Semiconductor Nanointerface Eigenstate-Photoevolution

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Abstract: - The dynamics of photonic evolution for the eigenstate of a generic semiconductor-nanointerface is studied in terms of its two-dimensional electron gas (2DEG) fundamental-sublevel eigenenergy's correlation with respective 2DEG areal density, versus instantaneous cumulative photonic intake. Application of this treatment to the experimental photoresponse of typical modulation – doped optoelectronic nanodevices leads to a realistic tracing of the nanostructure pertinent photodynamics.

Keywords: - nanotechnology, optoelectronics, functional eigenstate, nanodevice, photodynamics, two-dimensional electron gas.

1. Introduction

Semiconductor nanodevices, owing to the mesoscopic regime engineered, are outfitted with characteristic structural dimensions actually smaller than the appropriate mean free-paths for carrier mobility and wavefunction (WF) phase coherence. Epitaxial-growth techniques applied allow for incorporation of desired depth-profile quantum wells (QW) in the nanoheterointerfaces (NHI) being established. For total energy lower than the NHI QW potential-energy top, the carrier acquires a quasi-two-dimensionality perpendicular to the QW spatial bottom, a two-dimensional electron gas (2DEG) thus being formulated and exhibiting momentum and eigenenergy quantisation [1].

The major nanodevice-performance enhancement achieved through the introduction of modulation doping by Dingle et al. [2] has ever since been providing NHIs hosting separately a dense distribution of dopants on the wider-bandgap part of theirs and a high-mobility 2DEG along the QW extension, belonging to the narrower-bandgap side. Investigation of such NHIs has been designing and exploiting innovative nanodevices of the kind of the Bloch oscillator [3,4], the resonant-tunnelling double heterodiode [5], the hot-electron tunnelling-transistor [6], the revolutionary quantum-cascade LASER [7,8].

A major part of our research activity has been evolving within the field of designing, characterising, and analysing optoelectronic nanodevices [9 – 24]. In particular, monitoring frequently the photoconductive response of NHI structures has ultimately inspired us to assess the 2DEG-eigenstate photodynamics being effected within a generic modulation-doped nanoheterodiode by absorption of regulated successive photon-doses.

In this Work, this photonic modification is being studied in terms of the 2DEG fundamental-sublevel eigenenergy's correlation with the respective 2DEG areal density, versus instantaneous cumulative photonic intake for conventional nanoheterodiodes.

2. Photodynamics Model

Within the extension of the typical NHI, the energy-band bendings of the energetic-barrier portion and the conductive channel are being determined by its neighbouring (ionised-impurity) electric-charge density and overall field (with any effective non-built-in one incorporated). Thus, on the one hand the 2DEG confined sublevels are quantum-mechanically calculable and, on the other, the thermodynamic-equilibrium requirement mirrors an ultimate uniform Fermi-energy level throughout the nanoheterojunction to a realistic sheet-concentration of QW two-dimensional electrons.

At each instance of such dynamic equilibrium, the energetic top of actually filled NHI 2DEG states aligns with the uniform Fermi-level operative:

$$\mathrm{E}_0 + \frac{\zeta}{\rho} = \mathrm{E}_F , \quad (1)$$

with E_F being exactly the Fermi-energy level, E_0 being the energetic bottom of the 2DEG fundamental subband (considered as the only one occupied near the electric quantum limit, approached by conventional NHIs primarily functioning at ambient temperatures in the vicinity of absolute zero), ζ being the instantaneous 2DEG sheet- concentration within the NHI QW, and ρ being the theoretical two-dimensional per-unit-area (normal to the QW spatial extension) density of states accessible to conductivity electrons having their normal wavevector-component quantised, given [22, 24] in the parabolic approximation by

$$\rho = \frac{m^*}{\pi\hbar^2} , \quad (2)$$

where m* denotes the conductivity-electron effective mass at the NHI QW fundamental subband, and $\hbar$ Planck's action constant divided by 2π.

