Temperature and strain effects on polarization of light emitted by AlGaN bulk layers and quantum wells

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***Abstract*—We present a systematic analysis of the effect of temperature and tensile/compressive strain on polarization of light emitted from AlGaN bulk layers and quantum wells. For this purpose, a $\mathbf{k}\cdot\mathbf{p}$-based approach is used with rigorous treatment of the k-vector dependence of joint density of states and optical matrix elements. The latter is shown to be critical for accurate calculating the polarization degree of emitted light with and without account of strain effects. The results obtained are validated by comparison with available data.**

***Index Terms*—AlGaN, polarization degree, quantum well, $\mathbf{k}\cdot\mathbf{p}$ approach, numerical simulation**

I. Introduction

The external quantum efficiency of deep ultraviolet AlGaN-based light emitters generally decreases with the AlN fraction in the alloys. One of the reasons for the efficiency decline frequently discussed is a light extraction efficiency reduction caused by specific polarization of the emitted light.

The change of the polarization from a dominant transverse electric (TE) at low Al contents to a dominant transverse magnetic (TM) at large AlN fractions in AlGaN can be generally analyzed within a $\mathbf{k}\cdot\mathbf{p}$ approach [1], providing a reasonable agreement with experiments [2]. Unfortunately, the authors of [2] confined their study by room-temperature (RT) light emission from thin quantum wells (QW) coherently grown on an AlN substrate only. Therefore, general trends in polarization variation with elastic strain and temperature remained obscure. In this contribution, we present a systematic study of temperature and strain effects on degree of polarization (DoP) of light emitted by either a relaxed bulk [0001]AlGaN layer or a strained single quantum well (SQW).

II. Modeling approach

To find the photon emission rate assuming the momentum selection rule to be valid, we have applied a numerical approach where the joint density of states (JDOS) and optical matrix element (ME) corresponding to each of the valence subband, i.e. of heavy, light, or split-off holes, were calculated by $\mathbf{k}\cdot\mathbf{p}$ method with rigorous accounting for the hole energy dependence on the value and direction of the electron/hole k-vector. This enabled an accurate treatment of non-parabolicity and warping of the hole subbands, which were found to be rather strong in AlGaN alloys.

In order to get practically reasonable band alignments in bulk AlGaN layers and QW profiles, we have regarded a simple structure schematically shown in Fig.1. The structure contained an active $Al_xGa_{1-x}N$ region sandwiched between two 100 nm $Al_yGa_{1-y}N$ cladding layers. As the active region, we have considered (i) a strain-relaxed 20 nm bulk AlGaN layer or (ii) a 1 nm AlGaN SQW (similar to that studied in [2]). The AlN molar fraction in the active layer x was varied in a wide range, being kept smaller than that in the claddings y by a fixed value of 0.13. The bottom cladding layer was n-doped and the upper one was p-doped up to the donor/acceptor concentrations of 10^{19} cm^{-3}/10^{20} cm^{-3} respectively. For DoP calculating, we considered photon emission with two orthogonal polarizations. One, the transverse electric (TE) polarization, was that with the electric field normal to the plane spanned by the photon emission direction (e.g., red arrow in Fig.1) and the hexagonal axis of the AlGaN crystal (aligned with z-axis in Fig. 1). Another, the transverse magnetic (TM) polarization, was that with the electric field vector lying in the above plane. The DoP P was then defined as $P = (I_{TE} - I_{TM})/(I_{TE} + I_{TM})$, where $I_{TE/TM}$ was the intensity of TE/TM-polarized light.

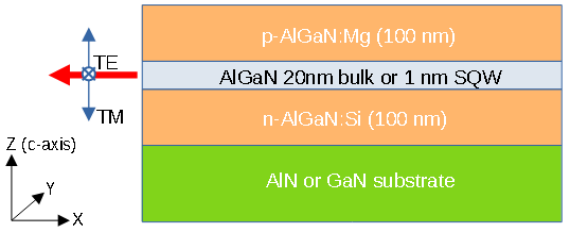

Fig. 1. Schematic structure used for DoP calculations.

The effect of strain was modeled by the lattice constant mismatch between the $Al_xGa_{1-x}N$ active layer and substrate. Either AlN or GaN substrate was assumed for simulating the impact of the compressive or tensile strain on the SQW polarization properties. Modeling of the structure with the

relaxed bulk active region was made by assuming a virtual AlGaN substrate with the AlN fraction equal to that of the active region.

In all the cases, the current density flowing through the structures was set to be of (200 ± 10) A cm^{-2}.

