COMPARISON OF THE MODELS OF POLARIZATION USED TO SIMULATE *I-V* CURVES OF AlGaN/GaN STRUCTURES

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1. Motivation

Polarization effects at material interfaces play a key role in the performance of devices based on nitride materials. We have focused on the effect of spontaneous and piezoelectric polarization in a real metal/GaN/AlGaN/GaN heterostructure used in the production of various types of sensors. Spontaneous polarization is due to the intrinsic asymmetry of the bonding in the equilibrium wurtzite crystal structure. Mechanical stress results in the so-called piezoelectric polarization. It is negative in tensile and positive in compressive strained AlGaN layers. The orientations of spontaneous and piezoelectric polarizations are parallel in the case of tensile strain and antiparallel in the case of compressive stress. We demonstrate the effect of tensile and compressive strain upon the *I-V* characteristics of metal/GaN/AlGaN heterostructures.

2. Theory

The effect of spontaneous and piezoelectric polarization charge $P^{\mathrm{TOTAL}}_{\mathrm{Al}_m\mathrm{Ga}_{1-m}\mathrm{N}}$ is reflected in the Poisson equation determining the shape of the sheet bound total interface charge

$$-\frac{\mathrm{d}}{\mathrm{d}x}\left(\varepsilon_0\,\kappa(x)\frac{\mathrm{d}\psi(x)}{\mathrm{d}x}-P^{\mathrm{TOTAL}}_{\mathrm{Al}_m\mathrm{Ga}_{1-m}\mathrm{N}}(x)\right)=q\left(p(x)-n(x)+N^{\mathrm{D+}}(x)-N^{\mathrm{A-}}(x)+N_{\mathrm{t}}^{\mathrm{D+}}(x)-N_{\mathrm{t}}^{\mathrm{A-}}(x)\right). \quad (1)$$

Here, κ is the relative permittivity, ψ is the electric potential, n and p are concentrations of free charge carriers, $N^{\mathrm{D+}}$ and $N^{\mathrm{A-}}$ are concentrations of shallow ionized donors and acceptors, $N_{\mathrm{t}}^{\mathrm{D+}}$ and $N_{\mathrm{t}}^{\mathrm{A-}}$ are concentrations of deep ionized donors and acceptors expressed, and m is the molar concentration of Al.

2.1 Spontaneous polarization

Spontaneous polarization is negative for all Ga-polarity heterostructures. The value of $P^{\mathrm{SP}}_{\mathrm{Al}_m\mathrm{Ga}_{1-m}\mathrm{N}}$ exhibits a nonlinear dependence on m which is described by introducing a bowing parameter b into the usual linear interpolation between the values for AlN and GaN

$$P^{\mathrm{SP}}_{\mathrm{Al}_m\mathrm{Ga}_{1-m}\mathrm{N}}=m\,P^{\mathrm{SP}}_{\mathrm{AlN}}+(1-m)P^{\mathrm{SP}}_{\mathrm{GaN}}+b_{\mathrm{AlGaN}}\,m(1-m), \quad (2)$$

where the bowing parameter is calculated as

$$b_{\mathrm{AlGaN}}=2\left(P^{\mathrm{SP}}_{\mathrm{AlN}}+P^{\mathrm{SP}}_{\mathrm{GaN}}-2P^{\mathrm{SP}}_{\mathrm{Al}_{0.5}\mathrm{Ga}_{0.5}\mathrm{N}}\right). \quad (3)$$

Since the Poisson equation (1) contains the derivative of polarization, one can eliminate spontaneous polarization in GaN as it is considered constant and Eqn. (2) can be rewritten as

$$P^{*\mathrm{SP}}_{\mathrm{Al}_m\mathrm{Ga}_{1-m}\mathrm{N}} = m\,P^{\mathrm{SP}}_{\mathrm{AlN}} + (1-m)P^{\mathrm{SP}}_{\mathrm{GaN}} + b_{\mathrm{AlGaN}}\,m(1-m) - P^{\mathrm{SP}}_{\mathrm{GaN}}. \tag{4}$$

Parameters of spontaneous polarization are summarized in Table 1.

