第 24 卷第 6 期 半 导 体 学 报 Vol. 24, No. 6
2003 年 6 月 CHINESE JOURNAL OF SEMICONDUCTORS June, 2003

Binding Energy and Photoionization of Hydrogenic Impurities in GaAs/$Ga_{1-x}Al_xAs$ Quantum Well Wires*

Liu Jianjun[1,2], Su Hui[3], Guan Ronghua[2,4] and Yang Guochen[2]

(1 *College of Physics, Hebei Normal University, Shijiazhuang* 050016, *China*)
(2 *Institute of Physics, Hebei University of Technology, Tianjin* 300130, *China*)
(3 *Institute of Physics, The Chinese Academy of Sciences, Beijing* 100080, *China*)
(4 *Department of Applied Physics, North China Electric Power University, Baoding* 071003, *China*)

Abstract: The binding energy and the photon energy dependence of the photoionization cross-section are calculated for a hydrogenic impurity in GaAs/$Ga_{1-x}Al_xAs$ quantum well wires. The correlation between confined and non-confined direction of the wire in the variational wave function is taken into account. The results show that the photoionization cross-sections are affected by the width of the wire and that their magnitudes are larger than those in infinite potential quantum well wires. In comparison with previous's results, the variational wave function improves the binding energy and decreases the value of photoionization cross-sections of the hydrogenic impurities, which makes the results more reasonable.

Key words: photoionization cross-section; binding energy; hydrogenic impurity; quantum well wire
PACC: 7865; 7320D; 7115P
CLC number: O471.1 **Document code**: A **Article ID**: 0253-4177(2003)06-0561-06

1 Introduction

The photoionization process is one of the powerful means to understand the optical properties of carriers in semiconductors. The study of the photoionization cross-section can be used for the characterization of the impurity states in the materials of semiconductors. There have been many studies that examine the binding energy and the behavior of the photoionization cross-section as a function of photon energy in low-dimensional electronic systems, such as quantum wells (QWs)[1~8], quantum well wires (QWWs)[9~11].

In 1997, Sali *et al*. investigated the photon energy dependence of the photoionization cross-section of a hydrogenic impurity located in a finite GaAs/$Ga_{1-x}Al_xAs$ QWW and they considered the case that the light was polarized along z-direction[10]. They have also worked on the similar object in the case that the light is polarized along x-direction and have found that the shape of the photoionization cross-section is entirely different from the case of the z-direction polarized light and the value of the photoionization cross-section is smaller[11]. The above two papers have a common ground that they both take variational approaches and adopt a simple form for the variational wave func-

* Project supported by Natural Science Foundation of Hebei Province (No. 102137), and Educational Committee Natural Science Foundation of Hebei Province (No. 200104)

Liu Jianjun male, was born in 1962, professor, PhD candidate. He is engaged in research on semiconductor superlattice physics and functional materials.

Su Hui female, was born in 1977, PhD candidate. Her major is semiconductor superlattice physics.

Received 13 November 2002, revised manuscript received 15 February 2003 ©2003 The Chinese Institute of Electronics

tion, in which the correlation between confined (x- and y- direction) and unconfined direction (z-direction) of the QWWs is not considered. So their results should be very approximate and can not embody the real situation. But the correlation has been shown to be negligible only for the region of small well width for QWWs[12], so it is necessary to make further theoretical study for the binding energy and the photoionization cross-section of the hydrogenic impurity in QWWs.

In this paper, we employ another variational wave function to recalculate the binding energy and photoionization cross-section, considering the correlation between confined and nonconfined direction of the QWWs, which is widely used to calculate the binding energy in many references[13~20]. Our results show that the binding energy of the impurities is improved and the photoionization cross-section is decreased in comparison with the previous results. It is arranged as following: first, the binding energy of the impurities is calculated by using our wave function; then, the photoionization cross-section is obtained from the wave function and the binding energy when the light is polarized along z-direction and x-direction; finally, a detailed analysis is made for the results.

