



# Chapter 1

## Introduction

### 1.1 A short story of GaN

The first gallium nitride (GaN) compounds were prepared by reacting ammonia gas with metallic gallium at high temperatures in 1932 by Johnson *et al.* [1]. Their work showed its remarkable stability toward heat, solutions of acids and bases. Almost four decades later Maruska *et al.* [2] and Pankove *et al.* [3] characterized the optical properties of GaN and determined the direct band gap to 3.36 - 3.39 eV at room temperature. A few years later the GaN bandstructure and its reflectivity were computed by the empirical pseudopotential method [4]. Bloom *et al.* predicted GaN as a promising material for luminescence devices and laser applications due to its wide direct band energy. In the following years, Ilegems and Montgomery [5] suggested that the n-type conductivity of GaN semiconductor behaviour is due to native defects. Their conclusions were widely debated. The question was whether n-type conductivity was due to native defects or impurities. Several groups continued their work intensively on point defects and most comprehensive point defects studies are contributed by Neugebauer and Van de Waal [6]. They proposed that unintentional donor impurities and gallium vacancies are responsible for n-type conductivity of GaN rather than the long believed-nitrogen vacancy [7]. Other noticeable work on charged point defects which control numerous defect properties of semiconductors have been published by Seebauer and Kratzer [8].

In early 90's, the first p-n junction LED GaN fabrication was reported by a Japanese group [9]. Earlier reports of improving crystalline quality of GaN by inserting a thin AlN nucleation layer to accommodate lattice constant mismatch of sapphire substrate was reported by Yoshida *et al.* and Akasaki *et al.* [10, 11]. In early 90's Khan *et al.* for the first time observed

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a 2-dimensional electron gas (2DEG) at the interface between AlGaN and GaN layers [12]. Since then, research of AlGaN/GaN high electron mobility transistors (HEMTs) towards improving technology for improved performance and novel application was intensively pursued by numbers of groups [13, 14, 15, 16, 17]- to mention a few.

Mishra's recent overview provided impressive data of RF performance of GaN HEMTs stand: 13.7 W/mm at 30 GHz, 10.5 W/mm at 40 GHz, and 2.4 W/mm at 60 GHz and the fastest GaN devices today at a cut-off frequency of 220 GHz and a maximum oscillation frequency of 400 GHz [18]. However, GaN-based devices have shown short-term instabilities including collapse of DC IV-characteristics, and high leakage currents. This urges comprehensive reliability studies which are the main purpose of this thesis. It is important to investigate the main cause of GaN HEMTs degradation i.e. temperature and/or electric field dependencies through detailed investigations from material growth to process technology.

## 1.2 GaN structure

Group III-nitrides can crystallize in three possible crystal structures: the wurzite (WZ) structure, the zinc-blende structure and the the rocksalt structure. The GaN WZ structure has a hexagonal unit cell and is thermodynamically more stable than other structures such as zinc blende or rocksalt structures [19]. The wurzite (WZ) structure is non-centrosymmetric (i.e. it lacks of inversion symmetry) and displays piezoelectric effect. The asymmetry of Ga-N bonding between the longer bond and the shortest bond in a tetrahedral atom arrangement leads to a permanent dipole along the c-axis (see Fig. 1.1b). Ga-N bond is highly polarized with the electrons located mostly near the nitrogen atom [20] (see Fig. 1.1c). The spontaneous polarization of GaN crystal by convention is along  $[000\bar{1}]$  direction [21] (see Fig. 1.2). Any stress accomodated during the heteroepitaxial GaN growth changes the lattice parameter along the c-axis, leading to an additional piezoelectric polarization. Piezoelectric constant of AlN, GaN and InN with WZ structure have are up to ten times larger than those of conventional III-V and II-VI semiconductor compound [22].

## 1.3 Substrate options

The sucessful growth of GaN epitaxial layer on foreign substrates has to consider several aspects: lattice mismatch, thermal conductivity and price.

