Full Band Simulation

Full Band Simulator [11] is used to simulate full electronic band structures for AlGaN epi-grown layer on GaN, the form factors interpolated from GaN and AlN form factors. The full electronic band structure includes bowing of band energies and their deformation potentials. The lattice constant extracted from epi-grown layers of GaN and AlGaN is used and given below:

Figures 4 and 5 depict the full electronic band structures for epi-grown GaN and AlGaN materials, respectively. The different physical parameters, e.g., carrier group velocity, different energies associated with different bands, effective mass, deformation potentials, and density of states for carriers have been traced on the full electronic band structures for simulation of carrier transport under external forces. The band-gaps at gamma valley are 3.2 and 3.41 eV for GaN and $Al_{0.37}Ga_{0.63}N$, respectively.



Material	GaN	Lattice Constant (a)	3.19
		Lattice Constant (c)	5.178
Vs (2.67)	-0.599	Va (2.67)	0.0
Vs (3)	-0.292	Va (3)	0.254
Vs (3.42)	-0.181	Va (3.42)	0.2482
Vs (5.67)	-0.1499	Va (5.67)	0.230
Vs (8)	0.029	Va (8)	0.10
Vs (9.42)	0.0587	Va (9.42)	0.03956
Vs (10.67)	0.031	Va (10.67)	0.20
Vs (11)	0.066	Va (11)	0.04
Vs (11.42)	0.05	Va (11.42)	0.006
Vs (12)	0.10	Va (12)	0.001
Vs (13.67)	0.42	Va (13.67)	0.4
Internal Parmeter (u)	0.377		
Band Gap	3.20190		

Material	AlGaN	Lattice Constant (a)	3.11
		Lattice Constant (c)	4.98
Vs (2.67)	-0.5	Va (2.67)	0.20
Vs (3)	-0.499	Va (3)	0.115
Vs (3.42)	-0.289	Va (3.42)	0.27850
Vs (5.67)	-0.2	Va (5.67)	0.0
Vs (8)	0.1	Va (8)	0.20
Vs (9.42)	0.199	Va (9.42)	0.0
Vs (10.67)	0.009	Va (10.67)	0.0
Vs (11)	0.1	Va (11)	0.2
Vs (11.42)	0.3	Va (11.42)	0.0216
Vs (12)	0.2	Va (12)	0.004
Vs (13.67)	0.195	Va (13.67)	0.645
Internal Parmeter (u)	0.3821		
Band Gap	3.41950		

Fig. 4 Full band structure of GaN

4 Mobility Characterization Simulation

Epi-grown layers are characterized with the help of Electron Mobility Simulator [12] to simulate the electron transport in AlGaN/GaN materials including different scattering mechanisms under the influence of electric field.

Figures 6 and 7 show the scattering rates at gamma valley and electrons occupation at different valleys under the application of external forces in the form of electric field. Initially, all electrons remain at gamma valley, as the electric field increases the transition of electrons starting from gamma valley to L- and X-valley. Since electrons effective mass is much higher in L-valley, electrons cannot transit to X-valley.