Tab. 1: Parameters of spontaneous polarization

Material	GaN	AlN	b_{AlGaN}
P^{SP} (C/m^2)	– 0.034	– 0.090	0.0182
Reference	[1]	[1]	[5]

2.2 Piezoelectric polarization

Group III nitrides, such as GaN, exhibit very strong piezoelectric polarization effects, greater by one order of magnitude than other III-V semiconductors [1]. Both in magnitude and orientation, piezoelectric polarization is directly related to the strain present in the material. Higher strain causes higher polarization. Compressive strain induces polarization oppositely oriented than tensile strain. This is illustrated in Fig. 1.

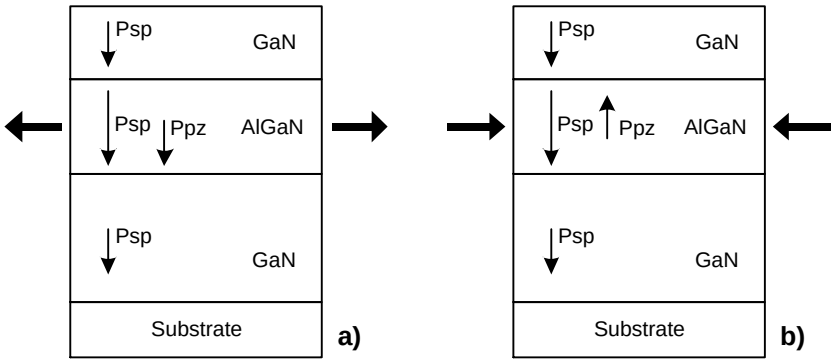

Fig. 1: The magnitudes and orientations of spontaneous and piezoelectric polarization components under tensile (a) and compressive strain (b).

Piezoelectric polarization sheet interface bound charge occurring due to the mismatch of the lattice constants at the heterointerfaces is determined as

$$P^{\mathrm{PZ}}_{\mathrm{Al}_m\mathrm{Ga}_{1-m}\mathrm{N}}(m) = e_{33}(m)\frac{c(m)-c(0)}{c(0)} + 2e_{31}(m)\frac{a(m)-a(0)}{a(0)}, \tag{5}$$

where e_{33} and e_{31} are piezoelectric constants. The relation between the lattice constants $a(m)$ and $c(m)$ in the hexagonal AlGaN system is given by elastic constants C_{13} and C_{33} as

$$\frac{c(m)-c(0)}{c(0)} = -2\frac{C_{13}(m)}{C_{33}(m)}\frac{a(m)-a(0)}{a(0)}. \tag{6}$$

Then the piezoelectric polarization sheet bound interface charge can be written as

$$P^{\mathrm{PZ}}_{\mathrm{Al}_m\mathrm{Ga}_{1-m}\mathrm{N}}(m) = 2\frac{a(m)-a(0)}{a(0)}\left(e_{31}(m) - e_{33}(m)\frac{C_{13}(m)}{C_{33}(m)}\right). \tag{7}$$

The elastic constants $C_{13,}$ C_{33}, piezoelectric constants $e_{31,}$ e_{33} and the lattice parameter a of the hexagonal unit cell of the wurtzite structure in dependence on the molar concentration m of aluminium in $Al_mGa_{1-m}N$ were linearly interpolated using the Vegard law by

$$y_{\mathrm{Al}_m\mathrm{Ga}_{1-m}\mathrm{N}} = m\,y_{\mathrm{AlN}} + (1-m)y_{\mathrm{GaN}}. \tag{8}$$

Parameters for piezoelectric polarization given in Table 2 were obtained from [1] and revised in accordance with [2].

