Effect of interdiffusion on electronic states of \textit{strain-free} \textit{gaussian-shaped} \textit{double quantum ring superlattice

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EFFECT OF INTERDIFFUSION ON ELECTRONIC STATES
OF STRAIN-FREE GAUSSIAN-SHAPED
DOUBLE QUANTUM RING SUPERLATTICE

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The effect of interdiffusion on band structure and Bloch amplitudes of three dimensional superlattice composed of Gaussian shaped double quantum rings is investigated using the Fourier transformation to the momentum space. It is shown that the sequence of the principal quasimomentum vectors which correspond to the energy increase depends on superlattice symmetry. Due to interdiffusion both the first and the second minibands of conduction band shift to the region of higher energies and broaden, meanwhile the difference between the behaviors of the dispersion curves in different directions of momentum space gradually disappears. The obtained results indicate to the opportunity of purposeful manipulation of structure characteristics by means of interdiffusion both quantitively and qualitatively.

**Keywords:** Gaussian Shaped Quantum Ring, Superlattice, Interdiffusion, Electronic States, Bloch Amplitudes

1. Introduction

Quantum rings (QRs) are a special class of nanostructures that have attracted a lot of attention due to the occurrence of the Aharonov–Bohm effect, which is specific to the doubly-connected topology of a ring [1–3]. Particularly interesting are the magnetic properties of such quantum systems, which are related to the possibility of inducing persistent currents. Recent development of nanofabrication technology allows us to create and assemble atomic units in an artificial manner, such as in the fabrication of quantum dots (QD) [4-7] molecule-like alignment of two QDs [8,9] and the formation and characterization of QR complexes [10], which open a new route, promised by ring geometry, to measurement of quantum interference effects [11,12]. Using droplet epitaxial technique, authors of [10] performed self-assembly of concentric double quantum rings (DQR) with high uniformity and excellent rotational symmetry. The generation and detection of terahertz (THz) radiation have gained importance for their potential applications in the areas of security, biomedical imaging, quality control, and submillimeter astronomy [13-16]. Semiconductor-based QD intersublevel detectors have been used for the detection of infrared radiation in the 15-100 THz range [17-21] but it is difficult to access the 3–10 THz range. QRs are derived from epitaxially grown self-organized QDs.*

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by post-growth annealing [22,23] and confinement in these nanostructures is stronger than that in QDs because of the altered shape [24]. In reference [25] it was found that the QR intersublevel detectors exhibit very low dark current and strong response in the 1–3 THz range, with the peak response at 1.82 THz in the temperature range of 5–10 K.

The potential application of QRs in nano-devices has given rise to theoretical investigation of their optoelectronic properties [26]. In some works the influences of spin-orbit coupling [27,28], hydrostatic pressure [29] and polaronic effects [30] are examined. Analytical treatments of electronic states in QRs with non-trivial geometry has also been suggested [31,32].

Recently, strain-free nanostructures grown by droplet epitaxy have been proposed and demonstrated for photovoltaic applications [33] and have also gained popularity in lasers and photodetectors [34,35]. In reference [36] strain-free DQR (SFDQR) solar cells were fabricated by droplet epitaxy. Rapid thermal annealing (RTA) was used to improve the optical quality of the solar cells. It was shown that RTA plays a major role in modifying the electronic structure and in the improvement of material quality.

In this work the effect of interdiffusion induced by RTA on electron energy levels and Bloch amplitudes in DQR superlattice (DQRSL) is modeled using the Fourier transformation to momentum space. The cases of SL of cubic and tetragonal symmetry are considered. Two shifted Gaussians are used as a shape function for DQRs, which can provide a reasonable representation of real DQRs obtained in [36] by choosing appropriate values of Gaussian parameters.

