Giant optical anisotropy in cylindrical self-assembled InAs/GaAs quantum rings

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Abstract – Using a single-particle atomistic pseudopotential method followed by a configuration interaction treatment to many-particle interactions, we investigate the geometry, electronic structures and optical transitions of a self-assembled InAs/GaAs quantum ring (QR), with its shape changing continuously from a lens-shaped quantum dot (QD) to a nearly one-dimensional ring. We find that the biaxial strain inside the ring is strongly asymmetric in the plane perpendicular to the QR growth direction, leading to a giant optical anisotropy.

Recently, a novel nano-structure, quantum ring (QR), has been fabricated via the self-assemble techniques [1] in various semiconductor systems, such as In(Ga)As/GaAs [1–5], InAs/InP [6,7], InP/GaInP [8], and Si/Ge [9] etc., with controlled sizes and shapes. Like the self-assembled quantum dots, the QRs have discrete energy levels due to 3D confinement effects. However, a QR differs from a QD because of its non-simply connected topology, and therefore offers a unique opportunity to study the physical effects, in addition to confinement effects, such as the Aharonov-Bohm effect [10,11], and quantized magnetic susceptibility [12].

The electronic structure of self-assembled QRs have been successfully explored via the electron charging spectra [13] and the photoluminescence (PL) spectra [14,15]. On the other hand, most of the theoretical studies on QRs are still using the continuum theories, such as the effective mass approximations (EMA) [12,16–20], k · p method [21], and the local spin density approximation [22], etc., assuming 1-dimensional, [16] 2-dimensional, [12,19,20] and 3-dimensional model confinement potentials [17,21,23]. These studies provide valuable qualitative knowledge about the single-particle electronic structures [20,21,23,24], as well as many-body effects [19,22,25] of QRs. However, it has been shown that one has to use atomistic theories to capture the subtle features, such as energy level splittings [26], shell filling [27] and exciton fine structures [28] etc., at single dot level. The atomistic effects are expected to be even more important for the QRs because the QRs have much larger surface area to volume ratio than the QDs of similar sizes. Furthermore, there are few theoretical studies on the optical transitions in QRs.

In this paper, we investigate the electronic structures and optical transitions of realistic self-assembled InAs/GaAs QRs by using an atomistic pseudopotential method [29]. We change the geometries of the QR from a lens-shaped QD to a narrow ring, by continuously increasing the inner radius of the ring. We then study the strain profiles, the single-particle energy levels, as well as the optical transitions of the QRs with respect to the inner radius. QRs have more complicated strain profiles than QDs, due to their complicated topology. We show that the biaxial strain of QRs is strongly asymmetric in the plane perpendicular to the QR growth direction, leading to single-particle energy level crossings and a giant optical anisotropy (even in cylindrical QRs).

Figure 1 depicts the cross-sections of the QRs with their structural parameters, embedded in a 60 × 60 × 60 GaAs matrix. The QRs are assumed to grow along the [001] direction, on the top of a 1-monolayer wetting layer. The outer radius \( R_{out} \) of the QR is measured from the center of the base to the outside edge of the ring, whereas the inner radius \( R_{in} \) is defined to be the distance from the center

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of the rings are obtained by solving the Schrödinger results. Alloy QRs and rings of larger outer radii give very similar 3nm, respectively. For the lens-shaped dot, the biaxial radius of the QRs, respectively. The QR heights \( h \) are fixed to be 2.5 nm.

![models of quantum rings](image)

**Fig. 1:** Cross-sections of the QRs for (a) \( R_{in} < 0 \) and (b) \( R_{in} > 0 \), where \( R_{in} \) and \( R_{out} \) are the inner radius and outer radius of the QRs, respectively. The QR heights \( h \) are fixed to be 2.5 nm.

of the base to the inner circle. At \( R_{in} = -R_{out} \), the QR is a lens-shaped quantum dot\(^1\). Therefore, by increasing the inner radius, we continuously change the QR from a lens-shaped quantum dot to a one-dimensional quantum wire as \( R_{in} \rightarrow R_{out} \). We fix the height of the quantum ring \( h = 2.5 \) nm, the outer radius \( R_{out} = 12.5 \) nm and vary the inner radius \( R_{in} \) from \(-12.5 \) nm (lens-shaped dot) to 6 nm. Alloy QRs and rings of larger outer radii give very similar results.

