Optical Gain Using the Three Band Model Taking into Account the Excitonic Effect

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Excitonic effects of optical gain in quantum wells has been studied theoretically in a three band model. It is shown that within the ladder approximation of the electronhole Coulomb interaction, the Wannier type excitons cannot directly contribute to the optical gain in the two band model. Taking into account an additional localized state within the energy gap, the optical gain due to the population inversion between the localized state and one of the subband states can be observed and it is enhanced extremely by the excitonic effect in terms of the electron-hole interaction of the subband states. Since the enhanced optical gain is obtained without the population inversion of the subband states, this gain might realized an very low threshold excitonic enhancement laser diode.

Recently, laser emission in (ZnCd)Se/ZnSe quantum wells at blue-green wavelength was observed under the resonant optical pumping into the lowest exciton resonance¹. The energy of the emitted light is less than that of the exciton peak energy. There is the argument how excitons can contribute to the optical gain. In this paper, we consider a donorlike localized state besides the band edge subband states and evaluate the optical gain of quantum well structure, to make it clarify the function of the exciton in the optical gain. In this three band model, there is the appropriate carrier concentration that the optical gain at the higher energy than that of the localized state and the excitonic absorption are observed simultaneously. This simple model might be able to explain the above experimental observation. Furthermore, we found the direct excitonic enhancement of the optical gain for the adequate localized state density in this system.

Absorption coefficient/optical gain is expressed by the current-current correlation function, whose current is caused by the recombination of electronhole pairs. We here make use of the temperature Green's function formalism to describe the currentcurrent correlation function and adopted the three band model in two dimensional system, as shown in Fig. 1. The energy dispersions of the conduction and the valence subband in-plane of the heterojunction are assumed to be parabolic. There are two channels of the transition; one is between the



Fig. 1. Two channels of electron-hole interaction.

localized state and the valence subband state (1) and the other, between the conduction and valence subband states (2). The current-current correlation function is the sum of the current-current correlation function of the each transition, given by,

$$\Pi(i\omega) = \sum_{k,j} w_{k,j}^* \pi_j(k, i\omega), \qquad (1)$$

where $w_{k,1} = \langle \phi_c | \frac{eA}{mc} \cdot p | vk \rangle$ and $w_{k,2} = \langle ck | \frac{eA}{mc} \cdot p | vk \rangle$ are the optical transition matrix elements, respectively. ϕ_c is the localized state wavefunction. $\pi_j(k, i\omega)$ are related to the pair Green's functions and are obtained from the Bethe-Salpeter equations^{2,3}

$$\pi_j(k,i\omega) = w_{k,j}P_j^0(k,i\omega) + P_j^0(k,i\omega)$$

$$\times \sum_{k',j'} V_{k,k'}^{j,j'} \pi_{j'}(k',i\omega),$$
 (2)

with

$$P_1^0(k, i\omega) = \frac{1 - f_d(\varepsilon_d^e) - f_h(\varepsilon_h^h)}{i\omega - \varepsilon_d^e - \varepsilon_k^h},$$

$$P_2^0(k, i\omega) = \frac{1 - f_e(\varepsilon_k^e) - f_h(\varepsilon_k^h)}{i\omega - \varepsilon_k^e - \varepsilon_k^h},$$

where ε_d^e , ε_k^e and ε_k^h are the localized state, the conduction subband and the valence subband energies, respectively. f_d , f_e and f_h are the distribution functions of the localized electron, the conduction electron and the valence hole, respectively. $P_1^0(k,i\omega)$ and $P_2^0(k,i\omega)$ are the noninteracting localized electron-valence hole and conduction electronvalence hole pair Green's functions, respectively. The approximation of eq. (2) corresponds to the coupled ladder diagrams in the two channels. $V_{k,k}^{ij}$ are the electron-hole Coulomb interactions and $V_{k,k'}^{1,2}$ is evaluated as $\langle \phi_c | ck'' = 0 \rangle V_{k,k'}^{2,2}$, where $\langle \phi_c | ck'' =$ 0 is the overlap integral between the localized state and the conduction subband state. Here, the conduction subband state at Γ point is remained since it is dominant in the linear combination of $|ck\rangle$, which describes the localized state $|\phi_c\rangle$. Note that the optical transition matrix element $w_{k,1}$ can be evaluated as $\langle \phi_c | ck'' = 0 \rangle w_{k,2}$ as well. To proceed the calculation analytically for a qualitative discussion, the wave number dependencies of $V_{k,k'}^{ij}$ and $w_{k,j}$ are ignored. Then, the current-current correlation function can be expressed explicitly as,