III. Simulation Results

The DoPs of light emitted by the relaxed bulk AlGaN layer at $T = 300$ K and $T = 77$ K are shown in Fig. 2 as a function of the alloy composition. One can see that DoP changes its sign at the AlN fraction $x \simeq 0.25$ irrespectively of temperature. The reason for this is approaching of two upper valence subband to each other at the Γ-point of the Brillouin zone just at this molar fraction. The position of the DoP zero-point is in excellent agreements with the experiments of Ref. [3] whereas general trend in the DoP variation with x agrees qualitatively well with the data of the paper. A lower temperature results in a more rapid transition from positive to negative DoP, which is due to a sharper Fermi distribution function at lower temperatures. In Fig.3 RT DoP vs. AlGaN

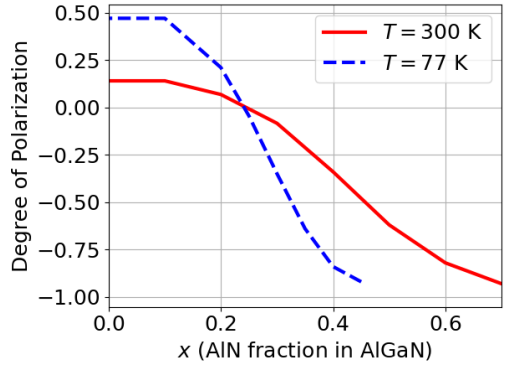

Fig. 2. DoP of light emitted by relaxed bulk AlGaN layer. Solid and dashed lined correspond to temperatures $T = 300$ K and $T = 77$ K, respectively.

composition is plotted for SQWs coherently grown on either AlN or GaN substrates. One can see that DoP zero-point shifts considerably to higher fractions x with respect to its value in the relaxed alloys in the presence of strain. In the

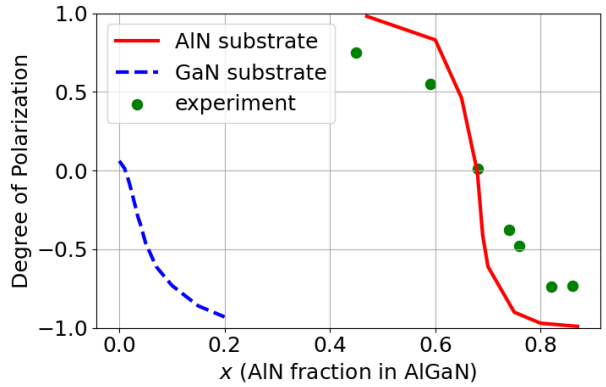

Fig. 3. RT DoP of light emitted by SQW on AlN (solid curve) and GaN (dashed curve) substrates. Circles on the upper plots are data from Ref. [2].

case of SQW on AlN (solid curve in Fig.3), the zero point approaches the value of $x \simeq 0.68$ which is in close agreement with the experiment (circles in Fig. 3) and simulation of Ref. [2]. In contrast, in the case of SQW on GaN (dashed curve in Fig.3) the DoP zero-point shifts to $x \simeq 0.01$. The latter actually means that ultraviolet LEDs coherently grown on GaN substrates are predicted to exhibit practically always a dominant TM-polarization.

The calculations of DoP obtained with the $\mathbf{k}$-dependent ME and with that taken at $\mathbf{k} = 0$ have provided very similar results. The temperature dependence of SQW's DoPs is found to exhibit nearly the same trend as the bulk AlGaN layer (see Fig.2).

The emission pattern is isotropic over the azimuthal angle. It is also isotropic over the polar angle in the case of TE-polarization but depends strongly on the angle in the case of TM-polarization. The patterns corresponding to both polarizations are shown in Fig.4 for SQWs on AlN with the compositions x on both sides of the DoP zero-point. One can see that change of the DoP sign is accompanied by a considerable redistribution of the partial and, thus, total emission patterns. In particular, only those SQWs which have the molar fractions x higher than the DoP zero point value provide dominant TM-polarized photons directed nearly parallel to the epitaxial layers. In summary, we have studied the effects of temperature

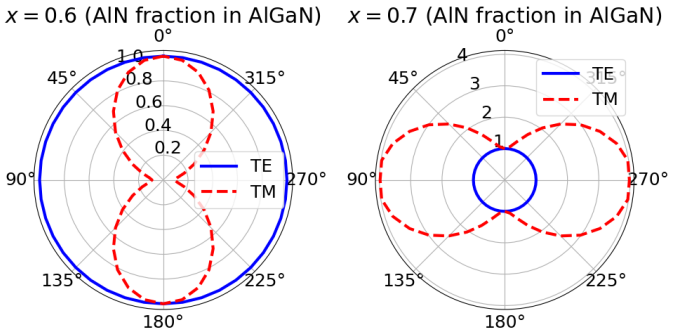

Fig. 4. RT Emission pattern of SQW with AlN molar fractions slightly below (left plot) and above (right plot) the DoP zero-point value.

and strain on the polarization degrees and emission patterns of photons emitted by either relaxed bulk AlGaN layers or SQWs coherently grown AlN or GaN substrates. Strain is found to be the major factor affecting considerably both DoP and emission patterns of TM-polarized photons. Accurate calculations of DoP require accounting for both non-parabolicity and warping of the AlGaN valence subbands.

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