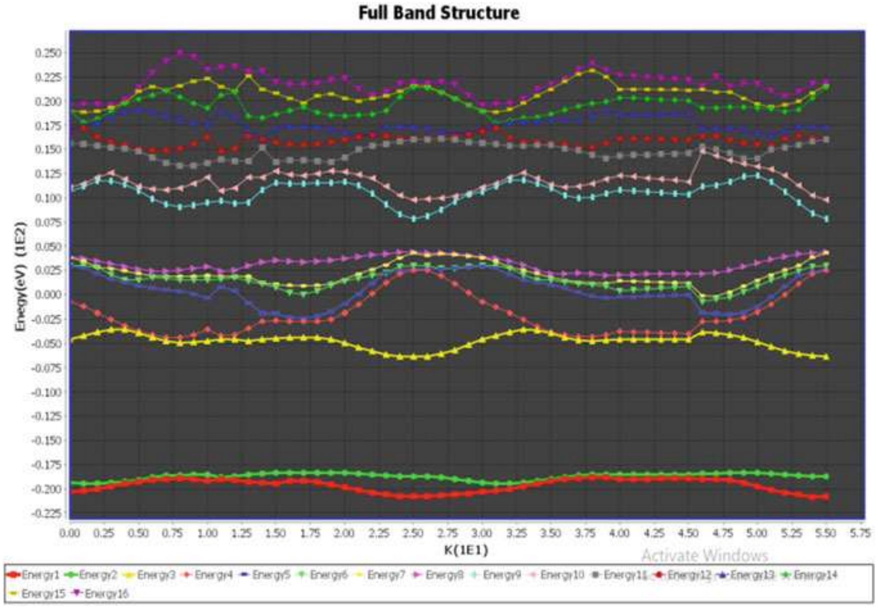


Fig. 5 Full band structure of AlGaN

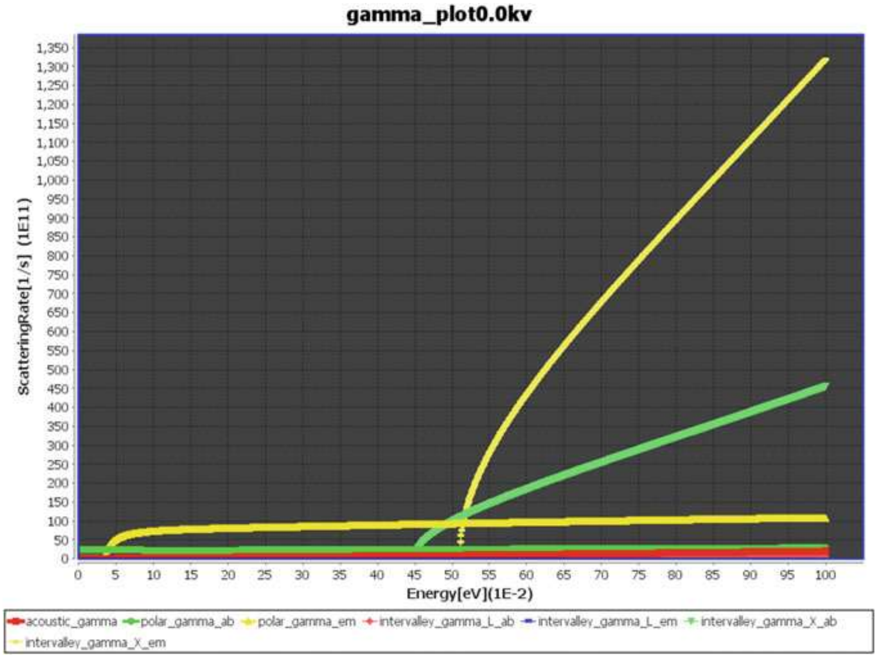


Fig. 6 Carrier scattering at gamma valley

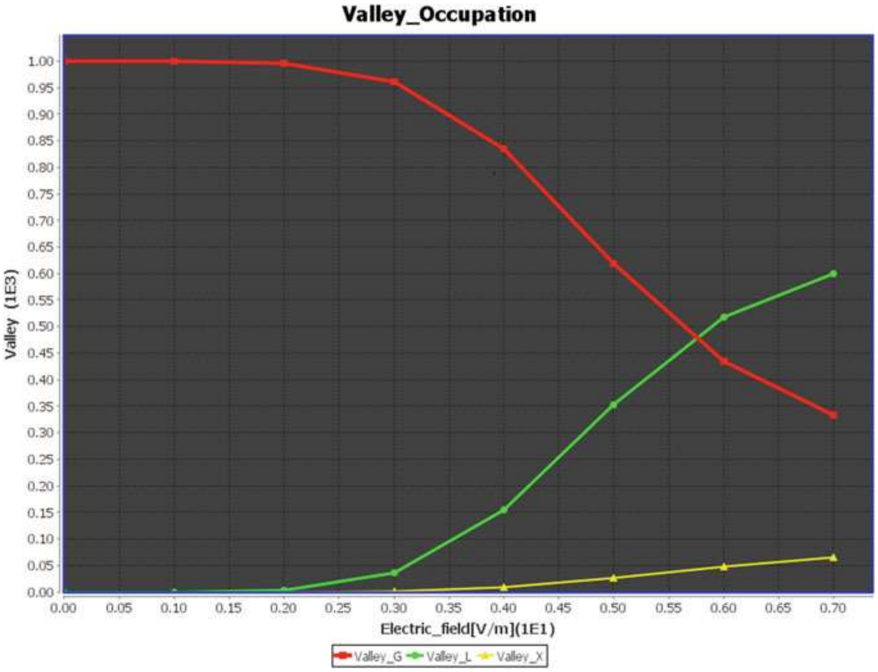


Fig. 7 Valley occupation variation with electric field

Figure 8 demonstrates the drift velocity of carriers under the application of electric field; the mobility of electrons increases as electric field increases and starts decreasing after attending the saturation values after which mobility starts to decrease due to different scattering mechanism and showing negative differential mobility. The mobility of carriers in epi-grown sample of AlGaN/GaN is coming out to almost 200 cm^2/V s which is reasonably agreed with the reported standard mobility of electrons in GaN/AlGaN sample ~300 cm^2/V s.

5 Device Simulation

A GaNFET with 190 nm gate length is chosen for device simulation as shown in Fig. 9. The device simulation includes the physical and electrical property study. The electrical performance has been studied in terms of I_d–V_g and I_d–V_d.

The I_d–V_g curve represents the standard current voltage characteristics for AlGaN/GaN on Si substrate. Under high reverse bias conditions, the current is almost negligible; in moderate to low reverse bias conditions, current starts rising linearly, and under forward bias conditions, it attains almost saturation as shown in Fig. 10 (Fig. 11).

