Electron and hole effective masses in self-assembled quantum dots

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Abstract. Electron and hole effective masses in self-assembled InAs/GaAs quantum dots are determined by fitting the energy levels calculated by a single-band model to those obtained by a more sophisticated tight-binding method. For the dots of various shapes and dimensions, the electron effective-mass is found to be much larger than that in the bulk and become anisotropic in the dots of large aspect ratio while the hole effective-mass becomes almost isotropic in the dots of small aspect ratio. For flat InAs/GaAs quantum dots, the most appropriate value for the electron and hole effective-mass is believed to be the electron effective-mass in bulk GaAs and the vertical heavy-hole effective-mass in bulk InAs, respectively.

PACS. 71.18.+y Fermi surface: calculations and measurements; effective mass, g factor – 73.22.Dj Single particle states – 73.21.La Quantum dots

1 Introduction

There have been many attentions focusing on the unique electronic and optical properties of self-assembled quantum dots due to their promising applications in opto-electronics devices. The understanding of the electronic structure of quantum dots is fundamental to master the detailed knowledge of their properties. A number of theoretical approaches, such as the effective-mass approximation, eight-band k · p [1–3], tight-binding [4,5], and empirical pseudopotential [6] methods have been developed to understand the experimental results. The single-band effective-mass approach [7–14], thanks to its simplicity, is the most widely used one believed to be able to explain the main features of many experimental observations. However, the value of electron effective-mass adopted in the calculations often varies largely from work to work. For an example of self-assembled InAs/GaAs quantum dots, the value in bulk InAs, $m_e = 0.023m_0$ or $0.026m_0$ is commonly used [7–10] while a much larger value, $0.04m_0$, is also seen in many works [11–13]. In spite that the electron states are known to be localized mostly in InAs islands, the value in bulk GaAs, $0.067m_0$, is adopted sometimes [14]. The large variation of the adopted effective-masses is apparently due to the lack of a guideline in the application of the effective-mass approach. In this work, we will investigate the applicability of effective-mass approach to the electronic structure of self-assembled quantum dots, which hopefully would provide a criterion on how to determine the effective-masses in its application.

2 Method

The Hamiltonian of the effective-mass model under this study is given by [15]

$$\hat{H}_e = -\frac{\hbar^2}{2m_e^\parallel} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) + \frac{\hbar^2}{2m_e^\perp} \frac{\partial^2}{\partial z^2} + V_e + V_e^\perp + V_p,$$

$$\hat{H}_h = \frac{\hbar^2}{2m_h^\parallel} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) + \frac{\hbar^2}{2m_h^\perp} \frac{\partial^2}{\partial z^2} - a_e H_s - b_e B_s + V_h + V_h^\perp + V_h^\parallel$$

where $V_e$ and $V_h$ are the band offsets (without strain) between the island (InAs) and matrix (GaAs) materials, $V_p$ is the piezoelectric potential. $H_s$ and $B_s$ are the hydrostatic and biaxial strain components, respectively, which modify the band edges through the deformation potential parameters, $a_e$, $a_h$, and $b_e$. Although the electron effective-mass is almost isotropic in most III-V semiconductors, two independent components $m_e^\parallel$ and $m_e^\perp$ are used to reflect the anisotropic geometries of the quantum dots. In spite of strong mixing between heavy- and light-hole bands, almost all the low-lying confined states in the valence bands in quantum dots are dominated by their heavy-hole components. Hence, this Hamiltonian takes into account only the heavy-hole band.

Since there is no a priori rule on how to choose the effective-masses within the model itself, $m_e^\parallel$, $m_e^\perp$, $m_h^\parallel$, and $m_h^\perp$ are treated as adjustable parameters and determined by fitting the calculated energy spectrum to that obtained...
by a more sophisticated approach like the tight-binding method described below. The Hamiltonian reads [16]

$$H(R_{\sigma \alpha}, R'_{\sigma \alpha}) = E_{s\sigma}^{000} \delta_{RR'} + E_{s\sigma}^{110} \delta_{R,\tau} + E_{s\sigma}^{200} \delta_{R,\lambda},$$

$$H(R_{\sigma \alpha}, R_{\sigma \alpha}) = E_{s\sigma}^{000} \delta_{RR'} + \delta_{R,\tau} [E_{s\sigma}^{110} - \tau_{p}^2] + E_{s\sigma}^{002} \delta_{R,\lambda} [E_{s\sigma}^{000} \tau_{p}^2 + E_{s\sigma}^{002} - \tau_{p}^2],$$

