行政院國家科學委員會專題研究計畫成果報告

次毫米波單載子共振態半導體雷射

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一、中文摘要

本計畫主要利用先進的奈米製程技術將原先單一量子井結構改進為多層量子井或長成超晶格，用以增加雷射的增益(gain)，再根據目前手中已完成的實驗資料與數據，將原本的δ-doped 位置由量子井中間改為量子井邊緣，用以降低由摻雜造成的自由載子束縛能，此由相關理論計算證實,並已發展出一套可以精確處理量子井中似氫原子雜質共振態的「多重次能帶」模型（multisubband model）。此模型是利用 Green function 計算在多重耦合量子井中受激雜質能態與連續次能帶能態的共振耦合。利用多重耦合量子井在元件的設計上，其自由度更高於單一量子井！

其次,研究在外加電場、外加光學幫浦作用或應力作用下，各種奈米結構產生的物理現象。譬如摻雜雜質的種類、元素(B、N、等)、摻雜濃度等都會影響能帶間各種光學現象的產生，而新的兆赫波段光學現象則與副能帶間自由載子的傳輸、光電流的傳輸、副能帶間單載子生命期等息息相關。

關鍵詞：理論計算、奈米、單載子

Abstract

The binding energy and the density-of-states spectrum of resonant impurity states in quantum well structure have been theoretically studied with variation of the impurity position taken into account, using the multi-subband model and the resolvent operator technique. Calculations for the $2p_o$ resonant state have been performed. It has been found that there can be a considerable resonant coupling in the $2p_o$ state. A theoretical model, which is based on the effective mass theory and the variation method with group-theoretical consideration for acceptor levels in both strained and unstrained semiconductors, has been developed in this project as well.

二、目的

The study of electronic states of a hydrogenic impurity in a semiconductor quantum-well structure has been a subject of considerable interest for the last two decades. There have been numerous reports on calculations of the impurity states in such a system. However, most of the studies are restricted to calculation of the binding energies of the ground state or some low-lying excited states attached to the first subband. The calculation relies on the variational technique accompanied with a proper trial function. For the ground state, a good trial function should keep the calculation not too complicated and give the expectation energy of the state as low as possible. The trial function for the $2p_o$ state, which is cylindrically symmetric and has a node along the growth direction, has to be chosen with caution. State is orthogonal to the other localized impurity states and can be obtained simultaneously with the ground state in a matrix diagonalization.

三、研究報告內容

(A) Theory of resonant states of hydrogenic impurity in quantum wells

The effective-mass Hamiltonian for an electron bound to a donor in an QW structure can be written as

$$H = H_0 + V_c(\mathbf{r})$$

where H_0 is the impurity-free Hamiltonian and can be written as

$$H_0 = -\frac{\partial}{\partial z}\frac{1}{m_r(z)}\frac{\partial}{\partial z} - \nabla_{\parallel}^2 + V_0(z)$$

where V_c is the coulomb potential energy of the impurity, having the following expression

$$V_c(r) = -\frac{2}{\kappa(z)\sqrt{\rho^2 + (z - z_i)^2}}$$

The Hamiltonian is written in the dimensionless form in which the energy and the length are in units of effective Rydberg R^* ($R^* = m_0^* e^4 / 2\epsilon_0^2 \hbar^2$) and effective Bohr radius a^* ($a^* = \hbar^2 \epsilon_0 / m_0^* e^2$) of the well material , respectively. (m_0^* *and* ϵ_0 are the effective mass and the static dielectric constant , respectively, of the material making up the well)

The wavefunction of the resonant states as $\rho \to \infty$ can be written in a linear combination of solutions of the Schrodinger equation, which can be regarded to be impurity-free, that is,

$$\psi = \psi_B + \psi_X$$

where

$$\psi_B = e^{im\phi} \sum_{n \ge \nu} C_n \frac{e^{ik_{\parallel n}\rho}}{\sqrt{\rho}} f_n(z)$$

The total Hamiltonian can be written as

$$H = H_U^{(\nu)} + H_C^{(\nu)} + (1 - P_\nu) V_c (1 - P_\nu)$$

where

$$H_U^{(\nu)} = P_\nu (H_0 + V_c) P_\nu + H_0 (1 - P_\nu)$$

and

$$H_C^{(\nu)} = (1 - P_\nu) V_c P_\nu + P_\nu V_c (1 - P_\nu)$$

where $H_U^{(\nu)}$ is the Hamiltonian of the uncoupled system in which there is no inter-subspace coupling. The bound part is obtained by use of the variational method with the trial function in the following form

$$\psi_B^{(\nu m)} = e^{im\phi} \rho^{|m|} \sum_{n > \nu} \sum_l C_{nl} e^{-\alpha_l \rho^2} f_n(z) .$$

