Calculation of polarization sheet charge density

This teaching module shows how to calculate the polarization sheet charge density at the interface between AlGaN electron blocking layer and a GaN spacer layer, pseudomorphically grown on relaxed AlGaN, GaN, and GaInN templates.

Basic equations for spontaneous polarization

The spontaneous polarization is determined by the material composition. The values of the spontaneous polarization for the binary III-N materials are listed as follows [1]:

$$P_{\mathrm{AlN}}^{\mathrm{SP}} = -0.0898\ \mathrm{C/m^2}$$

$$P_{\mathrm{GaN}}^{\mathrm{SP}} = -0.0339\ \mathrm{C/m^2}$$

$$P_{\mathrm{InN}}^{\mathrm{SP}} = -0.0413\ \mathrm{C/m^2}$$

In the case of ternary and quaternary III-N materials, the spontaneous polarization is expressed by using a second-order polynomial of the alloy composition [2].

$$P_{\mathrm{Al}_x\mathrm{Ga}_{1-x-y}\mathrm{In}_y\mathrm{N}}^{\mathrm{SP}} = x\,P_{\mathrm{AlN}}^{\mathrm{SP}} + y\,P_{\mathrm{InN}}^{\mathrm{SP}} + (1-x-y)P_{\mathrm{GaN}}^{\mathrm{SP}} + b_{\mathrm{AlGaN}}\,x\,(1-x-y) + b_{\mathrm{GaInN}}\,y\,(1-x-y) + b_{\mathrm{AlInN}}\,xy$$

The bowing parameters are listed as follows [3]:

$$b_{\mathrm{AlGaN}} = +0.0191\ \mathrm{C/m^2}$$

$$b_{\mathrm{GaInN}} = +0.0378\ \mathrm{C/m^2}$$

$$b_{\mathrm{AlInN}} = +0.0709\ \mathrm{C/m^2}$$

Basic equations for piezoelectric polarization

The piezoelectric polarization is determined by the induced strain on the material. The strain in an epitaxial layer pseudomorphically grown on a relaxed template is expressed as:

$$\varepsilon = \frac{a_{\mathrm{template}} - a_{\mathrm{epi}}}{a_{\mathrm{epi}}}$$

The in-plane lattice constants of the relaxed binary III-N materials are listed as follows [4]:

$$a_{\mathrm{AlN}} = 0.31095\ \mathrm{nm}$$

$$a_{\mathrm{GaN}} = 0.31986\ \mathrm{nm}$$

$$a_{\mathrm{InN}} = 0.35848\ \mathrm{nm}$$

The in-plane lattice constants of the relaxed ternary and quaternary III-N materials can be calculated by using Vegard's law.

$$a_{\mathrm{Al}_x\mathrm{Ga}_{1-x-y}\mathrm{In}_y\mathrm{N}} = x a_{\mathrm{AlN}} + y a_{\mathrm{InN}} + (1-x-y) a_{\mathrm{GaN}}$$

The piezoelectric polarizations in binary III-nitrides are expressed as follows [2]:

$$P_{\mathrm{AlN}}^{\mathrm{PZ}}(\varepsilon) = -1.808\,\varepsilon + 5.624\,\varepsilon^2\ [\mathrm{C/m^2}],\ \text{for}\ \varepsilon < 0$$

$$P_{\mathrm{AlN}}^{\mathrm{PZ}}(\varepsilon) = -1.808\,\varepsilon - 7.888\,\varepsilon^2\ [\mathrm{C/m^2}],\ \text{for}\ \varepsilon > 0$$

$$P^{\mathrm{PZ}}_{\mathrm{GaN}}(\varepsilon) = -0.918\,\varepsilon + 9.541\,\varepsilon^2\ [\mathrm{C/m^2}]$$

$$P^{\mathrm{PZ}}_{\mathrm{InN}}(\varepsilon) = -1.373\,\varepsilon + 7.559\,\varepsilon^2\ [\mathrm{C/m^2}]$$

In the case of ternary III-nitrides, the piezoelectric polarization is calculated from the piezoelectric polarization of binary III-nitrides and Vegard's law:

$$P^{\mathrm{PZ}}_{\mathrm{A}_x\mathrm{B}_{1-x}\mathrm{N}}(\varepsilon) = x\,P^{\mathrm{PZ}}_{\mathrm{AN}}(\varepsilon) + (1-x)\,P^{\mathrm{PZ}}_{\mathrm{BN}}(\varepsilon)$$