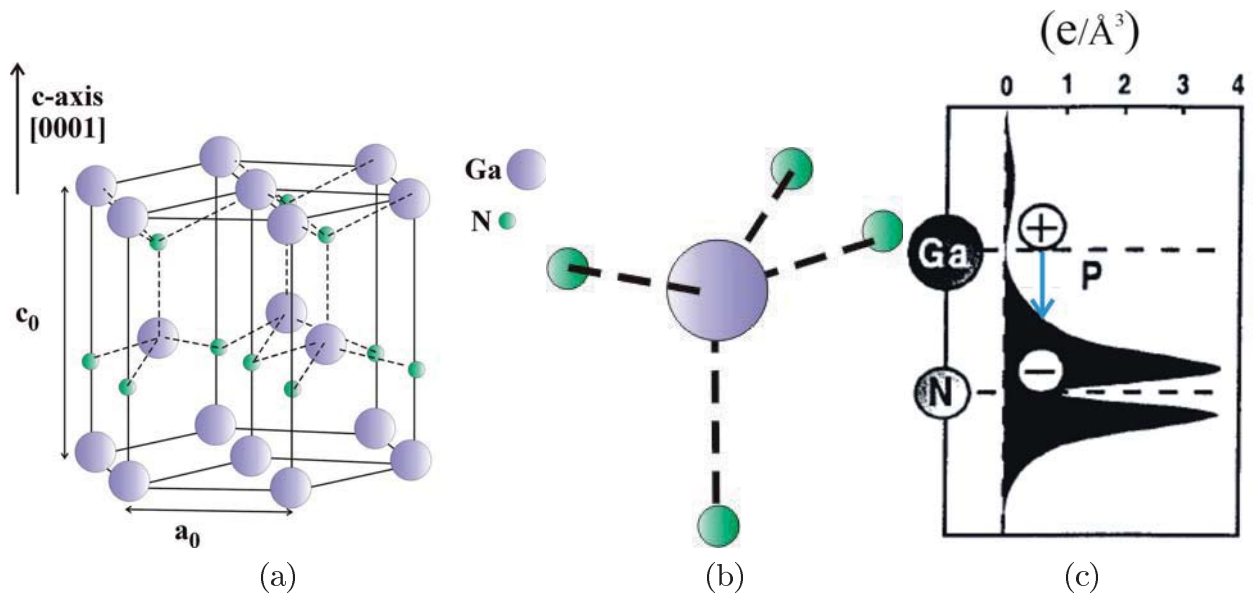


Figure 1.1 GaN (a) wurtzite structure, (b) tetrahedral configuration, and (c) charge distribution of valence electrons.

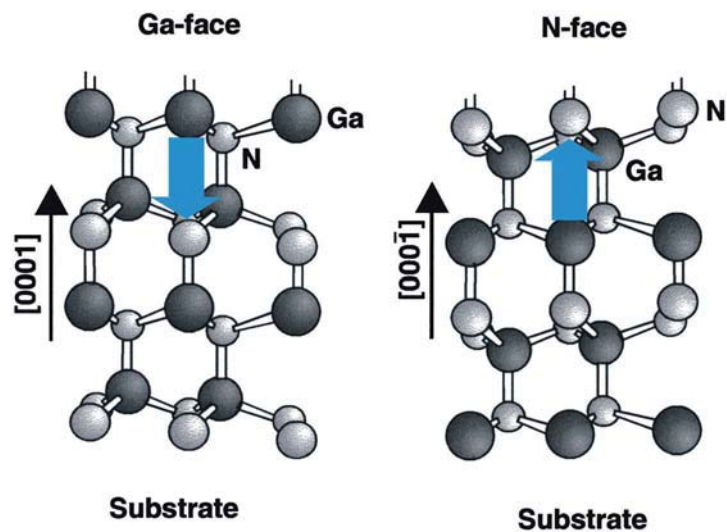


Figure 1.2 Ga-polarity and N-polarity crystals with each polarization direction (blue arrow)[13].

Historically, sapphire ( $\text{Al}_2\text{O}_3$ ) was the first substrate for GaN-based devices, but it is not that favorable for RF and high power device applications due to its poor thermal conductivity (0.2-0.5 W/cm K). Moreover, GaN growth on sapphire has big lattice mismatch 13-16 % [23, 24]. The most favorable GaN substrate for microwave applications is SiC which is good in terms of thermal conductivity of 5 W/cm K, less expensive and provides a comparable low

lattice mismatch  $\sim 3.4\%$  [25]. Growing GaN-based device on SiC substrate with AlN nucleation layer, the strain can be smaller  $\sim 0.5\%$  [26].