The resonant coupling between B_ν and X_ν can be treated with the technique of resolvent operators. Let $G^{(0)}$ and G be the resolvent operators for the uncoupled system
and the total system, have

$$G^{(0)} = (E - H_U^{(\nu)} + i0^+)^{-1}$$

and

$$G = (E - H + i0^+)^{-1}$$

related through the Dyson equation

$$G = G^{(0)} + G^{(0)} H_G^{(\nu)} G .$$

Finding the DOS spectrum of the impurity states as follows

$$n_B(E) = -\frac{1}{\pi} \mathrm{Im}[\langle \psi_B | G | \psi_B \rangle] \ ,$$

where

$$\langle \psi_B | G | \psi_B \rangle = [F(E) + i\Gamma(E)]^{-1}$$

With

$$F(E) = \pi \sum_{n<\nu} \sum_{k_\parallel} P \frac{\left| \langle \psi_B | V_c | \psi_{nk_\parallel} \rangle \right|^2}{E - E_{nk_\parallel}}$$

$$= E - E_I - \frac{1}{\pi} \sum_{n<\nu} P \int_{E_{n0}}^{\infty} \frac{\Gamma_n(E')}{E - E'} dE'$$

$$\Gamma(E) = \pi \sum_{n<\nu} \sum_{k_\parallel} \left| \langle \psi_B | V_c | \psi_B \rangle \right|^2 \delta(E - E_{nk_\parallel})$$

and

$$\Gamma_n(E) = \frac{A}{4} \left| \langle \psi_B | V_c | \psi_{n,k_\parallel = \sqrt{E - E_{n0}}} \rangle \right|^2 ,$$

here E_I is the energy of the impurity state in the absence of the resonant coupling. The resonant energy E_R of the impurity state is obtained by finding the peak position of the DOS spectrum.

In the presence of electric field, the bound impurity states are almost emptied through impact ionization. The free carriers are then accelerated toward the vicinity of the $2p_0$ impurity state, as illustrated in the inset of Fig. 1. The hot carrier near the $2p_0$ resonant state may have a large possibility to be captured into the impurity state due to the resonant coupling. As a result, a population inversion is achieved between the higher $2p_0$ state and the ground $1s$ state.

Fig. 1 shows the calculated binding energies of the $1s$ state and the $2p_0$ state of a shallow donor in $Al_{0.2}Ga_{0.8}As$/GaAs coupled wells separated by a 2-nm $Al_{0.2}Ga_{0.8}As$ arrier. It is found in Fig. 1 (a)

that the 1*s* state has a peak binding energy for the impurity in the left wider well. This is because there is a larger likelihood of finding the electron of the 1*s* state in the wider well, enhancing the Coulomb potential as the ionized donor stays in the wider well. Similarly, the $2p_0$ state has a peak binding energy for the impurity in the right narrower well. Fig. 2 shows the lifetime broadening and the energy shift of the resonant $2p_0$ state as results of the resonant scattering. The lifetime broadening reflects the strength of the resonant coupling or the capture rate of carriers into the impurity. It is found from Fig. 2 (a) that the capture lifetime can be as small as 94 fs. However, an improper design of the quantum wells and the impurity position can cause a small resonant coupling.

The resonance leads in general to a slight blue shift in energy. As the two wells have a small difference in their widths, the resonant state nevertheless becomes close to the first subband edge and a red shift of ~1 meV may result. Fig. 3(a) shows the intra-impurity transition energy from the $2p_0$ to the 1*s* states. It can serve as a useful guide to design the structure with a specific emission frequency. The design should be with a caution to prevent the difference between the $2p_0$ state and the first subband edge from being larger than the LO phonon energy. The high phonon emission rate will make it difficult to accelerate the electrons to the vicinity of the resonant state. Fig. 3 (b) gives a plot for such energy differences. As the figure shows, a 3-nm right well should be avoided in the device design.

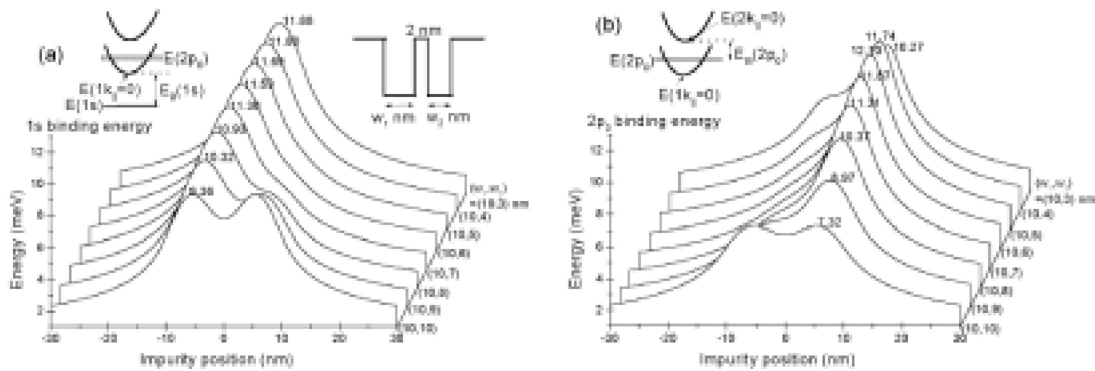

Fig. 1 The binding energies of (a) the 1*s* impurity state and (b) the $2p_0$ impurity state versus the impurity position with various widths of the coupled wells. The position origin is at the center of the 2 nm barrier.

