# Interface Phonon Spectrum and Electron-Phonon Interaction in GaN/AlGaN nanostructures

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This paper presents a theoretical investigation of the properties of electron states and interface phonon states in anisotropic wurtzite AlGaN/GaN/AlGaN nanostructures, key elements for IR photodetectors. Focusing on the influence of built-in spontaneous and piezoelectric polarization fields, the study employs self-consistent calculations to determine electron properties. The influence of electron-interface-phonon interaction on the spectral characteristics of electron states, specifically energy renormalization, is analyzed using Green's function theory. The dependence of these characteristics on the geometric parameters of the structure, such as quantum well width, is investigated.

## Introduction

Modern quantum cascade lasers (QCL) and detectors (QCD) are vital for infrared applications. While traditional III-V arsenide-based devices cover the mid- and far-infrared range [1, 2], they face limitations in the near-infrared. Over the past decade, anisotropic III-V nitride materials like GaN and AlN have emerged as promising alternatives for near- and mid-infrared QCLs/QCDs. Their deep potential wells and significant optical phonon energies (e.g., approx. 92 meV in GaN) support higher temperature operation, making them highly attractive [3, 4]. However, the wurtzite structure of nitrides introduces significant built-in spontaneous and piezoelectric polarization fields. Understanding the fundamental properties of electron states and interface phonons, and their interaction in these polarized nanostructures, is essential for optimizing future nitride-based nano-devices.

## 1. Electron States: Theory and Analysis

A GaN quantum well in $Al_xGa_{1-x}N$ barriers is considered. Assuming the crystallographic c-axis coincides with the nanostructure growth direction, the electron effective mass are position-dependent.

The electric field strengths depend on the polarization values in the well and barrier regions

$$F_1 = F_3 = \frac{\left(P^{(GaN)} - P^{(AlGaN)}\right)w}{(b_1+b_2)\varepsilon_\infty^{(GaN)} + w\varepsilon_\infty^{(AlGaN)}}; F_2 = \frac{(b_1+b_2)\left(P^{(AlGaN)} - P^{(GaN)}\right)}{(b_1+b_2)\varepsilon_\infty^{(GaN)} + w\varepsilon_\infty^{(AlGaN)}}$$

The effective electron potential is determined by the self-consistent solution of the coupled Schrödinger and Poisson equations:

$$\begin{cases}\left[-\frac{\hbar^2}{2}\frac{d}{dz}\frac{1}{m(z)}\frac{d}{dz} + V_{\text{eff}}(z) - E_{n\vec{k}} + \frac{h^2k^2}{2m^*}\right]\Psi(z) = 0, \\ \frac{d}{dz}\left[\varepsilon_\infty(z)\frac{dV_H(z)}{dz}\right] = -\frac{e}{\varepsilon_0}\left[-en(z) + \sigma\sum_{p=1}^{2}\delta(z-z_p)\right].\end{cases}$$

The solutions were found using an iterative procedure, incorporating the standard boundary conditions for the wave function and its derivative at the heterointerfaces and the wave function normalization condition.

The developed procedure determining the electron wave functions and nanostructure potential profiles (Fig. 1), with a fixed Al concentration of x=0.5 .

The calculated stationary electron energy spectrum as a function of the quantum well width w is presented in Fig.2. As seen in Fig. 2, the energy levels depend on the quantum well width approximately as $w^{-2}$.

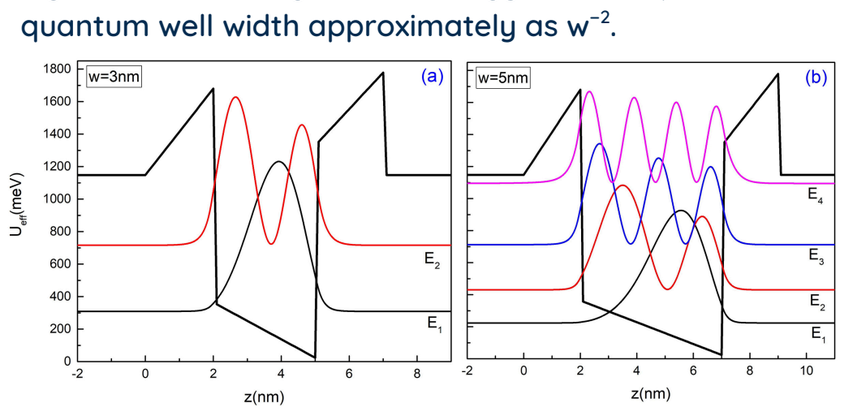


Fig. 1. Nanostructure potential profiles. The squares of the wave function moduli correspond to the electron energy levels.