Another option are Si substrates which are cheaper than SiC substrates and have a thermal conductivity of  $1.5\text{ W/cm K}$ . Disadvantage is the higher lattice mismatch about  $16.9\%$  [27] which causes strong tensile strain. The best substrate to grow GaN-based device is a freestanding GaN substrate with advantages, of course, no lattice mismatch and good thermal conductivity ( $1.3\text{ W/cm K}$ ). Recently, it was reported a very low thermal impedance of AlGaIn/GaN HEMTs on diamond substrate is  $4.1\text{ K mm/W}$  due to high diamond thermal conductivity of  $22\text{ W/cm K}$ ) [28]. However, GaN growth on diamond has large lattice mismatch which causes severe strain and wafer bowing [29] (see Table 1.1).

Fig. 1.3 shows estimations of the annual wafer production for each substrate type. For large volume production the Si substrate is the most attractive option for power electronics applications. Fre standing GaN substrates are good for optoelectronic applications since they are very sensitive to vertical dislocations. For microelectronic applications, still SiC substrate is favorable.

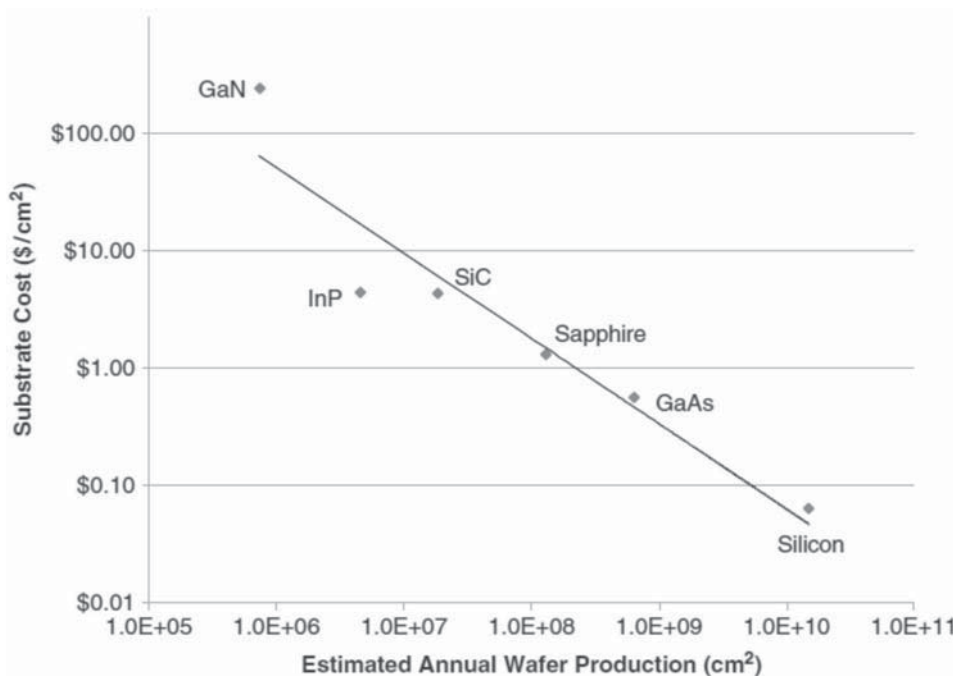


Figure 1.3 Substrate cost per square centimeter estimation in annual wafer production [30].

Table 1.1 Summary of alternative to SiC substrate for GaN-based device [29]

Substrate	Advantage	Disadvantage
GaN	lower relative defect density, lower leakage current, higher device yield, good for optoelectronic applications	difficult to produce large-diameter single-crystal GaN substrate, expensive
Diamond	high thermal conductivity, higher operating power density and temperature capabilities	large lattice mismatch causes severe strain and bowing, not easy to deposit GaN
Si	offers integration with Si IC technologies, large diameter substrate	lower thermal conductivity, big lattice mismatch

## 1.4 AlGaN/GaN high electron mobility transistors (HEMTs)

AlGaN/GaN HEMTs are fabricated at FBH by metal organic vapour phase epitaxy (MOVPE) in crystal direction (0001) with gallium face surface. On the top of the GaN buffer layer, a thin AlGaN layer is deposited. At the interface of this heterostructure, a 2DEG is formed (see Fig. 1.4). When two different semiconductors are in contact in the absence of an external bias voltage, the equilibrium is reached by lining up the Fermi level and bending the band diagram accordingly. This can create triangularly shaped quantum well structure at the interface. The necessary band bending is a consequent to the transfer of electrons from semiconductor with larger band gap (i.e. AlGaN) to lower band gap (i.e. GaN). The transfer of electrons to occupy lower energy states continues until the Fermi level is the same on both sides of heterostructures [31, 32]. The electrons occupy energy states in the triangular potential well the so called 2DEG such that electrons have quantized energy and are free to move in a two dimensional plane parallel to the interface.

