Renormalization of electron states by interaction with confined phonons in a wurtzite-type nanostructure

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The renormalisation of the energy spectrum and electron relaxation dynamics upon interaction with confined optical phonons in a wurtzite AlGaN/GaN/AlGaN nanostructure are studied theoretically. The model accounts for the macroscopic dielectric anisotropy of the crystal and the strong built-in internal electric field arising from spontaneous and piezoelectric polarisations at the heterointerfaces. Changes in the electron spectral characteristics due to the influence of confined phonons are calculated using the temperature Green's function method by computing the mass operator in the one-phonon approximation. Electron–phonon scattering rates are analysed based on quantum transition probabilities via Fermi's Golden Rule.

Introduction

Semiconductor nitride heterostructures based on GaN, AlN, and their solid solutions occupy a leading position in modern optoelectronics and power electronics. The wide direct bandgap, high thermal conductivity, large electron saturation velocity, and high breakdown voltage make these materials indispensable for fabricating blue and ultraviolet light-emitting diodes, laser diodes, high-electron-mobility transistors, high-power converters and IF quantum cascade detectors and lasers.

Alongside internal fields, an equally important factor governing carrier kinetics in nitride nanostructures is the interaction of electrons with optical phonons. Since the LO-phonon energy in GaN (~92 meV) is nearly three times that in GaAs (~36 meV), electron–phonon interaction in nitride structures is considerably stronger.

Despite significant progress in the study of optical phonons and electron–phonon interaction in nitride heterostructures, a number of important questions remain open. In particular, the influence of the multi-branch character of phonons in wurtzite symmetry on electron-spectrum renormalisation at finite temperatures, the comparative analysis of the contributions of LO- and TO-like subbands, and the investigation of the temperature dependence of spectral characteristics remain insufficiently studied theoretically.

1. Theoretical Foundations and Methods

Electron Hamiltonian

An electron in a wurtzite-type nanostructure grown along the crystallographic c-axis is considered. The structure consists of a GaN quantum well of thickness w surrounded by semi-infinite AlGaN barriers. In the effective-mass approximation, the Schrödinger equation of the electron subsystem is solved exactly in each region of the structure. The boundary conditions and normalisation condition uniquely determine the wave functions and lead to the dispersion equation for the electron energy spectrum.

In the second-quantisation representation, the electron Hamiltonian takes the form:

$$\hat{H}_e = \sum_{n\bar{k}} E_{n\bar{k}} a^+_{n\bar{k}} a_{n\bar{k}}$$

Phonon Hamiltonian

According to the Poisson equation within the anisotropic dielectric continuum model, the anisotropy of wurtzite systems gives rise to four types of polar optical modes: interface, confined, half-space, and propagating.

The existence condition for confined modes requires that the components of the GaN dielectric tensor have opposite signs. The dispersion equation for the confined phonon spectrum and the amplitude of the phonon potential are found from the continuity conditions for the normal component of the electric field vector and the tangential component of the displacement vector, and with the normalisation condition.

The Hamiltonian of confined phonons in the occupation-number representation takes the form:

$$\hat{H}_{ph} = \sum_{\lambda} \sum_{\bar{q}} \Omega_{\lambda\bar{q}} (b^+_{\lambda\bar{q}} b_{\lambda\bar{q}} + 1/2)$$

where the index λ labels the phonon branches with dispersion relations Ω(λ).

Electron–Phonon Interaction

The interaction of electrons with the dispersive branches of confined phonons is described by a Fröhlich-type Hamiltonian in the second-quantisation representation:

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

The coupling functions equal the overlap integral of the electron wave functions with the phonon potential and are evaluated by numerical integration.

For calculations of the electron spectrum renormalisation, the temperature Green's function method is used. The mass operator of electron states in the one-phonon approximation is computed accounting for the full configurational interaction:

$$M_n(\hbar\omega,\vec{k}) = \sum_{n',\lambda,\vec{q}} \left|\phi_{n',n}(\lambda,q)\right|^2 \left[\frac{1+\nu_{\lambda q}}{\hbar\omega - E_{n'}(\vec{k}-\vec{q}) - \Omega_{\lambda q} + i\delta} + \frac{\nu_{\lambda q}}{\hbar\omega - E_{n'}(\vec{k}+\vec{q}) + \Omega_{\lambda q} + i\delta} \right]$$

The real part determines the energy-level shifts, while the imaginary part determines the decay.