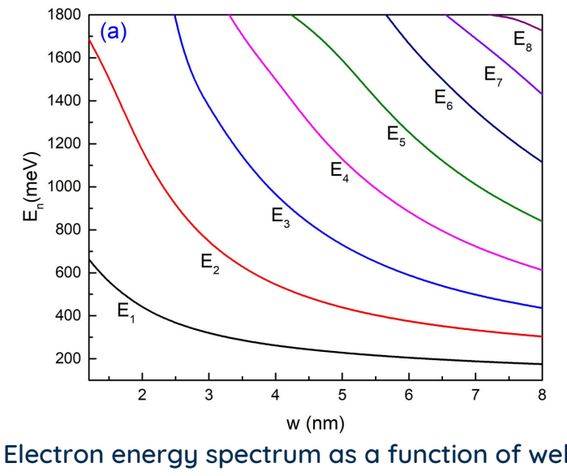


Fig. 2. Electron energy spectrum as a function of well width.

## 2.Interface Phonon States: Theory and Analysis

A system of equations for the optical phonon polarization field potential in each layer j has the form:

$$\left[\frac{\partial^2}{\partial z^2} - \gamma_j(\Omega)q^2\right]\Phi_j(z) = 0$$

Interface phonons exist when the condition

$$\gamma_j(\Omega) = \frac{\varepsilon_\perp^{(j)}(\Omega)}{\varepsilon_\parallel^{(j)}(\Omega)} > 0,\ \varepsilon_\parallel^{(j)}(\Omega)\,\varepsilon_\parallel^{(j+1)}(\Omega) < 0$$

is met simultaneously in all regions of the nanostructure.

The I-potentials in the different regions of the structure have the general form:

$$\Phi_j(z) = A_j e^{q_\perp\sqrt{|\gamma_j|}z} + B_j e^{-q_\perp\sqrt{|\gamma_j|}z}$$

These potentials satisfy the normalization condition and the boundary conditions at each interface for the continuity of the tangential component of the electric field and the normal component of the electric displacement vector.

The dependence of the I-phonon energy spectrum on the quasimomentum q is shown in Fig. 3. It can be seen that in one-well nanostructure I-phonons have four branches: two low-frequency and two high-frequency. These branches exhibit both positive and negative dispersion. Increasing the width of the GaN nanolayer leads to an increase in dispersion.

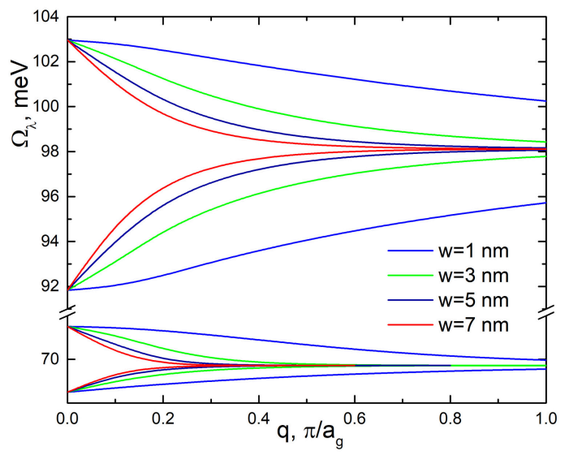


Fig. 3. Dependence of I-phonon energies on q.

Fig. 4 shows the evolution of the potentials for all I-phonon branches as a function of the z-coordinate, calculated for w=3 nm and three values of quasimomentum q=0.1,0.5,1 (in units of $\pi/a_{GaN}$). Analysis shows that the extrema of the absolute potential values occur at the interfaces. The potential of the highest energy branch is the largest, suggesting that the electron interaction with this specific branch will be the strongest.