The AlGaN crystal has a smaller lattice constant than GaN crystal because the Ga atom in GaN crystal is replaced by smaller sized Al atom. Consequently, the AlGaN a-axis lattice spacing must stretch to match to the underlying GaN lattice (see Fig. 1.5). This causes the c-axis of the AlGaN layer to contract and the lattice is unrelaxed and an additional piezoelectric polarization  $P_{PE}$  in AlGaN layer occurs. The total polarization field of both spontaneous polarization  $P_{SP}$  and piezoelectric polarization  $P_{PE}$  induces charges in 2DEG at the AlGaN/GaN interface with a high sheet charge density of  $\sim 10^{13} \text{ cm}^{-2}$ . It was shown that there is a minimum AlGaN thickness necessarily to induce charges in 2DEG [33] and that the Al concentration in

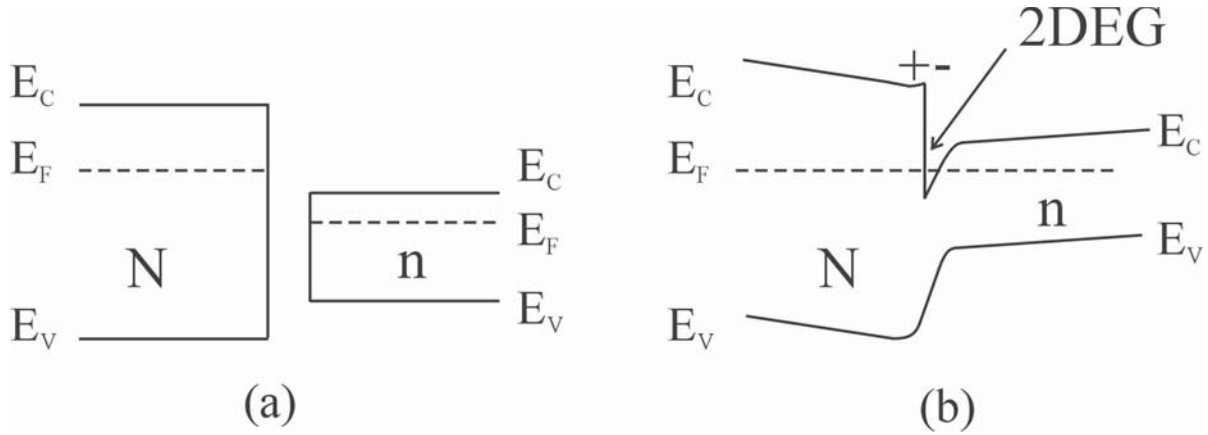


Figure 1.4 Schematic formation of 2DEG in the interface of heterostructure semiconductors due to the conduction band discontinuity in the interface (a) before contact, and (b) in contact reaching the equilibrium by lining up Fermi level. Electrons transfer from larger band gap semiconductor (N) to lower band gap semiconductor (n) results a positive donor space charge in larger band gap semiconductor.

AlGa<sub>x</sub>N layer determines the charge sheet density in the 2DEG channel [34]. Fig. 1.6 depicts the composition-dependent strain and the total polarization for a thin Al<sub>x</sub>Ga<sub>1-x</sub>N layer on a relaxed GaN layer.