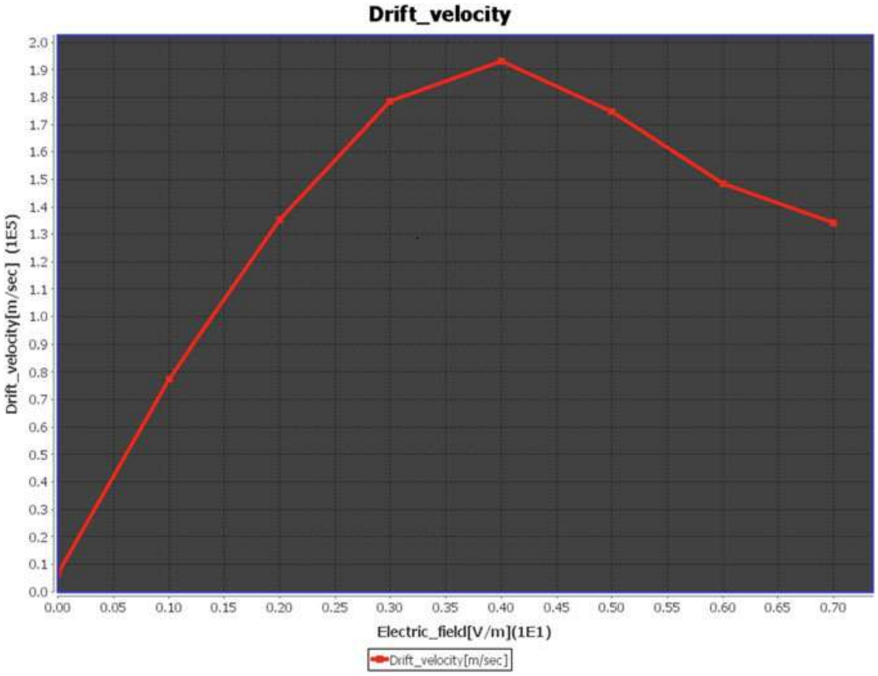


Fig. 8 Drift velocity versus electric field

The I_d–V_d curve matches with the standard I–V characteristics of GaN-FET devices under same operating conditions. At low forward bias condition, the current increases linearly showing ohmic type of dependence on the voltage, while as device starts operating at high forward bias conditions, the current attends saturation due to different scattering mechanisms, and hence, the mobility of carriers decreases.

6 Conclusion

The present paper shows the capabilities of innovative TNL TCAD simulators with atomistic level simulation starting from epi-growth, material characterization to device simulation. The TNL TCAD simulators use solution Boltzmann equation with Monte Carlo technique for material characterization and device simulation purposes. The carriers transport on full band structure under appropriate biasing conditions can provide valuable information of inside physical mechanisms which are not possible with the conventional drift-diffusion and hydrodynamic models.