The single-particle energy levels and wave functions of the rings are obtained by solving the Schrödinger equation

\[
\left[-\frac{1}{2} \nabla^2 + V_{ps}(r)\right] \psi_i(r) = \epsilon_i \psi_i(r),
\]

where the total electron-ion potential \( V_{ps}(r) \) is a superposition of local, screened atomic pseudopotentials \( v \alpha(r) \) [26], i.e.

\[
V_{ps}(r) = \sum_{\alpha} v \alpha(r - R_{\alpha}),
\]

The atom positions \( (R_{\alpha}) \) are obtained by minimizing the strain energies using the valence force field (VFF) method [30,31]. Equation (1) is solved using the “Linear Combination of Bloch Bands” (LCBB) method [29]. The exciton energies and optical transitions are calculated via a configuration interaction (CI) method [32], in which the exciton wave functions are expanded as the linear combination of Slater determinants constructed from the single-particle electron and hole wave functions.

**Strain profiles.** – Figure 2(a)–(d) depicts the biaxial strain,

\[
B = \sqrt{(\epsilon_{xx} - \epsilon_{yy})^2 + (\epsilon_{zz} - \epsilon_{xx})^2 + (\epsilon_{yy} - \epsilon_{zz})^2},
\]

of the QR, for \( R_{in} = -12.5 \) (lens-shaped dot), \(-3 \), 0 and 3 nm, respectively. For the lens-shaped dot, the biaxial strain is almost isotropic in the (001) plane. However, with the increasing of the inner radius \( R_{in} \), the biaxial strain becomes asymmetric in the (001) plane: the biaxial strain along the [110] direction becomes larger than that along the [110] direction. As the inner radius increases further, the difference of biaxial strain between the two directions becomes significant. One can clearly see the biaxial strain peaks around the inner edge of the ring along the [110] direction at \( R_{in} = 0 \) nm and \( R_{in} = 3 \) nm in fig. 2(c), (d). Since the hole confinement potential strongly depends on the biaxial strain, the strain-modified potentials for holes (not shown) are also asymmetric in the (001) plane.

**Single-particle energy levels and wave functions.** – The electron and hole single-particle energy levels are shown in fig. 3(a), (b) respectively, as functions of \( R_{in} \). The orbital labels \( s, p, d, 2s \) are given by continuously monitoring the characters of the wave functions (see fig. 4). We denote the \( p, d \) orbitals with peaks along the [110] direction \( p_1, d_1 \) and those of peaks along the [110] direction \( p_2, d_2 \). The lens-shaped dot, the \( s-p \) and \( p-d \) energy spacings are nearly equal. For electrons, the two \( p \) orbitals are nearly degenerate, so are the two \( d \) levels. However, for holes, the \( p, d \) levels show quite large (8–10 meV) energy splitting [26,33]). The 2s state is close in energy to the \( d \) states, suggesting that the confinement potential is close to a parabolic potential\(^2\). As we increase \( R_{in} \), we found that all the confined electron (hole) levels decrease (increase) first and then increase (decrease). We attribute

\(^1\)Rigously speaking, when \( R_{in} < 0 \), the QR is not a real ring. However, to simplify the discussion, we still call it a ring in this paper.

\(^2\)For a cylindrical QDs, the degeneracy of energy levels is at most two. However, for a dot with parabolic confinement, the 2s level also accidentally degenerate with the d levels.
the decreasing (increasing) of the energy levels at small $R_{in}$ to the strain effects after a close examination of the strained confinement potentials. The energy level turning points are indicated by the small arrows in fig. 3. The turning points $R_{in}$ of the $s$ and $2s$ levels are about $-2$ to $-3$ nm, whereas the turning points of $p$ states are at larger inner radius $R_{in} = -1$ nm. The turning points of the $d$ states are at about $R_{in} = 1$ nm for both electrons and holes, larger than those of $s$ and $p$ orbitals. Beyond the turning point, the confined energy levels increase rapidly with the increasing of $R_{in}$, especially for the $s$ and $2s$ states. The $2s$ states become unconfined at $R_{in} \sim 2$ nm.