The charge carriers in 2DEG channel due to total polarization ( $P = P_{SP} + P_{PE}$ ) is described by Poisson equation as the following [29],

$$\begin{aligned}\nabla \cdot D &= \nabla \cdot (\varepsilon E + P) = \rho \\ \nabla \cdot [\varepsilon(-\nabla\varphi)] + \nabla \cdot P &= \rho \\ \nabla \varepsilon &\rightarrow 0, \text{ then} \\ \nabla^2\varphi &= -\frac{\rho}{\varepsilon} + \frac{1}{\varepsilon} [\nabla \cdot P],\end{aligned}$$

At the interface between AlGa<sub>x</sub>N and GaN, the polarization results in a fixed polarization charge  $\rho^{Pol}$

$$\nabla^2\varphi = -\frac{\rho}{\varepsilon} - \frac{\rho^{Pol}}{\varepsilon}$$

The charge  $\rho$  in the semiconductor covers holes p, electrons n, ionized donors  $N_D^+$ , and ionized acceptors  $N_A^-$ ; and possibly the donor-acceptor traps. Thus a complete description of charged carried in semiconductor due to the response of a potential field as the following,

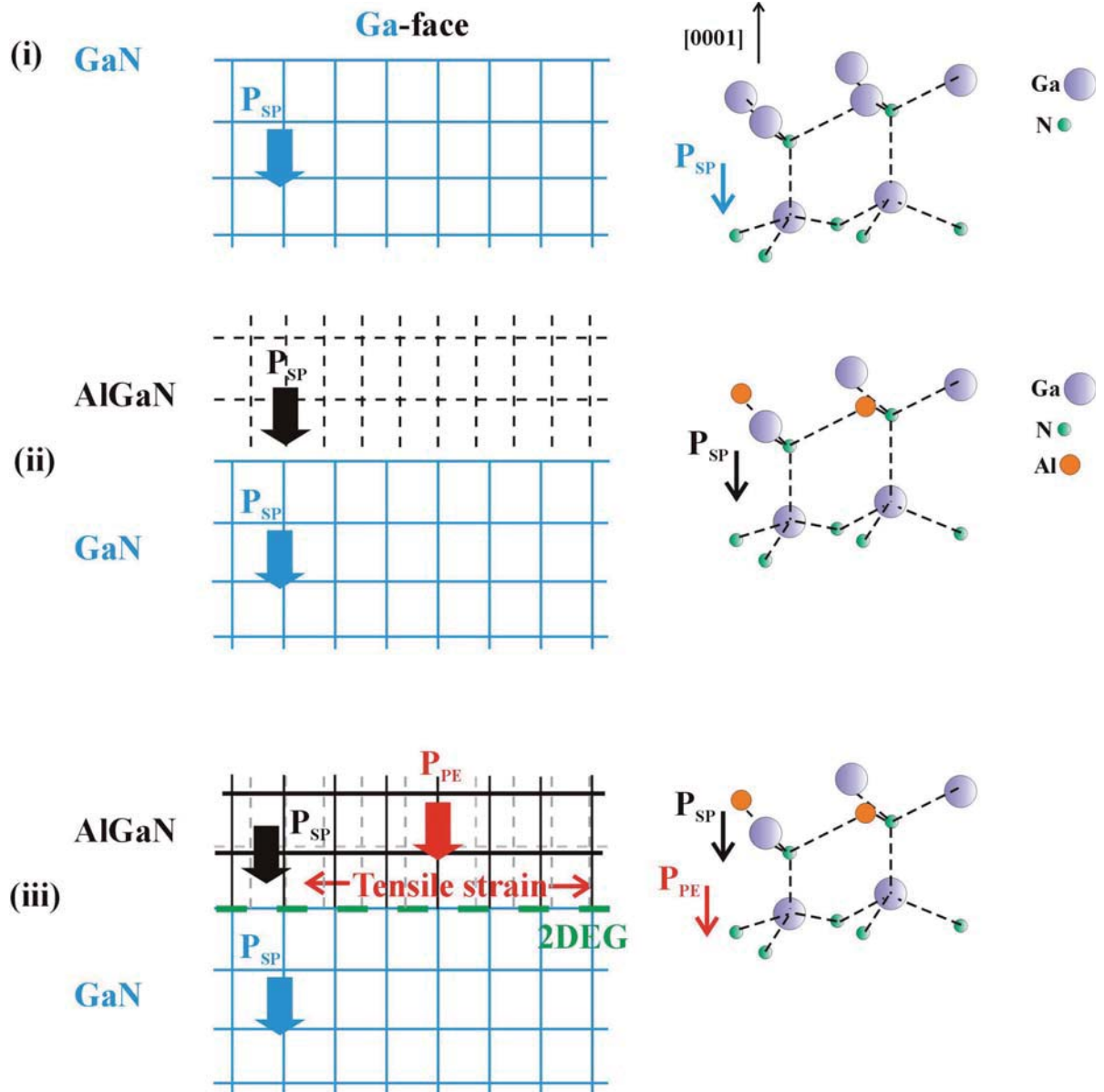


Figure 1.5 Schematic explanation of polarization induced charge creation (i) GaN growth with Ga-face has spontaneous polarization field  $P_{SP}$  along c-axis represented by a blue arrow (ii) before intimate contact- AlGaN layer with smaller lattice constant (dashed black lines) than GaN lattice constant due to smaller size of Al atom (iii) deposition of AlGaN layer on the top of GaN layer creates tensile strain along a-axis to match GaN lattice constant and consequently the lattice constant of AlGaN in c-axis is stretched. This creates piezoelectric polarization  $P_{PE}$  in AlGaN layer.

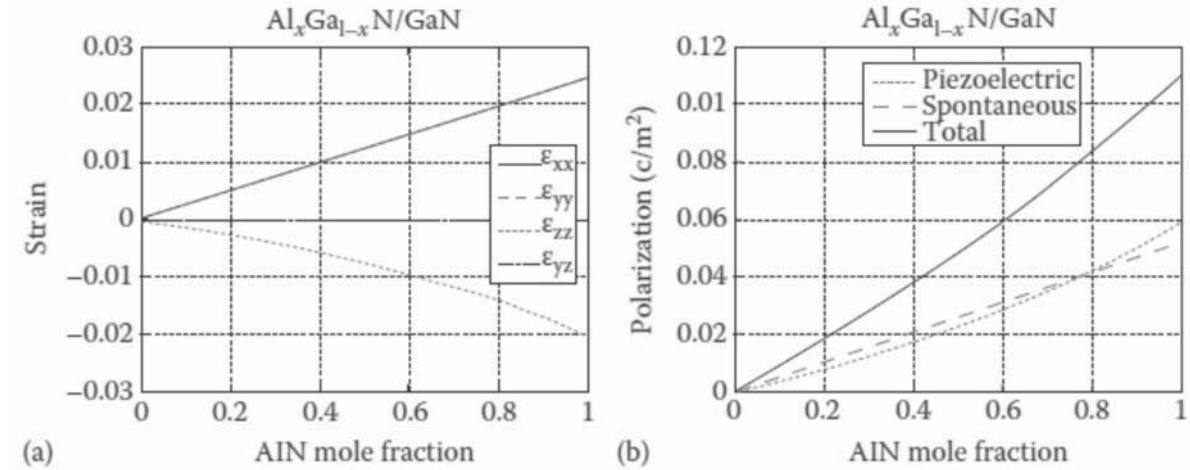