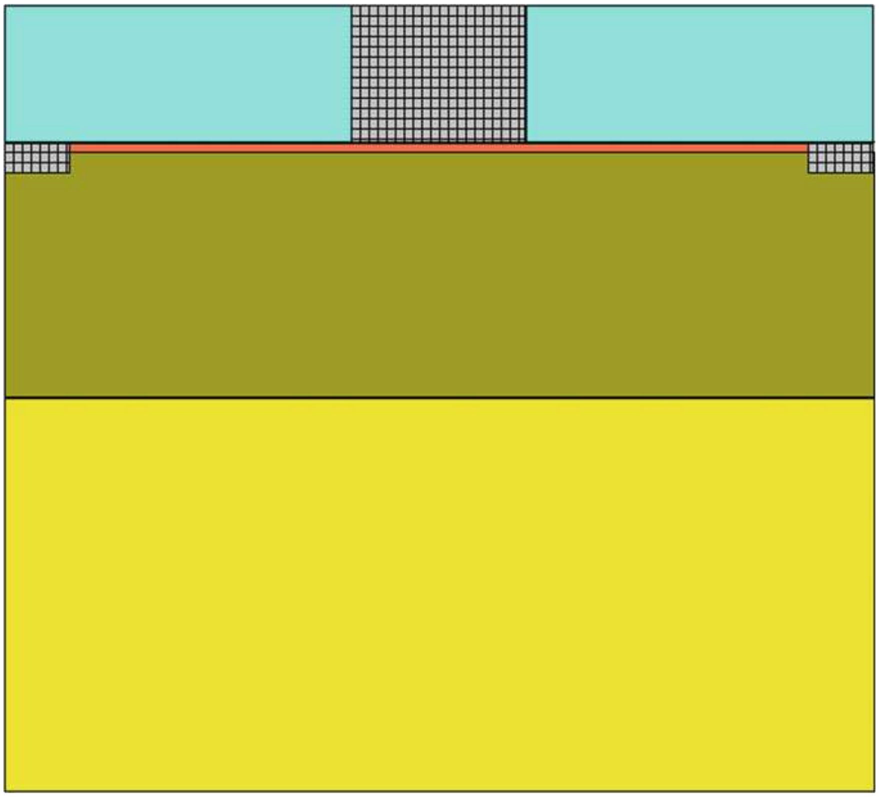


Fig. 9 Device structure with 25 nm thick AlGaN/GaN layer grown on SiC (100) substrate

Fig. 10 Output (I_d–V_g) characteristics

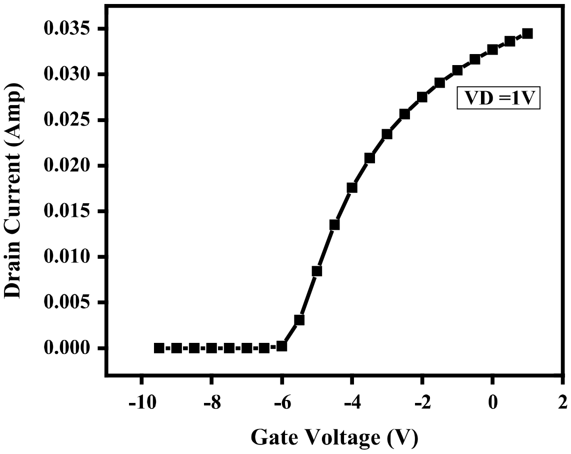
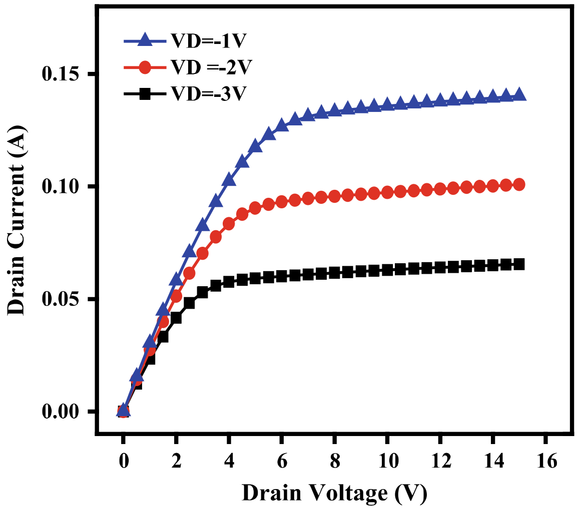


Fig. 11 Output (I_d–V_d) characteristics



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