The trend of the electron energy levels as functions of the $R_{in}$ of the QRs can be understood by examining the wave functions of each level. The six lowest confined electron and hole states are shown in fig. 4(a), (b). For lens-shaped QDs, the electron wave functions are the $s$ orbitals, whereas the $p$ orbitals have nodes at the dot center. The electron $2s$ orbital becomes unconfined after $R_{in} > 0$ nm, and $e_5$ is actually a $f$ state at $R_{in} = 3$ nm. The $s$, $2s$ states, having maximum density at the dot center, are very sensitive to $R_{in}$, as the states feel strong confinement potential from the inner circle of the ring with the increasing of $R_{in}$, leading to much faster increasing of the level energies than those of other states. Their wave functions also change dramatically from disk-like states at $R_{in} < 0$ nm (i.e., have the maximum at center of the ring), to ring-like ones (i.e., hollow at the center of the ring) at $R_{in} > 0$ nm. In contrast, the $p$ and $d$ orbitals have nodes at the ring center, and do not feel the confinement potential until at much larger $R_{in}$. Consequently, the electronic structures of the QRs deviate significantly from those of the QDs: i) the $s$-$p$ energy level spacing is much smaller than the $p$-$d$ energy level spacing; ii) the $2s$ level is no longer (nearly) degenerate with the two $d$ levels.

We observe several energy level crossings with respect to $R_{in}$ in fig. 3, including the level crossing between the electron $2s$ state and the $f$ state at $R_{in} = 0$ nm, the hole $2s$ state with two $d$ states at $R_{in} = -3$ and $0$ nm, as well as the two electron (hole) $p$ orbitals at $R_{in} = -3$ ($-4$) nm. The level crossing with different angular momentum (e.g. the $2s$ and $f$ states) is due to the confinement effect, as discussed above, whereas the level crossing between the two hole $p_1$ and $p_2$ states is due to the biaxial strain effects.

**Optical transitions.** – We calculate the optical transition spectra in QRs, and the results are shown in fig. 5(a)–(d) with $R_{in} = -12.5, 0, 3, 6$ nm, respectively. We show the polarized transition intensities in both [110] and [110] directions, as the transitions are almost linearly polarized in these two directions. The primary exciton energy is shifted to zero for each $R_{in}$ for clarity, and the transition peaks are marked by their leading transition characters. For example, the primary exciton transition is a $s$ (electron) to $s$ (hole) transition. We also show the
p-p and d-d transitions. As we see, the energy differences between the s-s, p-p and d-d transitions decrease significantly with the increasing of the inner radius, reflecting the change of single-particle level spacings. The transition intensities also change dramatically with respect to R_{in}. For example, the p-p and d-d transitions are much weaker in the QRs than in the dots. At R_{in} = 6 nm, a significant s to p transition appears, because the envelope wave functions of the electron s state and hole p states are no longer (nearly) orthogonal at this R_{in}.

Interestingly, even though the total transition intensity of the primitive exciton does not change much with respect to R_{in}, the transition intensity polarized along the [110] becomes much stronger than that of the [110] direction. We calculate the optical polarization anisotropy λ[26], defined as the ratio of the transition intensities along the [110] and [110] directions, i.e.,

$$ \lambda = \frac{I_{\{110\}}}{I_{\{110\}}} $$

for the s-s transitions. For lens-shaped QDs (fig. 5(a)), I_{\{110\}} is slightly smaller than I_{\{110\}} (λ_{s} = 1.09), which agrees well with previous calculations [26]. However, with the increasing of the inner radius, λ_{s} decreases dramatically. At R_{in} = 6 nm, λ_{s} is only about 0.30, i.e., the transition in the [110] direction is about 3 times stronger than that in the [110] direction. The giant optical anisotropy comes from the asymmetric biaxial strain. Since the QRs studied here are cylindrical, the anisotropy is an “atomic symmetry” effect [26].

To conclude, we have investigated via a single-particle atomistic pseudopotential and a many-particle CI methods, the electronic structures and optical transitions of self-assembled InAs/GaAs QRs. We find that even in cylindrical InAs/GaAs quantum rings, the biaxial strain is strongly asymmetric in the (001) plane, where the biaxial strain along the [110] direction is much larger than that along the [110] direction. The asymmetric strain induces single-particle energy level crossing, and lead to giant optical anisotropy. The optical anisotropy could be examined in future experiments and should be taken account of in designing QR devices.

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