2 Theory and calculation

2.1 Variational wave function and binding energy

We assume that a single impurity is located at the center of GaAs/$Ga_{1-x}Al_xAs$ QWWs, the Hamiltonian of the hydrogenic impurity can be written in the effective mass approximation as

$$H = \frac{p^2}{2m_i} - \frac{e^2}{\epsilon_i r} + V(x,y) \tag{1}$$

where

$$V(x,y) = \begin{cases} 0, & |x| < L_x/2, |y| < L_y/2 \\ V_0, & \text{else} \end{cases} \tag{2}$$

$m_i (i = 1, 2)$ represents the electron effective mass in the well and barrier, $\epsilon (i = 1, 2)$ is the dielectric constant in the well and barrier, and V_0 is the magnitude of the barrier.

We make use of the variational approach to get the eigenvalue of formula (1). Considering the correlation between the confined and unconfined directions of the QWWs, we choose the trial wave function of the ground state as

$$\psi_i(\vec{r}) = B\Phi_1(x)\Phi_1(y)\exp(-\lambda r) \tag{3}$$

where

$$\Phi_1(x) = \begin{cases} \cos(\alpha_{1x}x), & |x| < L_x/2 \\ \cos(\alpha_{1x}\frac{L_x}{2})\exp(\beta_{1x}\frac{L_x}{2})\exp(-\beta_{1x}|x|), & |x| > L_x/2 \end{cases} \tag{4}$$

$\Phi_1(y)$ is similar to $\Phi_1(x)$, which is the wave function of the electron first subband and in which $\alpha_{1x} = (\frac{2m_1E_{1x}}{\hbar^2})^{\frac{1}{2}}$ and $\beta_{1x} = [\frac{2m_2(V_0 - E_{1x})}{\hbar^2}]^{\frac{1}{2}}$, E_{1x} is derived from continuity of the wave function $\frac{\Phi_1(x)}{\Phi_1(x)}$ on the border of the well and barrier, as $m_1\beta_{1x} = m_2\alpha_{1x}\tan(\alpha_{1x}\frac{L_x}{2})$, in which λ is the variational parameter, B the normalization constant, and $r = \sqrt{x^2 + y^2 + z^2}$ the distance between the electron and the donor ion. The ground state energy of the hydrogenic impurity (or the initiate state energy of the system) is

$$E_i = \frac{\int \psi_i^* H \psi_i d\tau}{\int |\psi_i|^2 d\tau} \tag{5}$$

The binding energy of the hydrogenic impurity is the electron energy without impurity ion subtracting the hydrogenic impurity energy,

$$E_b = E_e - \min \langle \psi_i | H | \psi_i \rangle \tag{6}$$

2.2 Calculation of photoionization cross-section

The general expression for the photoionization cross-section associated with an impurity in the dipole approximation as[9~11]

$$\sigma(\hbar\omega) = \left| (\frac{E_{\text{eff}}}{E_0})^2 \frac{n_r}{\epsilon} \right| \frac{4\pi^2}{3}\alpha\hbar\omega \sum_f |\langle \psi_i | \vec{r} | \psi_f \rangle|^2 \times \delta(E_f - E_i - \hbar\omega) \tag{7}$$

where n_r is the optical index of refraction, ϵ is the dielectric constant, α is the fine structure constant

and E_f is the energy of final state. The factor $(\frac{E_{\text{eff}}}{E_0})^2$ is effective field ratio, which does not affect the shape of the photoionization cross-section and can be equal to 1[9~11].

(1) For the light polarized along z-direction, we consider the photoionization as an optical transition from the impurity ground state to the first subband state ($n_x = 1, n_y = 1$). The final state of wave function is taken as

$$\psi_f(\vec{r}) = \frac{1}{\sqrt{L}}\phi_1(x)\phi_1(y)\exp(ik_z z) \tag{8}$$

where the expressions of $\phi_1(x)$ and $\phi_1(y)$ are the same as that in the above expression (4).