2. Theory

Let us consider a three dimensional superlattice composed of GaAs/Al$_{0.33}$Ga$_{0.67}$As DQRs. Before the influence of RTA on the distribution of Al and Ga atoms at the heterojunction one can assume that there is an exact interface between the DQR and the surrounding area. The shape of DQR can be taken as a superposition of two shifted Gaussian functions [37] with the introduction of the shape function as follows:

\[
f(\rho,z) = \begin{cases} 
1, & 0 \leq z \leq z_0(\rho), \\
0, & z < 0 \text{ or } z > z_0(\rho),
\end{cases}
\]  

(1)  

where

\[
z_0(\rho) = A \exp(-\alpha^2(\rho - \rho_1)^2) + B \exp(-\beta^2(\rho - \rho_2)^2).
\]  

(2)  

In Fig.1 the image of surface of GaAs/Al$_{0.33}$Ga$_{0.67}$As SFDQR structure [36] (left) and a model
of DQR corresponding to Eqs. (1) and (2) (right) are presented. The values of parameters in (2) are taken to be \( A = B = \rho_2 = 2\rho_1 = a/3 \), \( \alpha = \beta = 25/a \), where \( a \) has the dimension of length and in further calculations is assumed to be the period of DQRSL in x and y directions \( (a_x = a_y = a) \). As is seen from the figure, Eqs. (1) and (2) provide a good description of real DQRs and the agreement can be improved choosing appropriate values of the parameters. It should be mentioned that the difference of the suggested model from the DQR model with rectangular profile used by most of authors is mainly expressed by the fact that the potential barrier between the concentric rings exists not for all values of \( z \). It means that electron can move from the inner ring to the outer one not only by tunneling. Of course, by choosing corresponding values for the parameters in \( z_0(\rho) \) one can obtain a DQR with the potential barrier between rings for all values of \( z \).

Assuming that before the interdiffusion there are no Al atoms in the region of DQRs and the concentration of Al atoms is constant \( (X_0) \) elsewhere one can solve the diffusion equation according to Fick’s low which leads to the following expression for the potential profile in conduction band of DQRSL subjected to RTA:

\[
V_c(x, y, z; L) = \frac{eQ_cX_0}{2} \left( 1 - \sum \frac{\text{erf}(t_a/L)}{2} + e^{-(t_a/L)^2} \int_0^{\infty} \frac{x}{L^2} \text{erf} \left( \frac{z_0(x) - \tau_z}{L} \right) dx \right),
\]

where \( L = 2\sqrt{Dt} \) is the diffusion parameter, \( D \) is the diffusion coefficient, \( t \) is time, \( t_a = 1247\, \text{meV} \) for the Ga\(_x\)Al\(_{1-x}\)As material, \( Q_c \) is the band offset \( (Q_c = 0.6 \) for GaAs\), \( \tau_\rho = \sqrt{(x-R_z)^2 + (y-R_z)^2} \), \( \tau_z = z-R_z \), \( R \) is the radial vector of the center of corresponding DQR base, \( \text{erf}(q) \) is the error function and \( I_0(q) \) is the modified Bessel function of zero order.

In Fig.2 the potential cross sections by \( z = 0.1a \) and \( x = 0 \) planes are illustrated for the DQRSL of cubic symmetry \( (a_x = a_y = a_z = a) \) at the above mentioned values of DQR. First of all it is clear that for the cases of smaller values of diffusion parameter \( (L/a = 0.03 \) and \( L/a = 0.1 \) the potentials of separate DQRs retain cylindrical symmetry (see the upper row of graphics), while for enough large values of diffusion parameter the rectangular symmetry of superlattice superimpose on the cylindrical symmetry of separate DQR. Secondly one can see that the potential barriers in the center and between the concentric rings decrease with the increase of \( L \) and finally vanish \( (L/a = 0.2) \).

The same features can be observed for the potential cross section by the \( x = 0 \) plane. Namely the abrupt profile smoothes out, the barriers between the concentric rings (for \( L/a = 0.03 \) and \( L/a = 0.1 \) and
The decrease of potential barrier between the DQRs makes possible the transport of electrons with the higher energy levels without tunneling. In other words the part of miniband which is closer to the barrier energy transforms to the lower part of continuous spectrum in conduction band.