Commonly, modulation doping of the epitaxially composed nanodevice embeds a heavily dense donor-distribution within the wider-bandgap-semiconductor part of the NHI being established, with the donor energy-level getting located sufficiently deep –with reference to the bandgap profile- for the Fermi level to be plausibly regarded as pinned to it and remaining there (with, effectively, negligible rate of change) for the entire regime of quantum-limit-like nanodevice functioning [28, 30, 18]. Such a Fermi-level immunity against evolving cumulative photonic intake (tantamount to increasing 2DEG population being hosted by the NHI QW) by the nanoheterostructure would be sustainable through a mechanism successively lowering the 2DEG fundamental sublevel E_0 (as well as the first excited sublevel, which nevertheless would not be participating in the hosting of QW conductivity electrons as always lying over the Fermi-energy demarcation) within the QW being commensurately broadened whilst keeping its energetic depth dictated by the invariable NHI conduction-band discontinuity.

Considering, therefore, the dynamics of energy-level positions against regulated successive photon-doses being absorbed by the probed NHI, we obtain through partial differentiation of (1) with respect to the instantaneous cumulative photonic dose δ:

$$\frac{\partial E_0}{\partial \delta} + \frac{1}{\rho}\frac{\partial \zeta}{\partial \delta} = \frac{\partial E_F}{\partial \delta} \cong 0 , \quad (3)$$

or,

$$\frac{\partial E_0}{\partial \delta} = - \frac{1}{\rho} \frac{\partial \zeta}{\partial \delta} ,$$
(4)

providing the photonic dose-rate of evolution of the 2DEG fundamental-eigenstate sublevel E_0 in terms of the experimentally traceable photon-dose-rate of augmentation of the 2DEG areal density ζ within the QW of the monitored NHI.

In this sense, (4) is following the photodynamics of the evolving photonic modification of the NHI fundamental-eigenstate, during the procedure of successive intakings of appropriate photon-transmissions: To each experimentally measurable Δζ(δ) for the augmentation of the 2DEG sheet-concentration ζ (with respect to its pre-illumination initial value ζ_d) consequent upon some instantaneous total photon-dose δ, the respective eigenstate-sublevel shift $\Delta E_0(\delta)$ (away from its dark locus E_{0d}) drawn by this cumulative dose δ is awaited, through to (4), to be:

$$\Delta E_0(\delta) = - \frac{1}{\rho} \Delta\zeta(\delta) .$$
(5)

This predicted gradual photolowering of NHI eigenstate-subband bottom is interpretable as quantum-mechanically compatible with previous studies of ours [13, 17] approximating the modification of a generic nanodevice's conductive-channel extension as positively linearly proportional to the respective 2DEG areal-concentration alteration.

With respect, now, to the generic situation of a conductivity electron being hosted by the QW of potential energy profile U(x) against the growth-axis coordinate x within a conventional semiconductor-nanodevice heterointerface, the pertinent Schrödinger equation, concerning the electron de Boglie time – independent wavefunction ψ (x) and taking into account the spatial variation m^* (x) of the carrier effective mass, reads:

$$-\frac{d}{dx}\left[\frac{\hbar^2}{2m^*(x)} \frac{d\psi(x)}{dx}\right] + U(x)\,\psi(x) = E\,\psi(x),$$
(6)

with E being the allowed energy-eignevalue conjugate to each physically meaningful wavefunction ψ (x), solving (6) and vanishing asymptotically at infinities, and $\hbar$ being Planck's action constant divided by 2π.
Performing, now, an independent variable transformation, namely,

$$x \equiv \alpha x^* \,\mathrm{Arctanh}\,(\xi) \leftrightarrow \varphi(\xi) \equiv \psi[x(\xi)] ,$$
(7)

we obtain in place of (7) the Sturm – Liouville differential equation

$$(d/d\xi)\,\{M(\xi)\,[d\varphi(\xi)/d\xi]\} - u(\xi)\varphi(\xi) + \lambda\sigma(\xi)\varphi(\xi) = 0 ,$$
(8)