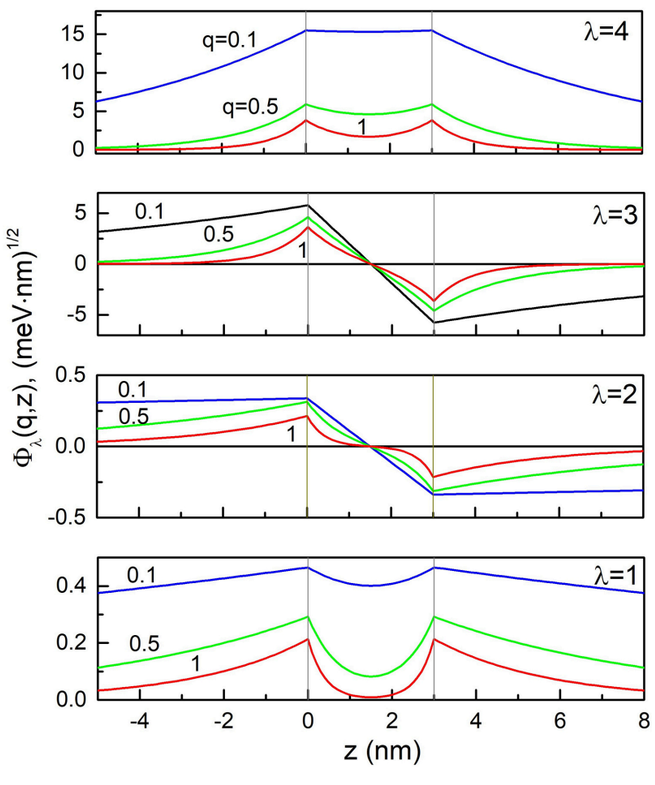


Fig.4. Evolution of I-phonon branch polarization potentials. Values q are given in units of $\pi/a_{GaN}$.

## 3. Electron-Phonon Interaction: Theory and Analysis

In the representation of second quantization, the Hamiltonians for the electron and interface phonon subsystems are [5]:

$$\hat{H}_e = \sum_{n\vec{k}} E_{n\vec{k}} a^+_{n\vec{k}} a_{n\vec{k}},\ \hat{H}_{ph} = \sum_{\lambda,\vec{q}} \Omega_\lambda(q)(b^+_{\lambda\vec{q}} b_{\lambda\vec{q}} + 1/2)$$

The electron-phonon interaction Hamiltonian is given by:

$$\hat{H}_{e-ph} = \sum_{\lambda,\vec{q}} \sum_{n,n',\vec{k}} F_{n'n}(\lambda,q) a^+_{n'\vec{k}+\vec{q}} a_{n\vec{k}} (b_{\lambda,\vec{q}} + b^+_{\lambda,-\vec{q}})$$

where

$$F_{n'n}(\lambda,q) = -\sqrt{\frac{4\pi e^2\hbar}{qSP(\lambda,q)}} \sum_{j=0}^{N+1} \int_{z_{j-1}}^{z_j} \Psi^*_{n'j}(z)\varphi_j(q,z)\Psi_{nj}(z)\,dz$$

is the coupling function.

The electron-phonon Hamiltonian allows calculation of the electron Green's function using the Dyson equation:

$$G_n(\vec{k},\hbar\omega) = [\hbar\omega - E_{n\vec{k}} - M_n(\hbar\omega,\vec{k})]^{-1}$$

with the mass operator calculated in the one-phonon approximation at T=0K

$$M_n(\hbar\omega,\vec{k}) = \sum_{n'}\sum_{\lambda,\vec{q}} \frac{F^*_{n'n}(\lambda,q)F_{n'n}(\lambda,q)}{\hbar\omega - E_{n'}(\vec{k}-\vec{q}) - \Omega_\lambda(q) + i\eta}$$

By converting the sum over two-dimensional phonon quasimomenta to an integral, the mass operator is calculated. According to Green's function theory, the real part of the mass operator determines the energy shift and the imaginary part determines the decay rate of the n-th electron level, caused by the interaction with all interface phonon modes (λ).

Electron-phonon interaction leads to the renormalization of the electron energy spectrum. Table 1 shows that the main contribution to the magnitudes of the electron state energy shifts is due to intra-level configuration interaction involving phonons. The absolute magnitudes of the shifts decrease with increasing quantum well width.

Table 1. Energy shifts for the ground and first excited electron states at different quantum well widths.

| | w=3 nm | w=5 nm | w=7 nm |
|---|---|---|---|
| **$\Delta_1$ (meV)** | **−23.16** | **−18.30** | **−15.73** |
| $\Delta_{11}$ (meV) | −22.55 | −17.56 | −15.04 |
| **$\Delta_2$ (meV)** | **−24.84** | **−16.68** | **−13.25** |
| $\Delta_{22}$ (meV) | −23.73 | −17.77 | −13.48 |

## Conclusions and Results

A study investigated electron states, interface phonons, and their interaction in anisotropic wurtzite AlGaN/GaN quantum wells, emphasizing built-in polarization effects and geometry dependence.

Self-consistent calculations determined polarization-affected electron states. The interface phonon spectrum and localized potentials were found using a dielectric continuum model.

Analyzing electron-phonon interaction via Green's function theory revealed energy renormalization. Key findings include dominant coupling to the highest interface phonon branch and major energy shifts from intra-level scattering.

These results provide crucial insights into scattering mechanisms essential for optimizing nitride-based infrared nano-devices.

## Reference

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