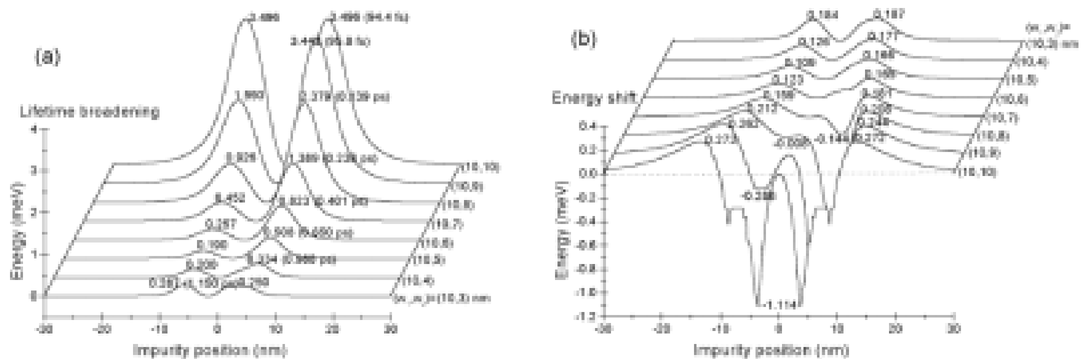

Fig. 2 (a) The lifetime broadening and (b) the energy shift of the $2p_0$ impurity state versus the impurity position with various widths of the coupled wells. The position origin is at the center of the 2 nm barrier.

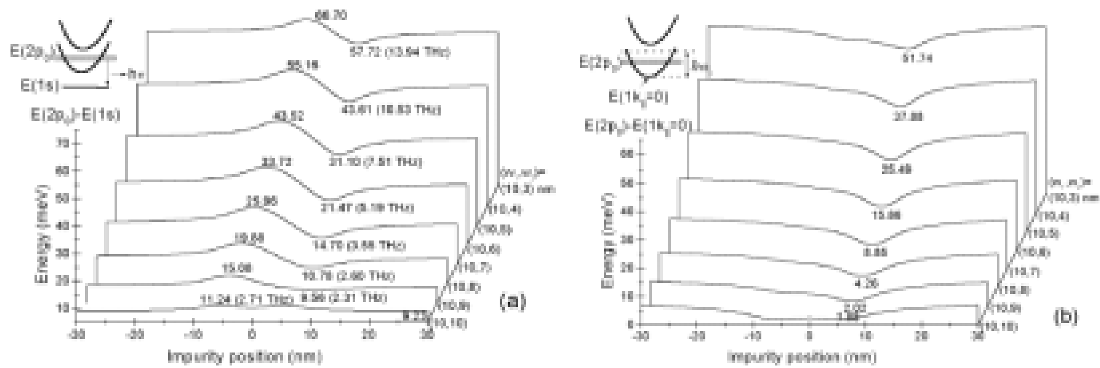

Fig. 3 (a) The intra-impurity transition energy and (b) the energy separation between the $2p_0$ state and the first subband edge versus the impurity position with various widths of the coupled wells. The position origin is at the center of the 2 nm barrier.

四、文獻

1. G. Bastard , Phys. Rev. B **24,** 4714 (1981).
2. C. Mailhiot, Y.-C. Chang, and T. C. McGill, Phys. B **26**,4449 (1982)
3. R. L. Greene and K. K. Bajaj, Sold State Commun. **45,** 825 (1983).
4. S. Chaudhuri, Phys. Rev. B **28**, 4480 (1983).
5. K. Tanaka, M. Nagaoka, and T. Yamabe, Phys. Rev. B **28**, 7068 (1983).
6. S. Chaudhuri and K. K. Bajaj, Phys. Rev. B **29**,1803 (1984).
7. R. L. Greene and K. K. Bajaj, Phys. Rev. B **31,** 913 (1985).
8. R. L. Greene and K. K. Bajaj, Phys. Rev. B **31,** 4006 (1985).
9. F. J. Betancur and I. D. Mikhailov, Phys. Rev. B **51** 4982 (1995).
10. J.-L. Zhu, Phys. Rev. B **40**, 10529 (1989).
11. J.-B. Xia, Phys. Rev. B **39,**5386 (1989).
12. C. Priester, G. Allan, and M. Lannoo, Phys. Rev. B **29,** 3408 (1984).
13. K.Jayakumar, S.Balasubramanian, and M. Tomak, Phys. Rev. B **34**, 8794 (1986).
14. S. Fraizzoli, F. Bassani, and R. Buczko, Phys. Rev. B **41,** 5096 (1990).
15. S. T. Yen, Phys. Rev. B, with referees.
16. T. A. Perry, R. Merlin, B. V. Shanabrook, and J. Comas, Phys. Rev. Lett. **54**, 2623, (1985).
17. F. Bassani, G. Ladonisi, and B. Preziosi, Rep. Prog. Phys. **37**,1099 (1974).
18. M. A. Odnoblyudov, I. N. Yassievich, M. S. Kagan, Yu. M. Galperin, and K. A. Chao, Phys. Rev. Lett.**83**, 644 (1999).