under the boundary conditions

$$\varphi(-1) = 0 \ \&\ \varphi(+1) = 0,$$
(9)

with functions M(ξ), u(ξ), and σ(ξ) in the new dimensionless variable ξ (belonging to the universal interval [-1, +1]) defined as

$$M(\xi) = (1/\alpha)\,(1 - \xi^2)\, m_0/m^*[x(\xi)] ,$$
(10)

$$u(\xi) = [2\,\alpha/(1 - \xi^2)]\, U[x(\xi)]/E^* ,$$
(11)

$$\sigma(\xi) = 2\,\alpha/(1 - \xi^2) ,$$
(12)

and dimensionless new, "reduced-energy", eigenvalue λ defined as

$$\lambda = \frac{E}{E^*},$$

(13)

where E^* denotes a convenient energy-scale

$$E^* \equiv \frac{\hbar^2}{m_o x^{*2}} \equiv 1\,\mathrm{e\,V},$$

(14)

rendering the characteristic confinement-length x^* entering the independent variable transformation (7) after the dimensionless scale factor α equal to 2.76043 $\overset{0}{A}$, m_o

giving the electron rest mass.

For converting the Sturm – Liouville differential equation concerning the NHI 2DEG transformed wavefunction $\varphi(\xi)$ via a linearised system of difference equations into a tridiagonal-matrix eigenvalue-problem, we have previously [23, 24] composed a finite-difference-method iterative algorithm. Therewith, the opposite of the eignvalues of this matrix lead to the approximations to the NHI WF exact reduced-energy eigenvalues λ, thus computing (Eq.(13)) the allowed QW 2DEG subband-energies $E = \lambda E^*$. On the other hand, the determined Strum – Liouville eigenvectors $|\varphi(\xi)>$ conjugate to these numerical eigenvalues unveil through transformation (7) the quantum-mechanically allowed wavefunctions $\psi(x)$ for the 2DEG dwelling within the nanodevice heterointerface QW and underlying the crucial optoelectronic effects exhibited by the generic semiconductor-nanostructure. In particular such determinations would facilitate the prediction of 2DEG mobility behaviour and, furthermore, the consideration of quantum-mechanical-tunnelling transmission probability [28, 29] for conductivity electrons escaping the heterointerface and travelling through the nanodevice – especially at nanoelectronic cryogenic ambient temperatures.

This finite-difference-method algorithm is incorporated in the following procedure, repeatedly performed for each successive experimental cumulative photon-dose δ:

1. Extraction from predictive-scheme Eq.(5) of the awaited 2DEG fundamental-sublevel photolowering conjugate to experimentally measured 2DEG sheet-density PPE driven by current total photonic intake.
2. Deduction of current 2DEG fundamental sublevel by subtraction of the absolute value of current fundamental-sublevel photolowering from sublevel dark (prior to exposure to photonic doses) locus.
3. Iterative applications of the algorithm with respect to a sought-for 2DEG QW spatial width compatible with the respective fundamental-eigenstate sublevel predicted for the current cumulative photonic dose. The entailed potential-energy profile $U(x\,;\,\delta)$ is simplifyingly simulated by a rectangular one, of energetic depth always expressible by the NHI conduction-band discontinuity and resting on the boundaries of the photowidened QW spatial extension. Thus, the parametrisation of the QW potential-energy profile by total photonic intake δ is effected through letting a simulative fixed-energetic-depth rectangular model-QW expand spatially at a rate induced by each current intaken cumulative photon-dose.
4. Once the iterative algorithm has converged for the optimum QW spatial width conjugate to the current total photonic intake, the adjoint 2DEG fundamental-eigenstate wavefunction $\psi_0(x\,;\,\delta)$ is obtained, thus exhibiting its traceable penetration-length [31] into the NHI energetic-barrier part.