The quantum transition probabilities calculated via Fermi's Golden Rule

$$W_{n,n'}(\lambda,\vec{k}) = \frac{2\pi}{\hbar} \sum_{\vec{q}} \left|\phi_{n',n}(\lambda,q)\right|^2 \left(\nu_{\lambda q} + \frac{1}{2} \pm \frac{1}{2} \right) \delta\left(E_n(\vec{k}) - E_{n'}(\vec{k} \mp \vec{q}) \mp \Omega_{\lambda q}\right)$$

2. Results and Discussion

To analyse the influence of confined optical phonons on the electron energy spectrum and relaxation dynamics, numerical calculations were performed for a AlGaN/GaN/AlGaN nanostructure with Al concentration x = 0.5 in the barrier layers. The varied geometric and thermodynamic parameters are the quantum well width w and the temperature T.

It can be seen (Fig. 1) that the phonon modes form two distinct allowed subbands: a high-energy LO-like subband and a low-energy TO-like subband. Unlike isotropic cubic crystals, confined phonons in the wurtzite nanostructure exhibit a q-dependence due to mixing of longitudinal and transverse polarisations. Both subbands contain an infinite number of confined modes.

Absolute values of electron energy shifts and decay increase with well width (Fig. 2). Intra-level interactions with the high-energy LO-like subband provide the main contribution to the renormalisation.

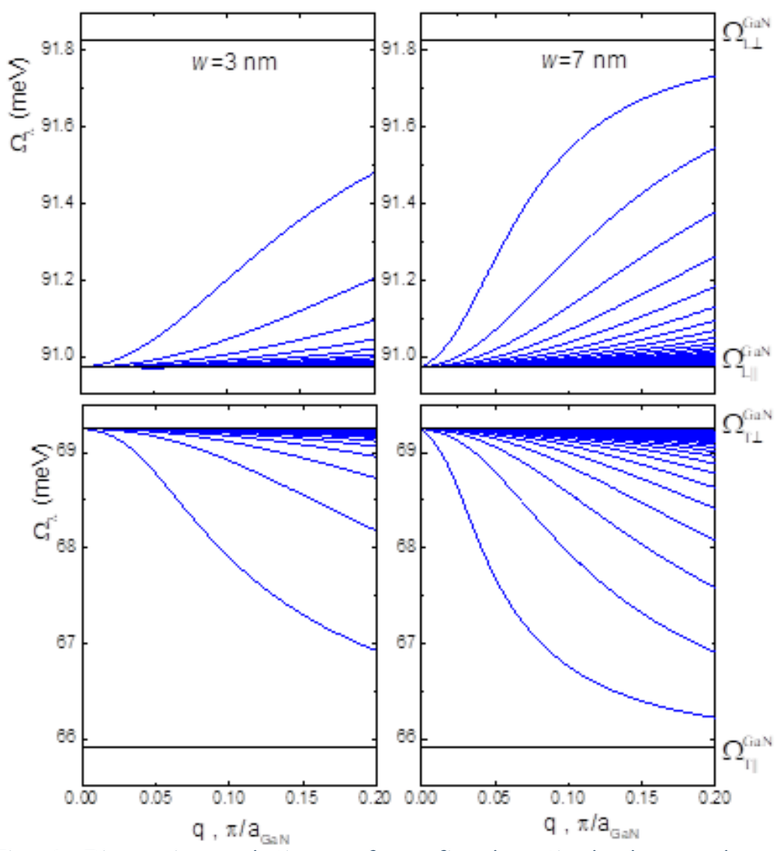

Fig. 1. Dispersion relations of confined optical phonon branch energies Ω vs. wave vector q in the nanostructure for two quantum well widths (w).

The TO-like subband contribution is negligible. This finding may have important practical significance for modelling the transport and optical properties of wurtzite nanostructures.