Basic equations for polarization sheet charge density

When an epitaxial layer, **A**, is pseudomorphically grown on a template, **T**, the polarization sheet charge density between two different layers can be expressed as:

$$\sigma = -\left(P^{\mathrm{total}}_{\mathrm{A}} - P^{\mathrm{total}}_{\mathrm{T}}\right) = -\left(P^{\mathrm{SP}}_{\mathrm{A}} + P^{\mathrm{PZ}}_{\mathrm{A}} - P^{\mathrm{SP}}_{\mathrm{T}} - P^{\mathrm{PZ}}_{\mathrm{T}}\right)$$

When an epitaxial layer, **B**, is inserted between layer **A** and template **T**, the polarization sheet charge density between layer **A** and **B** can be expressed as:

$$\sigma = -\left(P^{\mathrm{total}}_{\mathrm{A}} - P^{\mathrm{total}}_{\mathrm{B}}\right) = -\left(P^{\mathrm{total}}_{\mathrm{A}} - P^{\mathrm{total}}_{\mathbf{T}}\right) + \left(P^{\mathrm{total}}_{\mathrm{B}} - P^{\mathrm{total}}_{\mathrm{T}}\right)$$

Figure 1 shows the polarization sheet charge density between the GaN QB and GaInN QW (left-hand ordinate) and the AlGaN EBL and GaN spacer (right-hand ordinate) pseudomorphically grown on ternary III-nitride templates (GaInN and AlGaN).

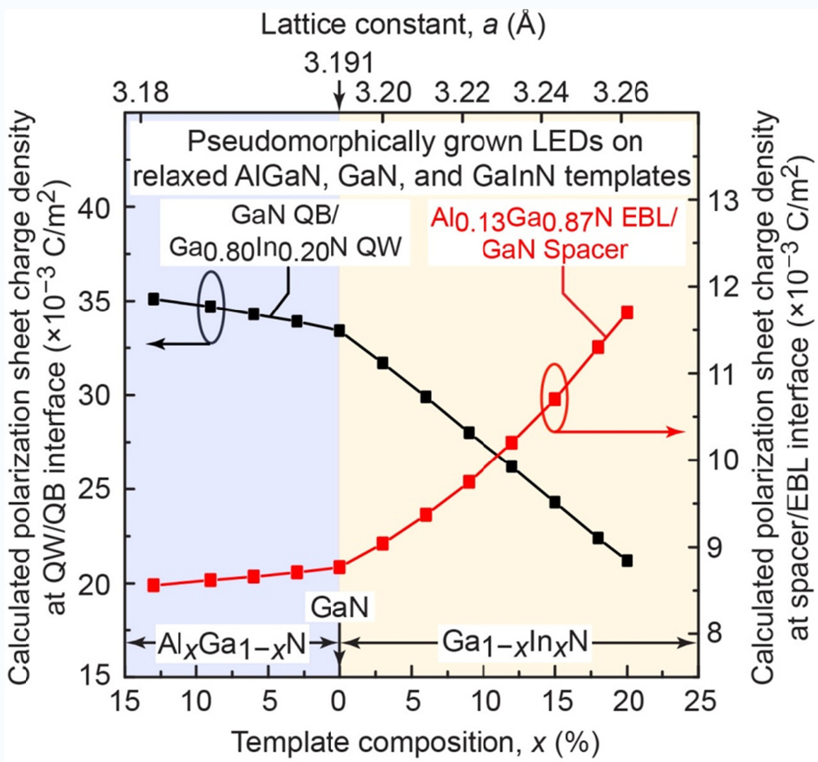

Figure 1: Relation between the template composition and the calculated polarization sheet charge densities at the interface between $Ga_{0.80}In_{0.20}N$ QW and GaN QB and between GaN spacer and $Al_{0.13}Ga_{0.87}N$ EBL. The active-region (including the EBL) layers are grown pseudomorphically on the templates and the templates are assumed to be relaxed.

References

[1] F. Bernardini *et al*. "Accurate calculation of polarization-related quantities in semiconductors" *Phys. Rev. B* **63**, 193201 (2001)

[2] F. Bernardini "Spontaneous and piezoelectric polarization: basic theory v. practical recipes" in J. Piprek (Ed.) *Nitride Semiconductor Devices: Principles and Simulation* (Wiley-VCH Verlag GmbH & Co. KGaA 2007)

[3] F. Bernardini *et al*. "Nonlinear behavior of spontaneous and piezoelectric polarization in III-V nitride alloys", *Phys. Stat. Sol*. (a) **90**, 65 (2002)

[4] V. Fiorentini *et al*. "Evidence for nonlinear macroscopic polarization in III-V nitride alloy heterostructures" *Appl. Phys. Lett*. **80**, 1204 (2002)