Therefore, tracing the fundamental-eigenstate penetration-length in the optimum wavefunction

$\psi_0(x\ ;\ \delta)$ obtained by convergence (with respect to the optimum QW width compatible with predicted photoredefined eigenstate locus) of the iterative algorithm for each total photon-dose intaken, we manage to map its photodynamics.

3. Additional Application

The present algorithm has been additionally applied to our proposed novel LASER action nanoheterosturcture [23] operational principle based on remotely optically pumped dual resonant tunnelling (OPRT) unipolar change transport mechanism materialisable within the framework of two communicating quatum wells (CQWs), asymmetric *both* in the their spatial extension *and* energetic barrier height aspect, hosting a total of five partially localised subbands – two (the fundamental **If>** and first excited **If '>**) on the part of the envisaged device front [F] QW and the remaining three (the fundamental **Ib>**, the first excited **Ib'>**, and the second excited **Ib">**) on the other part, of the OPRT device back [B] QW-, a band gap engineering designing meant to have established two selective, achievable by a nanostructure respective growth procedure, energy matchings; one between the uppermost subbands **If '>** and **Ib">** of the two CQWs and another concerning the two neighbouring QWs innermost fundamental sublevels **If >** and **Ib>.**

The two LASER action OPRT nanodevice levels are designed to be the second excited **Ib">** back [B] QW subband and the local next lower first excited **Ib'>** one:

The upper OPRT LASER action level is predicted to be being provided with conductivity electrons resonantly tunnelling [17, 18] into it out of its energetically matched device front [F] QW first excited **If '>** subband, being populated through remotely ignited optical intersubband pumping from its local fundamental **If>**, front QW, subband. The lower OPRT nanostructure LASER action level is, on the other hand, expected to be directly delivering its radiatively de – excited electrons to the local, device back [B] QW, fundamental **Ib>** subband via a particularly fast longitudinal optical (LO) phonon scattering, almost vertical in the reciprocal space, favoured by a band gap – engineered energetic proximity of the entailed **Ib'>** ↔ **Ib>** intersubband separation with the characteristic LO phonon energy valid under the device operational conditions entailed within the [B] QW semiconductor material.

The considered OPRT LASER nanostructure resonant microcavity functionality [19, 21] is, furthermore, determined by the above LO phonon scattering of radiatively down – converted conductivity electrons (from the LASER action lower level to the local [B] QW fundamental subband) being succeeded by their being recycled back to the OPRT LASER nanostructure [F] QW fundamental **If>** subband by virtue of a second – reverse sense – resonant tunnelling – mediated normal charge transport mechanism.

The rate equation modelling of the LASER action functionality of subband levels **Ib''>** and **Ib'>** is taken of the form:

$$\frac{dN_{Ib''\succ}}{dt} = \frac{1}{T_{FB}} N_{If'\succ} - \frac{1}{\tau_{Ib''\succ}} N_{Ib''\succ} \qquad (15),$$

$$\frac{dN_{Ib'\succ}}{dt} = \frac{1}{\tau} N_{Ib''\succ} - \frac{1}{\tau_{Ib'\succ}} N_{Ib'\succ} \qquad (16),$$

with $N_{If\,'>}$, $N_{Ib'>}$ and $N_{Ib''>}$ being the sheet electron concentration of nanostructure resonator level If '>, Ib'> and Ib''>, respectively, $\frac{1}{T_{FB}}$ being the temporal rate of achieving the resonant tunnelling charge transport from the [F] QW first excited subband If '> onto the energetically commensurate [B] QW second excited subband Ib''>, $\tau_{Ib''>}$ being the total lifetime of upper LASER action level Ib''> - expressible by means of the combined radiative and non-radiative Ib''> → Ib'> down – conversion rate $\frac{1}{\tau}$ and the non – radiative direct Ib''> → Ib> relaxation rate $\frac{1}{\tau_{Ib''\succ \to Ib\succ}}$ as

$$\frac{1}{\tau_{Ib''\succ}} = \frac{1}{\tau} + \frac{1}{\tau_{Ib''\succ \to Ib\succ}} \qquad (17),$$

and $\frac{1}{\tau_{Ib'\succ}}$ being the non – radiative, fast vertical longitudinal optical phonon scattering rate of electrons received by the lower LASER action subband Ib'> to the local, [B] QW, fundamental subband Ib>.