Following the method developed in the work of Gunawan et al. [38] we present the wave function and the confining potential in the form of Fourier series:

\[ \psi(\mathbf{\rho}, L) = \sum_{\mathbf{g}} u_{\mathbf{g}}(L)e^{i(k+\mathbf{g})\cdot\mathbf{\rho}}, \]

\[ V(\mathbf{\rho}, L) = \sum_{\mathbf{g}} V_{\mathbf{g}}(L)e^{i\mathbf{g}\cdot\mathbf{\rho}}, \]

where \( \mathbf{g} \) is the reciprocal lattice vector, \( \hbar\mathbf{k} \) is the quasimomentum vector, after which a set of the following equations is obtained from the Schrödinger equation:

\[ \sum_{\mathbf{g}} \left\{ V_{\mathbf{g}} - \delta_{\mathbf{g}, \mathbf{g}'} + \left[ \frac{\hbar^2(k + \mathbf{g})^2}{2m} - E \right] \delta_{\mathbf{g}, \mathbf{g}'} \right\} u_{\mathbf{g}'} = 0, \]  

where

\[ V_{\mathbf{g}} = \frac{Q_{z}t_eX_0}{\Omega_0} \frac{L^2g^2}{4} \int_{\Omega_0} [1 - f(\mathbf{r})] \exp(-ig\mathbf{r})d\mathbf{r} \]  

is the Fourier transform of the SL potential, \( u_{\mathbf{g}} \) is the Fourier transform of the Bloch amplitude of wave function, \( \mathbf{g} \) is the reciprocal lattice vector, \( \Omega_0 \) is the volume of unit cell, \( \delta_{\mathbf{g}, \mathbf{g}'} \) is the Kronecker delta and \( m \) is the effective mass of electron. It should be mentioned that the expression of Fourier transform (5) is obtained automatically from the solution of diffusion equation in reciprocal space and there is no need to calculate integrals which contain expression (3) for the potential [38]. The integral in (5) can be calculated easily if we make the following approximation:

\[ \int_{\Omega_0} f(\mathbf{r}) \exp(-ig\mathbf{r})d\mathbf{r} = \int_{0}^{\rho} \int_{0}^{z_\Omega(\rho)} \exp(-ig\mathbf{z}) \int_{0}^{\rho} \exp(-ig\rho\cos\varphi)d\varphi dz d\rho, \]

i.e. the upper limit of the integral by \( \rho \) which corresponds to the borders of the unit cell in the left hand side of (6) is replaced by infinity. This approximation is reasonable if the shape function \( f \) defers from zero only in the region of the unit cell. After some calculations we finally obtain:

\[ V_{\mathbf{g}, \mathbf{g}'}(L) = \frac{Q_{z}t_eX_0}{\Omega_0} \frac{L^2g^2}{4} \left\{ \Omega_0 \delta_{\mathbf{g}, \mathbf{g}'} - 2\pi \int_{0}^{\rho} z_\Omega(\rho) I_0(g\rho) \rho d\rho, \text{ if } g_z = 0, \right. \]

\[ -\frac{4\pi}{g_z} \int_{0}^{\rho} \exp\left(-i\frac{g_zz_\Omega(\rho)}{2}\right) \sin\left(\frac{g_zz_\Omega(\rho)}{2}\right) I_0(g\rho) \rho d\rho, \text{ if } g_z \neq 0. \]
3. Discussion

As was mentioned above we obtain the band structure of SL by the exact diagonalization of the system (4) for different values of the quasimomentum. All calculations are carried out for the following values of parameters: \( A = B = (2/3)R, \alpha = \beta = 25/a, \rho_1 = (1/3)R, \rho_2 = (2/3)R, X_0 = 0.33, \) where \( R \) is the characteristic radius of DQR.