Tab. 2: Piezoelectric polarization parameters

Material	a (Å)	e_{31} (C/m^2)	e_{33} (C/m^2)	C_{13} (GPa)	C_{33} (GPa)
GaN	3.189	– 0.37	0.67	68	354
AlN	3.112	– 0.62	1.50	94	377
Reference	[4]	[1]	[1]	[1]	[1]

The values provided in Table 2 are inserted into Eqn. (8). This yields

$$a_{\mathrm{Al}_m\mathrm{Ga}_{1-m}\mathrm{N}} = 3.189 - 0.077\,m, \tag{9}$$

$$e_{31\mathrm{Al}_m\mathrm{Ga}_{1-m}N} = -0.37 - 0.25\,m, \qquad e_{31\mathrm{Al}_m\mathrm{Ga}_{1-m}\mathrm{N}} = -0.37 - 0.25\,m, \tag{10, 11}$$

$$C_{13\mathrm{Al}_m\mathrm{Ga}_{1-m}\mathrm{N}} = 68 - 26\,m, \qquad C_{33\mathrm{Al}_m\mathrm{Ga}_{1-m}\mathrm{N}} = 354 - 23\,m. \tag{12, 13}$$

Since the second term is constantly negative, it is clear that $P^{\mathrm{PE}}_{\mathrm{Al}_m\mathrm{Ga}_{1-m}\mathrm{N}} < 0$ under tensile strain, $a(m) > a(0)$, and $P^{\mathrm{PE}}_{\mathrm{Al}_m\mathrm{Ga}_{1-m}\mathrm{N}} > 0$ under compressive strain, $a(m) < a(0)$.

The total sheet interface bound charge due to spontaneous polarization and piezoelectric polarization is given as

$$P^{\mathrm{TOTAL}}_{\mathrm{Al}_m\mathrm{Ga}_{1-m}\mathrm{N}} = \left(P^{\mathrm{SP}}_{\mathrm{GaN}} - P^{\mathrm{SP}}_{\mathrm{Al}_m\mathrm{Ga}_{1-m}}\right) \pm \left(P^{\mathrm{PZ}}_{\mathrm{GaN}} - P^{\mathrm{PZ}}_{\mathrm{Al}_m\mathrm{Ga}_{1-m}\mathrm{N}}\right). \tag{14}$$

3. Simulation

We have focused on the effect of spontaneous and piezoelectric polarization in a real metal/GaN/AlGaN/GaN heterostructure shown in Fig. 2.

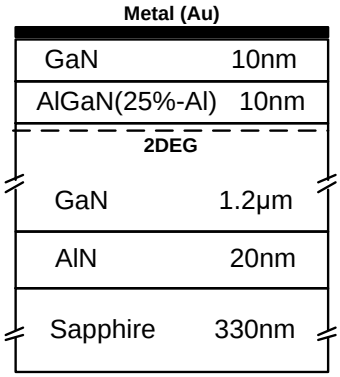

Fig. 2: Metal/GaN/AlGaN/GaN heterostructure.

The dependences of the magnitudes of spontaneous and piezoelectric polarizations of $Al_mGa_{1-m}N$ on the molar fraction m of aluminium are shown in Fig. 3, and the dependences of the total polarization under tensile and compressive stress on the molar fraction of aluminium are shown in Fig. 4.

Due to the tensile stress induced charge the band diagram in thermodynamic equilibrium has a roof-shaped maximum on the first GaN/AlGaN interface, Fig. 5. This "roof" presents a mighty barrier for the thermionic emission-drift-diffusion electron current. This is why the simulated current densities of such a structure are lower by many orders of magnitude than the experimentally observed values.

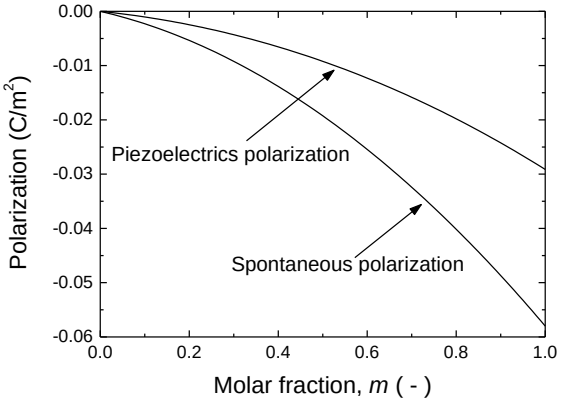

Fig. 3: Dependences of spontaneous (4) and piezo-electric polarizations (7) on the molar fraction of Al in $Al_mGa_{1-m}N$.