(1) and (2) form a system in five unknowns, namely $N_{Ic>}$ (c = f, f', b, b', b'') – the areal electron densities of the five nanostructure resonator levels Ic> - , along with the following equations:

$$\frac{dN_{If\succ}}{dt} = \frac{1}{T_{BF}} N_{Ib\succ} - \frac{I\Sigma}{\hbar\Omega} N_{If\succ} \qquad (18),$$

$$\frac{dN_{If'\succ}}{dt} = \frac{I\Sigma}{\hbar\Omega} N_{If\succ} - \frac{1}{T_{FB}} N_{If'\succ} \qquad (19),$$

$$\frac{dN_{Ib\succ}}{dt} = \frac{1}{\tau_{Ib''\succ \to Ib\succ}} N_{Ib''\succ} + \frac{1}{\tau_{Ib'\succ}} N_{Ib'\succ} - \frac{1}{T_{BF}} N_{Ib\succ} \qquad (20),$$

where $\frac{1}{T_{BF}}$ denotes the temporal rate at which the (reverse sense) Ib> → If> resonant electron tunnelling is effected within the CQWs, I the optical pumping intensity, Ω the pumping photon cyclic frequency, and Σ the optical absorption cross section exhibited by electrons initially resting upon [F] QW fundamental subband level If> to incoming pumping photons.

On the other hand, the quantum mechanically thus designed stimulated optical yield Y is determined as

$$Y = \frac{1}{L}\sigma\Delta N \qquad (21),$$

with L being the spatial extension of the entire CQWs configuration, σ the LASER stimulated emission cross section, for producing the secondary, coherent photons (of energy $\hbar\omega = \Delta E_{Ib''\succ \rightarrow Ib'\succ} = \Delta E$), and ΔN the LASER action population inversion between levels Ib''> and Ib'> obtained from the above electron concentration rate equation system solved at the steady state of the concurrency of the different charge transport mechanisms within the OPRT nanoheterostructure.

The aforementioned model formalism employed – based upon the rate equation monitoring of the proposed OPRT LASER action level population evolution and inversion – incorporates the transmission coefficient determination for the resonant tunnelling inter – QW communication mechanism consecutive steps.

For studying the applicability of the herewith proposed optically pumped dual resonant tunnelling LASER action unipolar charge transport mechanism we now consider an indicative generic semiconductor nanoheterostructure based on the conventional Al_xGa_{1-x} As/GaAs material system.

In particular, we employ two totally asymmetric – both in the spatial width and in the energetic barrier height –, communicating through an intervening barrier layer, approximately rectangular quantum wells, both formulated within (different portions of) the GaAs semiconductor: The front QW [F] of spatial width 96 ^{o}A and energetic barrier height 221 meV, contained between a surface $Al_{0.3}$ $Ga_{0.7}$ As slab and the inter – QW communication barrier layer, and the back QW [B] of growth axis extension 162 ^{o}A and energetic confinement hill 204 meV, spanning the region between the inter – QW communication barrier layer and a botton Al $_{0.33}$ $Ga_{0.67}$ As slab. The intervening, inter – QW communication barrier layer may non – exclusively be regarded as the succession (either abrupt or graded) of two rather equithick sublayers of $Al_{0.3}$ $GA_{0.7}$ As and $Al_{0.33}$ $Ga_{0.67}$ As.