In Fig. 3 the first miniband energies at the different fixed values of the diffusion parameter for the values of quasimomentum vector which coincide with the vertices of the Brillouin zone are presented. Fig. 3a corresponds to the case of SL of cubic symmetry while Fig. 3b is for SL of tetragonal symmetry. It should be mentioned that the directions \( z \) and \(-z\) are not equivalent in contrast to the directions \( x(y) \) and \(-x(-y)\). Furthermore in the considered case of \( a_x = a_y \) the directions \( x \) and \( y \) are equivalent. It is clear that the sequences of the high symmetry points (\( \Gamma\{0, 0, 0\}; X\{\pi/a, 0, 0\}; Z\{\pi/a, 0, 0\}; M\{0, \pi/a, \pi/a\}; R\{\pi/a, \pi/a, 0\}, A\{\pi/a, \pi/a, \pi/a\} \)) which correspond to the energy increase in the cases (a) and (b) are different. For small values of diffusion parameter (\( L \leq 0.25a \)) in the case (a) the change in the energy value when the values of \( k_x \) or \( k_y \) change by \( \pi/a \) is more significant comparing with the corresponding energy change due to the change of \( k_z \) by \( \pi/a \). As a result we observe a dupletic-like sequence of energy values. In the case (b) one can observe a tripletic-like sequence of energy values in contrast with the case (a). This is because of larger increase in the energy when the value of \( k_z \) increases by \( \pi/a_c = 2\pi/a \) comparing with the energy increase due to the corresponding changes in \( k_x \) or \( k_y \). However the further increase of \( L \) due to interdiffusion results in to the disappearance of this regularity because of the increase of electron tunneling in \( z \) direction, which results in to the increase of the influence of quasimomentum change on the value of energy. The shift of the first miniband to the higher energies region and the increase of its width are obvious in both cases. This is due to the potential increase in the regions of wells and its reduction in the regions of barriers.

Fig. 4 illustrates the dispersion curves for the first and the second minibands in the principal directions in reciprocal space for various values of diffusion parameter. The general form of these curves, excepting curves in Fig. 4d, coincide with ones obtained for bulk materials in the framework of the nearly free electrons model [39]. This coincidence takes place because of the diminishing role of the potential profile for the value of quasimomentum near the Brillouin zone edge (energy increases monotonically with the increase of \( k \) in the extended band diagram). However for the considered structure the energy in extended band diagram is not a monotone function of \( k_z \). This fact can be
explained by the resonant interaction between the potential wells and the electronic wave for enough large (small) values of $k_z$ (wave length in $z$ direction). The last fact results in to the increase of the second miniband energy with the increase of $k_z$ (the lowest three curves in the second miniband in Fig.4d). However with the increase of diffusion parameter a region of energy decrease appears and becomes as large as large is $L$. For enough large values of $L$ the region of energy increase disappears and the dispersion curves get conventional form. It is clear from Fig.4 that both the first and the second minibands shift to the higher energy region and broaden. Moreover the dependences on quazimomentum become more significant for all five directions. We can also conclude from the figure that the inhenced tunneling due to the diffusion leads to the significant decrease of the SL band gap.

In Fig.5 the sections of the first miniband Bloch amplitude’s modulus square by the plane $z = 0.2a$ in the region of the unit cell for parameter values $R = 100\,\text{Å}$, $a_x = a_y = a_z = a = 200\,\text{Å}$, $L = 0.01a$ and the values of $\vec{k}$ corresponding to the vertices of the first Brillouin zone are shown. The superposition of the DQR cylindrical symmetry with the cubic symmetry of SL is observed in all cases. The concavity of the surface (due to the potential barrier in the DQR center) is surrounded by four maxima in the diagonal directions (the directions of the weakest tunneling) and by four minima in the directions of the lattice translation vectors (the directions of the strongest tunneling). In the outer ring an opposite arrangement is observed. The maxima and the minima in the outer ring are expressed much more slightly because of its larger volume. In the cases of (100) or (101) directions the minima in the inner ring over the $x$ ($y$) axis become more (less) pronounced due to the appearance of a selected direction for the tunneling. This kind of directions appear also in the cases of (110) and (111) but they are expressed very smoothly due to the significant scattering of electron on the barriers in diagonal directions. It is also clear from the figure that with the increase of $\vec{k}$ the section of $|U|^2$ increases. This increase is more sensible to the changes in $k_x$ or $k_y$.