(2) For the light polarized along x-direction, the photoionization is the optical transition from the impurity ground state to the second subband state ($n_x = 2, n_y = 1$) and the final state wave function is taken as

$$\psi_f(\vec{r}) = \frac{1}{\sqrt{L}}\phi_2(x)\phi_1(y)\exp(ik_z z) \tag{9}$$

where $\phi_2(x)$ is the electronic wave function of the second subband in the x-direction of the wire.

$$\phi_2(x) = \begin{cases} -\sin(\alpha_{2x}\frac{L_x}{2})\exp(\beta_{2x}\frac{L_x}{2})\exp(\beta_{2x}x), & x < -L_x/2 \\ \sin(\alpha_{2x}x), & |x| < L_x/2 \\ \sin(\alpha_{2x}\frac{L_x}{2})\exp(\beta_{2x}\frac{L_x}{2})\exp(-\beta_{2x}x), & x > L_x/2 \end{cases} \tag{10}$$

where $\alpha_{2x} = (\frac{2m_1E_{2x}}{\hbar^2})^{\frac{1}{2}}$ and $\beta_{2x} = [\frac{2m_2(V_0 - E_{2x})}{\hbar^2}]^{\frac{1}{2}}$, E_{2x} is the second subband energy and satisfies the transcend equation, $m_1\beta_{2x} = -m_2\alpha_{2x}\cot(\alpha_{2x}L_x/2)$.

For every uncontinuous E_x and E_y, there is a subband caused by the continuous E_z and the final state density is $\rho_z = \frac{L}{4\pi\sqrt{E_z}}$, which leads the sum in the matrix element of the dipole transition in Eq. (7) to the numerical integral.

$$\sum_f |\langle\psi_i|\vec{r}|\psi_f\rangle|^2\delta(E_f - E_i - \hbar\omega) = \int |\langle\psi_i|\vec{r}|\psi_f\rangle|^2\delta(E_f - E_i - \hbar\omega)\frac{L}{4\pi\sqrt{E_z}}\mathrm{d}E_z \tag{11}$$

where the final state energy is $E_f = E_x + E_y + E_z$ and the initial state energy $E_i = \langle\psi_i|H|\psi_i\rangle$.

Due to the conservation of energy in the above equation, the integral variable

$$E_z = \hbar\omega - (E_x + E_y - E_i) = \hbar\omega - E_s \tag{12}$$

where E_s is the threshold energy of the photoionization.

The parameters of the GaAs/$Ga_{1-x}Al_xAs$ QWWs are[20]: $x = 0.3$, the effective mass $m_1 = 0.0665m_0$ in the well and $m_2 = (0.0665 + 0.083x) \times m_0 = 0.0914m_0$ in the barrier, m_0 is the mass of a free electron, the dielectric constant $\epsilon_1 = 12.58$ in the well and $\epsilon_2 = 12.58(1 - x) + 10.1 = 11.836$ in the barrier, the barrier height is V_0, the refractive index $n_r = 3.6$. In our calculation, we use units of the effective donor Bohr radius and the effective Rydberg, respectively, given by $a^* = \frac{\epsilon_1\hbar^2}{m_1e^2} = 10\text{nm}$ and the energy $R_y^* = \frac{e^2}{2\epsilon_1 a^*} = 5.72\text{meV}$.

3 Results and discussion

Figure 1 shows that the binding energy varies with the wire width L_x in the two cases of the square ($L_x = L_y$) and the rectangular ($L_y = 2L_x$) cross-section QWWs. From Fig. 1, it can be seen that the binding energy has a peak at a certain wire width $L_{x(\text{peak})}$ (about 2.5nm) for the square cross-section QWWs because the finite barrier height determines the maximum allowable Coulomb interaction. Reducing L_x leads to a greater effective interaction between the electron and the ion, but also a greater likelihood that the electron will be found out of the wire (in the barrier), thus the binding energy decreases from the peak. Increasing the wire width beyond $L_{x(\text{peak})}$ weakens the Coulomb interaction because the barrier no longer forces the electron near the impurity, which makes the binding energy decline with the wire width L_x increasing.