The major goal attempted by the above employment is the establishment of a specific band gap engineering depicting the desired novelty of *double* (both spatial *and* energetic trench – wice) asymmetry between the two successive communicating QWs embodying the crucial nanostructure hosting the prescheduled five in all conduction subbands fulfilling the dual energy matching (both between the uppermost energy levels of the two QWs and between the lowest two, fundamental, subbands of theirs) needed for the possibility of the (optically ignited) dual resonant tunnelling inter – QW communication.

For the computational technique utilised for self – consistently depicting the energy eigenvalues above, the Sturm – Liouville eigenuvalue problem comprising the quantum mechanical Schroedinger differential equation and the appropriate exact boundary conditions conjugate with the entailed eigenfucntion vanishing asymptotically at infinities is treated by the finite difference method after the employment of an independent variable transformation restricting the integration domain to the finite, universal, dimensionless interval [-1, 1]. The handling of the problem evolves into the numerical calculation of the eigenvectors and respective eigenvalues of a specific tridiagonal matrix hosting the three successions of coefficients appearing in the kind of finite difference equations selected to convergingly approach the initial Strum – Liouville differential equation.

In this manner, the partially localised conductivity electron eignestates accommodated by the couple of communicating QWs in the model application under study correspond to the energy eigenvalues (measured within each QW from its energetic bottom upwards): E (**If>**) = 32 meV, E (**If ’>**) = 136 meV – for the front QW fundamental and first excited bound state, respectively, - and E (**Ib>**) = 14 meV, E (**Ib’>**) = 55 meV, and E (**Ib’’>**) =121 meV – for the back QW fundamental, first excited, and second excited bound state, respectively.

Notably, against this predicted energy eigenvalue configuration, the fundamental back QW eigenstate **Ib>** elevated by 14 meV over the back QW energetic botton finds itself well aligned with the conjugate fundamental eigenstate **If>** of the front QW raised above its QW energetic botton by an amount corresponding to the inter – QW energetic bottom discrepancy plus, about, the former fundamental eigenstate **Ib>** height over its local QW bottom.

In an analogous manner, the uppermost bound eigenstates of the two communicating QW, emerge aligned, as the difference in the height of each over its local QW bottom almost cancels the energetic height asymmetry of the two QW bottoms.

The ensuing calculations incorporate the determination of the effective dipole lengths associated with the intersubband transitions collaborating or antagonising with one another through the optoelectronic structure, an intersubband transition lifetime engineering thus emerging as a conformal mapping of the original heterosturcture wavefunction-engineering attempted. The determined intersubband transition (ISBT) effective dipole lengths, furthermore, demonstrate the oscillator strengths supporting the different ISBT events, whereas the LASER action population inversion predicted leads to the device stimulated optical gain.

Our preliminary results (radiative transition time constant around 45 ns, corresponding to an ISBT dipole length $\langle b'' | z | b' \rangle$ around 1 nm), trace a LASER far mid – infrared emission OPRT functionality in the 65 meV / 15 THz range, with a stimulated optical gain Y sensitivity $\frac{\partial Y}{\partial I}$ to the pumping illumination power I around $11\frac{\mathrm{cm}^{-1}}{10^5\,\mathrm{W/cm^2}}$.

4. Conclusion

The photodynamics of the NHI 2DEG eigenstate by absorption of regulated successive photon-doses is studied for the generic case of a conventional nanoheterodiode, in terms of the 2DEG fundamental-sublevel eigenenergy's correlation with respective 2DEG areal density, versus instantaneous cumulative photonic intake. The scheme is applicable to the experimental photoresponse of typical modulation-doped NHDs and also allows for the deduction of the NHI 2DEG wavefunction penetration-length, as computed through an iterative algorithm converting the Sturm – Liouville differential equation concerning the NHI 2DEG transformed wavefunction into a tridiagonal-matrix eigenvalue-problem.

The predicted trend, thus, of evolving red photoshift for the NHI eigenstate sublevel would be compatible with a proceeding NHI QW-extension photowidening, on the one hand, and a NHI wavefunction penetration-length shrinking, on the other.

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