Figure 1.6 (a) Elastic strain calculation in  $\text{Al}_x\text{Ga}_{1-x}\text{N}$  layer as a function of Al concentration on a relaxed GaN crystal, and (b) total polarization from piezoelectric and spontaneous polarizations as a function of Al concentration [29].

$$\nabla^2\varphi = -\frac{q}{\epsilon} [N_D^+ - N_A^- + p - n] - \frac{\rho^{Pol}}{\epsilon}$$

Fig. 1.7 describes high concentration of charged carries in 2DEG as a response to the potential field. The standard AlGa<sub>N</sub>/Ga<sub>N</sub> HEMTs is characterized by a high sheet charge density of electrons at the interface even without any intentional doping. Depending on specific design the sheet charge density can be almost one order of magnitude higher than standard AlGaAs/GaAs HEMTs.

## 1.5 The status of GaN reliability

Literature of GaN device reliability has some decisive questions: what is the real cause of GaN degradation? Is it due to material intrinsic properties, substrate and/or GaN growth quality, process related effects or a combination of all of them? The most important question is: what is physics behind it?

Presently, there are two main streams of degradation mechanism explanations: hot electron [35, 36] and inverse piezoelectric effect [37]. Hot electrons by definition are electrons with higher energy than the lattice thermal energy. They can get kinetic energy from high electric field when the device is turned on. These "hot" electrons can get injected into the AlGa<sub>N</sub> barrier layer and might be trapped or create interface states or bulk traps [35]. Defect creation by hot electrons in GaN and other similar materials is controlled