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Intersubband linear and nonlinear optical response of the delta-doped SiGe quantum well

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ABSTRACT

The degree of ionization, controlled by external fields, of delta-doped layers inside the quantum wells can affect their energy structure, therefore delta-doped QWs can be used to engineer different kinds of tunable THz optical devices on intersubband transitions. Here it is calculated and analyzed the linear and nonlinear (Kerr-type) optical response, including absorption coefficient and refractive index change of 20 nm-wide $Si_{0.8}Ge_{0.2}/Si/Si_{0.8}Ge_{0.2}$ QW structures *n*-delta-doped either at the center or at the edge of the well under different temperatures. The conduction subband energy structure was found self-consistently, including the calculation of the impurity binding energy. Our results show that the degree of ionization of the impurity layer as well as the heterostructure symmetry has a strong influence on optical properties of the structures in THz region.

1. Introduction

Intersubband transitions in semiconductor quantum-confined structures are the perspective basis for the engineering of optical devices covering the terahertz range of spectrum [1]. One possible configuration to work with is stressed Si/SiGe quantum well structure, n-delta-doped inside the well. It should be noted that long (in comparison to GaAs and other III–V materials, where nonradiative polar scattering dominates) intersubband relaxation times are one of the key factors making SiGe structures perspective for developing devices on the base of intersubband transitions [2,3]. The other notable advantage is the absence of intensive polar absorption in THz region persistent in III–V materials, that makes Si/Ge non-quantum-confined layers transparent for the THz radiation. As for the doping inside the well, the shallow impurity of delta-layer within the quantum well can easily be ionized with external parameters like temperature and/or electric field. Free electrons and ionized donors make the Hartree potential that distorts the well energy profile, thus efficiently changing the structure of subbands (including transition energies) of the system [4]. Consequently, the effect can be used to tune the frequency of the presumable devices based on quantum-well-delta-doping configuration. All the above makes study of

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optical properties of such structures interesting, including non-linear properties as they are much more pronounced in quantum confined structures than in bulk semiconductors.

Previously [5] the self-consistent technique was developed to obtain numerically electronic structure of such a configuration. The technique allows for the Hartree potential distortion of energy profile and takes into account the change of impurity binding energy, which is found within the approach described in [6]. In the present work using that technique it is calculated and analyzed the linear and Kerr-type nonlinear optical response, such as absorption coefficient and refractive index change of Si/SiGe QW structures delta-doped either at the center or at the edge at different temperatures.

2. Materials and methods

The linear $\alpha_{ij}^{(1)}(\omega)$ and nonlinear $\alpha_{ij}^{(3)}(\omega, I)$ parts of the absorption coefficient for the transitions between i-th and j-th subbands were found following [7] with reference to [8] as:

$$\alpha_{ij}^{(1)}(\omega) = \frac{\omega\mu_0 c}{n} \mid M_{ji}\mid^2 \frac{\sigma_{ij}\Gamma}{(E_{ji}-\hbar\omega)^2+\Gamma^2}$$

$$\alpha_{ij}^{(3)}(\omega, I) = -\frac{\omega\,\mu_0 I}{2\,n^2\varepsilon\varepsilon_0} \mid M_{ji}\mid^2 \frac{\sigma_{ij}\Gamma}{\left\{(E_{ji}-\hbar\omega)^2+\Gamma^2\right\}^2} \times \left[4 \mid M_{ji}\mid^2 - \frac{|M_{jj}-M_{ii}|^2\left\{(E_{ji}-\hbar\omega)^2-\Gamma^2+(E_{ji}-\hbar\omega)\right\}}{E_{ji}^2+\Gamma^2}\right]$$

where ω is the angular frequency of the absorbed photon, ε permittivity (11.7 for silicon), ε_0 vacuum permittivity, μ_0 vacuum permeability, $n=\sqrt{\varepsilon}$ refractive index of the material (3.4926 for the silicon), E_i and E_j are energy levels of initial and target subbands of absorptive transition, $E_{ji}=E_j-E_i$ transition energy, I - incident electromagnetic wave optical intensity (was taken the same for all frequencies $I=0.5$ MW/cm^2 as reasonable value), $\Gamma=\hbar/\tau$ is the absorption broadening (Γ = 2 meV [9] for all transitions for simplicity), where τ is the intersubband nonradiative relaxation time. σ_{ij} is the concentration difference between i-th and j-th subbands,

$$\sigma_{ij} = \frac{m^* k_B T}{L\pi\hbar^2} \ln\left[\frac{1+\exp E_f - E_i)/k_B T}{1+\exp(E_f-E_j)/k_B, T}\right]$$

where m^* is an effective mass of electrons, k_B Boltzmann constant, T lattice temperature, L quantum well width. The dipole matrix element

$$M_{ab} = \int \psi_a^*(z) \mid e \mid z\psi_b(z)\, dz \quad (a,b = 1\ \ldots\ N_S),$$

where N_S is a number of lowest subbands taken into account, z is a coordinate along the structure growth direction, e unit charge, $\psi_a(z)$ and $\psi_b(z)$ – wave functions of corresponding subbands. The number of subbands accounted for was selected as $N_S=7$. It is big enough to provide acceptable precision in calculations of impurity binding energy embedded to our self-consistent technique: the difference between impurity binding energies found allowing for 6 and 7 subbands makes less than 0.1 meV. Also the absolute majority of free electrons in our structures are distributed within the first 7 subbands even for the higher temperatures so they are enough for THz absorption-based optical effects.

The complete absorption coefficient correspondingly is

$$\alpha_{ij}(\omega, I) = \alpha_{ij}^{(1)}(\omega) + \alpha_{ij}^{(3)}(\omega, I)$$

where

$$\alpha^{(1)}(\omega) = \sum_{i=1}^{N_S-1}\sum_{j=i+1}^{N_S} \alpha_{ij}^{(1)}(\omega) \text{ and } \alpha^{(3)}(\omega, I) = \sum_{i=1}^{N_S-1}\sum_{j=i+1}^{N_S} \alpha_{ij}^{(3)}(\omega, I)$$

Linear $\frac{\Delta n_{ij}^{(1)}(\omega)}{n}$ and nonlinear $\frac{\Delta n_{ij}^{(3)}(\omega, I)}{n}$ changes of the refractive index provided by the transitions between i-th and j-th subbands were calculated as [7]:

$$\frac{\Delta n_{ij}^{(1)}(\omega)}{n} = \frac{1}{2\,n^2\varepsilon\varepsilon_0} \mid M_{ji}\mid^2 \frac{\sigma_{ij}\,(E_{ji}-\hbar\omega)}{(E_{ji}-\hbar\omega)^2+\Gamma^2}$$

$$\frac{\Delta n^{(3)}(\omega, I)}{n} = -\frac{\mu_0\, c I}{4\,n^3\,\varepsilon\varepsilon_0} \mid M_{ji}\mid^2 \frac{\sigma_{ij}}{\left[(E_{ji}-\hbar\,\omega)^2+\Gamma^2\right]^2}$$

$$\times \left[4(E_{ji}-\hbar\,\omega) \mid M_{ji}\mid^2 - \frac{(M_{jj}-M_{ii})^2}{E_{ji}^2+\Gamma^2} \times \left[(E_{ji}-\hbar\omega)[(E_{ji}-\hbar\omega)E_{ji}-\Gamma^2] - \Gamma^2(2E_{ji}-\hbar\omega)\right]\right]$$