In Fig.6 the sections of $|U|^2$ are presented in the case of smeared potential ($L = 0.2a$) for the same values of other parameters as in Fig.5. These surfaces remind the probability distributions in cylindrical disk without any inner barriers. As in the case of $L = 0.01a$ the superposition of the DQR and the SL symmetries, the appearance of selected directions in the cases when $\vec{k} \neq 0$ and the changes in the magnitude of probability with the increase of diffusion parameter are observed. Comparison of Fig.5 and Fig.6 shows that the increase in the absolute value of quasimomentum effects on the probability density in the unite cell more significantly in the case of smeared potential profile.

Summarizing, we investigate the effect of interdiffusion on band structure and Bloch
amplitudes of three dimensional SL composed of Gaussian-shaped DQRs using the Fourier transformation to the momentum space. It is shown that the sequences of the values of quasimomentum which correspond to the increasing values of energy are different for SLs of cubic and tetragonal symmetry. The symmetry of the SL results in to additional maxima and minima of the Bloch amplitude’s modulus square in the inner and outer rings over the diagonal directions and the directions of translation vectors. Due to interdiffusion the symmetry of the SL potential superimpose on the cylindrical symmetry of DQR in unite cell. The shape of Bloch amplitudes smears tending to the one for the SL of cylindrical disks. Both the first and the second minibands of conduction band shift to the region of higher energies and become wider. Initially the form of dispersion curves in $k_z$ direction qualitatively differs from the corresponding curves in other “main” directions in momentum space. However because of interdiffusion this difference gradually disappears due to the enhanced tunneling of electron in $z$ direction. The obtained results indicate to the opportunity of purposeful manipulation of structure characteristics by means of interdiffusion both quantitatively and qualitatively.

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References
Fig. 1 The atomic force microscopy image of DQR obtained by Wu et al. [36] (left) and the model of DQR obtained by using of two shifted Gaussians (the lengths are presented in the unites of $a$).
Fig. 2 The dependences of potential in conduction band on $x$ and $y$ coordinates for $z = 0.1a$ (the upper row of graphics) and on $x$ and $z$ coordinates for $y = 0$ (the lower row).
Fig. 3 Dependence of the energy values in the first miniband at the high symmetry points of Brillouin zone on diffusion parameter for the parameter values $A = B = (2/3)R$, $\alpha = \beta = 25/a$, $p_1 = (1/3)R$, $p_2 = (2/3)R$. a) $R = 100\text{Å}$, $a_x = a_y = a_z = a = 200\text{Å}$, and the sequence of the high symmetry points $\Gamma$; $Z$; $X$; $R$; $M$; $A$ corresponds to the energy increase. b) $R = 80\text{Å}$, $a_x = a_y = a_z = 175\text{Å}$, $a_z = a/2$, and the sequence $\Gamma$; $X$; $M$; $Z$; $R$; $A$ corresponds to the energy increase.
Fig. 4 Dependences of the first and the second minibands’ energy on the quazimomentum for the five principal directions in momentum space a) (100), b) (110), c) (111), d) (001), e) (101) and for the parameter values $R = 100\text{Å}$, $a_x = a_y = a_z = a = 200\text{Å}$. The curves corresponding to a fixed miniband are arranged from bottom to top by the values of diffusion parameter $L/a = 0.01, 0.05, 0.1, 0.15, 0.2, 0.25, 0.3, 0.35, 0.4$ respectively.
Fig. 5 The section of the first miniband Bloch amplitude’s modulus square by the plane $z = 0.2a$ in the region of the unit cell for parameter values $R = 100\text{Å}, a_x = a_y = a_z = a = 200\text{Å}, L = 0.01a$. 
Fig. 6 The section of the first miniband Bloch amplitude’s modulus square by the plane $z = 0.2a$ in the region of the unit cell for parameter values $R = 100\text{Å}$, $a_x = a_y = a_z = a = 200\text{Å}$, $L = 0.2a$. 
1. The effect of interdiffusion on electronic states in a quantum ring superlattice is studied.
2. The Gaussian-Shaped double quantum rings have been considered.
3. Both the cases of superlattice of cubic and tetragonal symmetry have been considered.
4. The first two minibands shift to the region of higher energies due to interdiffusion.
5. As a result of interdiffusion the minibands become wider.