$$\Pi(i\omega) = |w_2|^2 \frac{\alpha P_1 + 2\alpha \Re(V^{2,2}) P_1 P_2 + P_2}{1 - \alpha |V^{2,2}|^2 P_1 P_2}, (3)$$

with

$$P_j(i\omega) = \frac{\sum_k P_j^0(k, i\omega)}{1 - V^{j,j} \sum_k P_j^0(k, i\omega)}, \qquad (4)$$

where $\alpha = |\langle \phi_c | ck = 0 \rangle|^2$ is the square of the overlap integral, which is proportional to the density of the localized state. According to the recipe of the temperature Green's function, the optical spectrum $I(\omega)$ is given by the imaginary part of the current-current correlation function $\Pi(\omega + i\delta)$. P_j are the pair Green's functions in the absence of the coupling $V^{1,2}$. In the two band model, where the conduction subband and the valence subband are considered, the optical spectrum is proportional to the P_{2i} , given by

$$P_{jr} + iP_{ji} = P_j(\omega + i\delta), (j = 1, 2).$$

In general, the Wannier type electron-hole bound state in doped systems, so called 'Mahan exciton⁴', is obtained from the pole of P_2 . However, there is no pole at $\omega < E_g$ when the occupation factor $1 - f_e(\varepsilon_k^e) - f_h(\varepsilon_k^h)$ is negative. The condition of $1 - f_e(\varepsilon_k^e) - f_h(\varepsilon_k^h) < 0$ exactly corresponds to the yield of the optical gain in the single particle picture. Thus, the electron-hole pair of the exciton cannot contribute to the optical gain directly in the two band model and it has nothing to do with the strength of the electron-hole Coulomb interaction.

On the other hand, in the three band model. where the two channels are coupled through the $V^{1,2}$, there is an appropriate carrier concentration such that the population inversion occurs only between the localized and the valence subband states. In such a case, the optical gain can be observed from the channel (1) transition $(P_{1i} > 0)$ and the excitons at the subband states can be constructed $(P_{2i} < 0)$ simultaneously. From eq. (3), it can be shown that the excitonic effect of the channel (2) excitons can enhance the oscillator strength of the channel (1) transition. It may cause the extremely enhanced optical gain at the exciton peak energy E_x when the optical gain spectrum in terms of the channel (1) transition becomes broad to E_x , that is, at least the total chemical potential satisfied with $E_x < \mu_e + \mu_h < 0.$

Figure 2 shows the optical gain spectra calculated from eq. (3) for the various α , which is proportional to the density of the localized state N_t , defined as $N_t = \frac{\alpha}{8\pi a_b^2}$ in the two dimensional system. a_b is the Bohr radius. α is closely related to $V^{1,2}$ and the optical transition matrix element of the channel (1), as well. The physical constants used here are indicated in Table 1. The Coulomb interaction $V^{2,2}$ is measured by $\frac{2\pi e^2}{\epsilon_0 q_s}$, where q_s is the screening parameter. The dash lines show the gain spectra P_{1i} by the channel (1) transition. The carrier concentration is chosen for the only channel (1) transition to yield the optical gain. Both for the low and high temperature cases, the excitonic peak in terms of the channel (2) transition changes from the absorption to the optical gain as α is increased.

Table 1. Physical constants for the calculation.

m_e	m_h	$V^{1,1}$	$V^{2,2}$	$E_g(eV)$	index
0.15	0.15	1.0	1.0	2.7	2.7



Fig. 2. Optical spectra as function of the localized states density.

When N_t is low, the optical gain of the channel (1) and the excitonic absorption of channel (2) are observed simultaneously and this gain spectrum is consistent with the experimental result of the laser emission by the optical pumping. In order to realize the excitonic optical gain, stronger coupling between the two channels or higher localized density is necessary. Note that for higher temperature case, the optical phonon scattering with the excitons are not include, so the excitonic enhancement might be overestimated in this calculation.

In summary, we have studied the role of the excitonic effects in the optical gain. Within the ladder approximation of the electron-hole interaction, the excitons cannot directly contribute to the optical gain in the two band model. Thus, the analysis of the optical gain, assuming the existence of exciton line for doped materials from the beginning, may not the correct treatment. Even if the excitonexciton interaction or exciton-free electron interaction is considered, the population inversion seems to be necessary to obtain the optical gain in the two band model according to the Ref. 2. To investigate the excitonic enhancement of the optical gain, an additional localized state is considered. When total chemical potential lie below the energy gap and within the exciton binding energy, the sharp and huge enhanced optical gain at the band edge exciton transition is obtained. This optical gain might realize a very low threshold laser diode.

References

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