In the case of the rectangular cross-section QWWs, the shape of binding energy varies with the wire width L_x. The variation is similar to that of the square cross-section QWWs, and only the max-

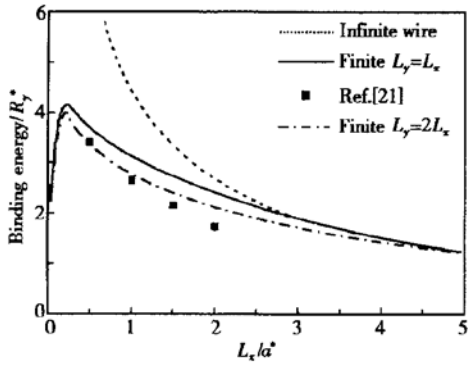

Fig. 1 Binding energy versus well width L_x

imum value of the binding energy and corresponding peak position are different. In the former, the distribution of the electron wave function is more extensive and the impurity binding energy is smaller. For the same reason, when the same width of the square wire is same, the binding energy of the impurity in the infinite QWWs is greater than that of the finite QWWs. It can be seen that as the size of the wire is very small, the wave function can not penetrate into the infinite barrier and the binding energy approaches infinity with the wire width decreasing. But with the size of the wire width L_x increasing, the confinement of barriers in the infinite QWWs has similar effect on the binding energy of the impurity as that in the finite QWWs, thus the binding energies for the wider wires in the two cases are close to the same value.

Comparing our results with that in Ref. [21] (the solid dot in Fig. 1), the binding energy we obtained is larger for the moderate and wider wire width. One reason for this is our consideration of the dismatch of effective mass and dielectric constant, another is that the correlation between confined and unconfined directions can not be neglected for the case of wider wire width. Thus, we demonstrate the validity of the results of Ref. [12].

When the light is polarized along the axis of the wire (z-direction), the final state is the first continuum subband. Figure 2 shows the results we have obtained in three different cases: finite wire ($L_x = 0.5a^*$, $L_y = 1.0a^*$) and ($L_x = L_y = 1.0a^*$), infinite wire ($L_x = L_y = 1.0a^*$). It can be seen from the Fig. 2 that the photoionization cross-section rises from zero absorption at the photoionization threshold, and peaks at the larger photon energy and then decreases monotonically for much larger photon energies, which has accordance with Ref. [10]. From the equations (6) and (12), we can see that the threshold energy is just the binding energy of the hydrogenic impurity. So the greater E_b is, the stronger the electron is bound and the smaller the photoionization cross-section is. It also can be known that the binding energy of the impurity in the finite square cross-section wire is larger than that in the finite rectangular cross-section wire (Fig. 1), so the photoionization cross-section is smaller in the square cross-section than in the rectangular cross-section for the same wire width (Fig. 2).

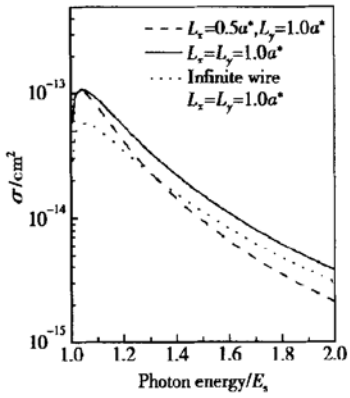

Fig. 2 Photoionization cross-section as a function of photon energy for three cases: finite wire ($L_x = L_y = 1.0a^*$), ($L_x = 0.5a^*$, $L_y = 1.0a^*$) and infinite wire ($L_x = L_y = 1.0a^*$) Final state is the first subband.

The same reason is used to explain that the value of photoionization cross-section is larger in finite wires than that in infinite wire for the same size of QWWs.