$$H(R_{\sigma \alpha}, R'_{\sigma \alpha}) = E_{s\sigma}^{110} \tau_{p} \delta_{R,\tau},$$

$$H(R_{\sigma \alpha}, R'_{\sigma' \alpha}) = E_{s\sigma}^{110} \tau_{p} \delta_{R,\tau}.$$  \hspace{1cm} (2)

where $\Delta R = R - R'$, and $\tau_{p}$ and $\lambda_{p}$ are the positions of the nearest and next nearest neighbors, respectively. Table 1 lists the next nearest-neighbor tight-binding parameters for GaAs and InAs. Other material parameters like the band offset, deformation and piezoelectric potential parameters are taken from reference [2]. Compared with conventional empirical tight-binding approaches [17,18], this formalism has the advantage that the effective masses of electrons and holes at the $\Gamma$ point, conduction and valence band edges at both the $\Gamma$ and $X$ points can be exactly reproduced.

As the ground state energy is mainly controlled by the vertical effective-mass component while the energy separation between the ground state and first excited state is governed by the in-plane component, we choose to fit the ground state and first excited state energies by minimizing $|\Delta E_1| + |\Delta E_2|$ where $\Delta E_i$ is the difference between the energies of the $i$th state calculated by the effective-mass and tight-binding methods. The criterion for convergence is set to be $10^{-7}$ meV. Another algorithm by fitting the first six energy levels gives a very close result: the difference for $m_{\perp}^e$ and $m_{\parallel}^e$ is less than 4% and 10%, respectively.

### Table 1. Next nearest-neighbor parameters (in eV).

<table>
<thead>
<tr>
<th>Integral</th>
<th>GaAs</th>
<th>InAs</th>
</tr>
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<tbody>
<tr>
<td>$E_{s\sigma}^{000}$</td>
<td>3.581011</td>
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<tr>
<td>$E_{s\sigma}^{510}$</td>
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<td>$E_{s\sigma}^{662}$</td>
<td>0.495500</td>
<td>0.525000</td>
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</tbody>
</table>

### 3 Results and discussions

Figure 1 plots the vertical and in-plane components of the electron effective-mass calculated as a function of the diameter of InAs/GaAs quantum dots. The lens-shaped dot has a height of 2.8 nm which includes a 2 ML thick wetting layer. For the calculations of the height of the dots from that in bulk InAs but close to

that in bulk GaAs. For a dot of a large diameter, the electron effective-mass is seen almost isotropic ($\approx 0.063$), close to the experimental value (0.053) [19]. As the dot shrinks laterally, the vertical component of the effective-mass is found to decrease slowly while the in-plane component increases more than twice as fast. As a result, the effective-mass is seen to be more and more anisotropic. At the diameter of about 14.1 nm, $m_{\parallel}^e/m_{\perp}^e$ reaches as large as 1.25.

The renormalization of the electron mass in solids is due to the band-mixing effect. By the second-order perturbation theory, the electron effective-mass in bulk semiconductors with direct band-gap can be expressed as [20]

$$\frac{m_{o}}{m_{e}} = 1 + E_{P} \frac{3E_{g} + 2\Delta_{so}}{3E_{g}(E_{g} + \Delta_{so})},$$  \hspace{1cm} (3)

where $E_{g}$ is the band-gap, $\Delta_{so}$ is the spin-orbit splitting, and $E_{P}$ is the parameter for the mixing between the conduction and valence bands. As $m_{o}/m_{e} \ll 1$ in most of III-V semiconductors, we see that $m_{o}/m_{e} \approx 3E_{g}/(3E_{g} + 2\Delta_{so})(E_{g} + \Delta_{so})/E_{P}$ which means a larger band-gap would lead to a larger electron effective-mass. The effective band-gap in those dots shown in Figure 1 is between 0.973 to 1.086 eV, which is much larger than 0.43 eV in bulk InAs. Substituting these values with $E_{g}$ in equation (3), we have the resulting effective-mass ranged from 0.0476 to 0.0525, which qualitatively explains why the electrons in quantum dots have much larger effective-masses than in the corresponding bulk material [21]. If one assumes the mixing effect between the conduction and valence bands is reduced in quantum dots, the behavior of the in-plane effective-mass can be well reproduced with $E_{P}$ modified from 21.5 eV in bulk InAs to 16.5 eV.

To see further the anisotropy of the electron effective-mass, Figure 2 plots $m_{\parallel}^e$ and $m_{\perp}^e$ calculated as a function of the height of the dots with a fixed diameter of 19.8 nm. As the height increases, it is seen that the difference between the two effective-mass components becomes larger. Combining these results with those shown in Figure 1, we