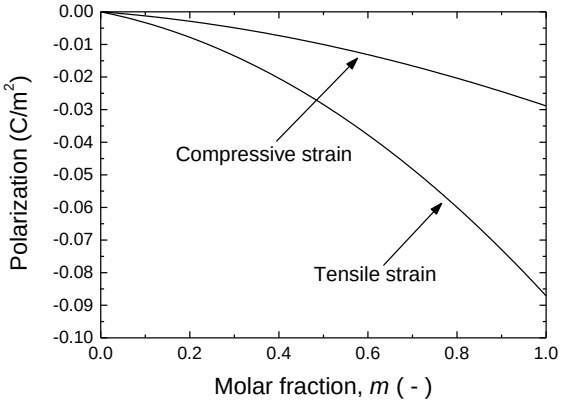

Fig. 4: Dependences of the total polarization (14) under tensile and compressive strain on the molar fraction of Al in $Al_mGa_{1-m}N$.

On applying a reverse voltage, the roof decreases and finally vanishes at V_a>1 V. However, if the spontaneous and piezoelectric polarizations are antiparallel (the effect compressive stress), no roof-shaped maximum is created on the conduction band and the simulated currents match well with the experiment, see Fig. 6. The further growth of the current is caused by the contribution of direct and trap-assisted tunnelling. For reverse voltages higher than 1 V the contribution of tunnelling is higher than that of thermionic emission-drift-diffusion.

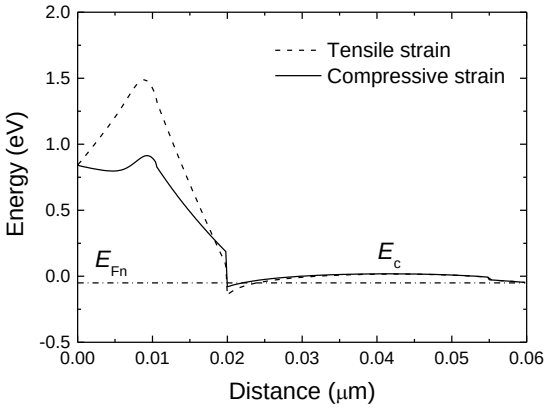

Fig. 5: Band diagram of metal/GaN/AlGaN/GaN structure in thermodynamic equilibrium under tensile and compressive strain.

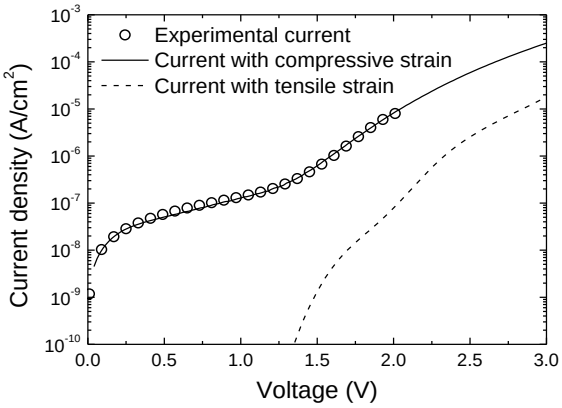

Fig. 6: Comparison of simulated reverse currents of metal/GaN/AlGaN/GaN structure under tensile and compressive strain with experimental data (circles) obtained at *T*=300 K.

4. Conclusion

A question arises about the orientations of spontaneous and piezoelectric polarizations. According to literature [3-5], AlGaN layers grown on GaN buffers are always under tensile strain. Our simulations match with the experimentally obtained *I-V* curves only under assumption of compressive strain [6].

Acknowledgment

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