When the light is polarized perpendicularly to the axis of the wire (e. g. x-direction), the final state is the second subband because of the asymmetry of the wave functions of the transition between the initial and final states. Figure 3 shows the results of three different cases: finite wires (L_x

$= L_y = 1.0a^*$) and ($L_x = 1.0a^*$, $L_y = 2.0a^*$), infinite wires ($L_x = L_y = 1.0a^*$). It can be seen that as

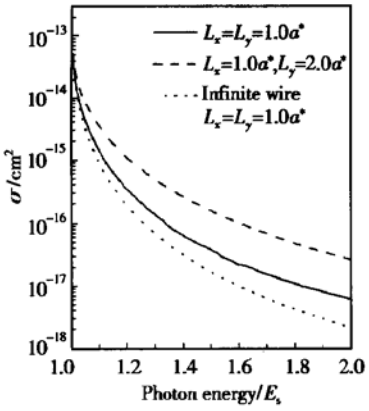

Fig. 3　Photoionization cross-section versus photon energy for three cases: finite wire ($L_x = L_y = 1.0a^*$), ($L_x = 1.0a^*$, $L_y = 2.0a^*$) and infinite wire ($L_x = L_y = 1.0a^*$)　Final state is second subband.

the photon energy is threshold energy, the photoionization cross-section is maximum and then decreases monotonically from the maximum absorption with the increase of photon energy, it is entirely different from the case of z-direction polarized light (Fig. 2). Because under this condition, for the same wire width, the second subband energy is much greater than the first subband energy, the threshold energy is enhanced and greater than the ground state binding energy of the hydrogenic impurity. Similarly, the difference between the binding energy of the impurities for square and rectangular cross-section QWWs results in the distinction in the photoionization cross-section.

References

[1] El-Said M, Tomak M. Photoionization of impurities in infinite-barrier quantum wells. J Phys Chem Solids, 1991, 52: 603

[2] El-Said M, Tomak M. Photoionization of impurities in quantum well. Solid State Commun, 1992, 82: 721

[3] El-Said M, Ilaiwi K F. Photoionization of shallow donor impurities in finite-barrier quantum wells. Phys Status Solidi B, 1995, 187: 93

[4] Sali A, Fliyou M, Loumrhari H. The effect of a strong magnetic field on the impurity photoionization in semiconductors. Phys Status Solidi B, 1996, 197: 119

[5] Li Shushen, Jiao Shanqing. Binding energy calculation of hydrogenic impurities in GaAs-$Ga_{1-x}Al_xAs$ quantum well in vertical magnetic field. Chinese Journal of Semiconductors, 1990, 11: 647 (in Chinese) [李树深, 焦善庆. 垂直磁场中 GaAs-$Ga_{1-x}Al_xAs$ 量子阱内类氢杂质束缚能的计算. 半导体学报, 1990, 11: 647]

[6] Li Shushen. Binding energy calculation of hydrogenic impurities in GaAs-$Ga_{1-x}Al_xAs$ quantum well in vertical electric field. Chinese Journal of Semiconductors, 1991, 12: 715 (in Chinese) [李树深. 垂直电场中 GaAs-$Ga_{1-x}Al_xAs$ 量子阱内类氢杂质束缚能的计算. 半导体学报, 1991, 12: 715]

[7] Li Shushen, Yuan Wei, Liu Jianjun, et al. Calculation of binding energy and effect of image potential on binding energy of hydrogenic impurity near GaAs-$Ga_{1-x}Al_xAs$ heterojunction. Chinese Journal of Semiconductors, 1994, 15: 223 (in Chinese) [李树深, 袁伟, 刘建军, 等. GaAs-$Ga_{1-x}Al_xAs$ 异质结附近类氢杂质束缚能及其受像势的影响. 半导体学报, 1994, 15: 223]

[8] Liu Jianjun, Su Hui, Yang Guochen. Scaling of hydrogenic impurity binding energy and virial theorem in semiconductor quantum wells and wires. Chinese Journal of Semiconductors, 2002, 23: 925 (in Chinese) [刘建军, 苏会, 杨国琛. 半导体量子阱和量子线中杂质束缚能的度规法则与维里定理. 半导体学报, 2002, 23: 925]