Fig. 2. Dependences of the energy shift and decay of electron states on quantum well width w. Solid curves: full calculation including all confined phonon branches. Symbols ■ : partial contributions from the upper subband only.

In the low temperature range T < 200 K, the shift and decay remain practically constant (Fig. 3). At low temperatures, thermal energy is insufficient to excite phonons, fully "freezing out" absorption processes. At 0 K, the ground state broadening is strictly zero because spontaneous phonon emission is forbidden by energy conservation.

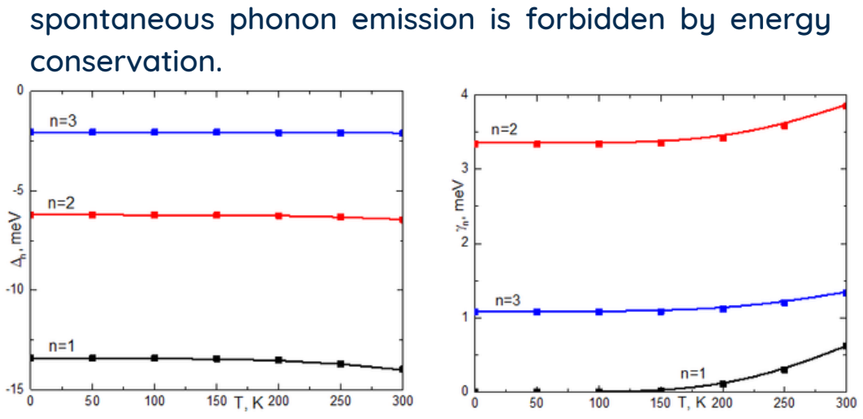

Fig. 3. Temperature dependences of the shift and decay of electron states in the well of 3 nm. Solid lines: all c-phonon branches; ■: partial contributions from the upper subband.

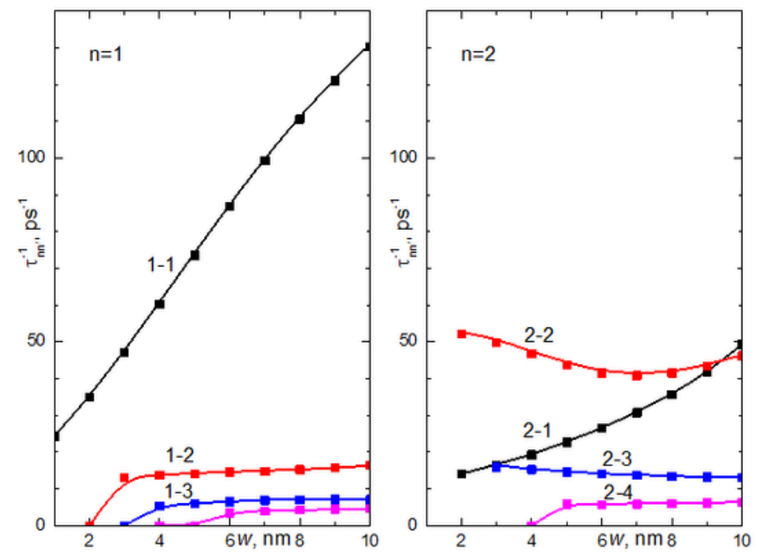

Fig. 4. Dependences of scattering rates (inverse relaxation times) on well width w at T = 300 K. Solid lines: all c-phonon branches. ■: partial contributions from the high-energy subband only.

At small well widths, the scattering dynamics are governed by the dominance of intrasubband transitions (Fig. 4). As the well width increases, fundamentally different behaviour is observed for ground and excited states. The 1-1 scattering probability increases gradually, in contrast, the 2-2 and 3-3 rates decrease.

Conclusions

- Renormalised characteristics of electron states in wurtzite nanostructures are entirely determined by the high-energy LO-like confined phonon subband.
- Intra-level electron-phonon transitions dominate the configuration interaction.
- At room temperature (300 K), electron relaxation times reach ~100 picoseconds, confirming the fast nature of charge carrier kinetics.