[9] Sali A, Fliyou M, Loumrhari H. The effect of the electron-longitudinal optical phonon interaction on the photoionization in quantum well wires. Phys Status Solidi B, 1997, 200: 145

[10] Sali A, Fliyou M, Loumrhari H. Photoionization of shallow donor impurities in finite-barrier quantum-well wires. Phys B, 1997, 233: 196

[11] Sali A, Fliyou M, Loumrhari H. Photoionization of impurities in quantum-well wires. Phys Status Solidi B, 1999, 211: 661

[12] Bastard G, Mendez E E, Chang L L, et al. Exciton binding energy in quantum wells. Phys Rev B, 1982, 26: 1974

[13] Bryant G W. Hydrogenic impurity states in quantum-well wires. Phys Rev B, 1984, 29: 6632

[14] Brum J A. Position-dependence of the impurity binding energy in quantum well wires. Solid State Commun, 1985, 54: 179

[15] Brown J W, Spector H N. Hydrogen impurities in quantum well wires. J Appl Phys, 1986, 59: 1179

[16] Takikawa M, Kelting K, Brunthaler G, et al. Photoionization of deep traps in AlGaAs/GaAs quantum wells. J Appl Phys, 1989, 65: 3937

[17] Latge A, Porras-Montenegro N. Infrared transitions between hydrogenic states in cylindrical GaAs-(Ga, Al) As quantum-well wires. Phys Rev B, 1992, 45: 9420

[18] Spiros V Branis, Gang Li, Bajaj K K. Hydrogenic impurities in quantum wires in the presence of a magnetic field. Phys Rev B, 1993, 47: 1316

[19] Montes A, Duque C A. Electric field effects on the states of a donor impurity in rectangular cross-section vacuum/GaAs/

vacuum quantum-well wires. J Appl Phys, 1998, 84: 1421

[20] Villamil P, Porras-Montenegro N, Granada J C. Infrared transitions between hydrogenic states in cylindrical GaAs quantum-well wires under applied magnetic fields. Phys Rev B, 1999, 59: 1605

[21] Osorio F A P, Degani M H, Hipolito O. Bound impurity in GaAs/GaAlAs quantum-well wires. Phys Rev B, 1988, 37: 1402

$GaAs/Ga_{1-x}Al_xAs$ 量子阱线中类氢杂质的束缚能和光致电离截面*

刘建军[1,2] 苏 会[3] 关荣华[2,4] 杨国琛[2]

(1 河北师范大学物理学院, 石家庄 050016)

(2 河北工业大学物理所, 天津 300130)

(3 中国科学院物理研究所, 北京 100080)

(4 华北电力大学应用物理系, 保定 071003)

摘要: 通过在波函数中考虑量子线的限制方向和非限制方向的相关性, 计算了 $GaAs/Ga_{1-x}Al_xAs$ 量子阱线中类氢杂质的束缚能和光致电离截面. 结果表明光致电离截面的大小受量子线尺寸的影响, 并且对于相同尺寸的量子线, 有限深势阱中杂质态的光致电离截面要比无限深势阱中的大. 与他人的结果比较发现, 所选波函数改进了体系的束缚能, 并使光致电离截面减小, 这使得结果更为合理.

关键词: 光致电离截面; 束缚能; 类氢杂质; 量子阱线

PACC: 7865; 7320D; 7115P

中图分类号: O741.1 **文献标识码**: A **文章编号**: 0253-4177(2003)06-0561-06

* 河北省自然科学基金(No. 102137)及河北省教育厅自然科学基金(No. 200104)资助项目

刘建军 男, 1962 年出生, 教授, 博士研究生, 从事半导体超晶格物理和功能材料研究.

苏 会 女, 1977 年出生, 博士研究生, 从事半导体超晶格物理研究.

2002-11-13 收到, 2003-02-15 定稿

©2003 中国电子学会