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Resonant Auger recombination in HgTe/CdHgTe quantum wells for mid infrared lasers

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Theoretical estimations are made for the resonant behavior of Auger recombination processes in heterostructures with Hg(Cd)Te/CdHgTe quantum wells designed for middle infrared range. Detailed calculations of the localized and delocalized (above-barrier) hole states are carried out in Hg(Cd)Te/CdHgTe quantum wells. The most probable mechanism of the resonant Auger recombination is established. Optimized structure designs are suggested to suppress the resonant non-radiative recombination processes.

Keywords: Auger recombination, Mercury–Cadmium–Telluride, quantum well, middle infrared, semiconductor laser.

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The development of interband semiconductor lasers of the mid-infrared range, which are formed on the basis of narrow-band heterostructures with quantum wells (QWs) and emit at wavelengths of $3-8\,\mu$m, is important for practical applications in gas spectroscopy, environmental monitoring, and security [1]. It is common knowledge that the lasing thresholds in such long-wavelength lasers are almost always set by non-radiative Auger recombination [2]. Various scenarios of Auger processes, some of which are shown schematically in Fig. 1, may be implemented in this case. First of all, these are „classical“ *eeh*-type processes, where the energy of interband recombination is carried away by an electron that passes into higher-energy states in the same subband of size quantization ($1'$ in Fig. 1). Such processes have a certain energy threshold and, consequently, may be suppressed partially at moderate temperatures. However, competing Auger processes, where a third („heated“) particle passes into another subband of size quantization or into the continuum states of barrier layers, are also feasible (*ehh* in Fig. 1). Depending on the energy gaps between different subbands in a QW and the magnitudes of the band discontinuities at the heterointerfaces, such processes may become thresholdless (resonant) and play a critical part in the interband dynamics of nonequilibrium carriers [3].

We have already investigated [4] the temperature dependence of the integrated intensity of spontaneous emission of Hg(Cd)Te/CdHgTe QWs emitting at wavelengths of $3.5-4.5\,\mu$m and observed indirectly a resonance peak in the non-radiative recombination rate in scanning through temperature within the range of $T = 10-300$ K. Preliminary calculations of the band structure of the studied QWs revealed that this resonance corresponds qualitatively to a match between the band gap width in QWs (the energy of radiative transitions) and the ionization energy of the ground hole state in QWs. As a result, the experi-

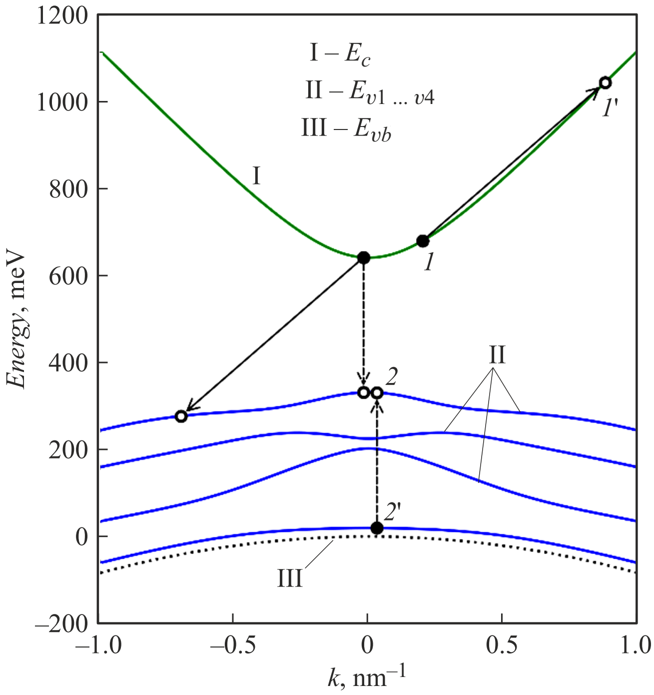

Figure 1. Positioning of energy bands for an $Hg_{0.89}Cd_{0.11}Te/Cd_{0.85}Hg_{0.15}Te$ QW with width $d_{QW} = 3.5$ nm. The ground electron subband (E_c) and several hole subbands ($E_{v1...v4}$) are shown. The energy is measured from the top of the valence band of barriers E_{vb}. Solid and dashed arrows represent transitions corresponding to the classical *eeh*-type (threshold) Auger recombination and the resonant (thresholdless) *ehh* recombination, respectively. The band energies were calculated in accordance with the procedure detailed in the present study.

mentally observed features of the luminescent response were associated with *ehh*-type Auger processes. At the same time, it remained unclear which hole states (*2′* in Fig. 1) enable such resonant processes: these may be either high-lying localized states in QWs or above-barrier states (resonant or free). In the present study, we perform a detailed calculation of the energies and structure of hole states in Hg(Cd)Te/CdHgTe QWs with the same parameters as in [4]. Note that microscopic calculations of the probabilities of various Auger processes, which are needed for a quantitative analysis of interband dynamics, are beyond the scope of this work. At the same time, qualitative data reveal specific implementations of resonant Auger processes and allow one to outline the ways to optimize QW designs for their suppression and, consequently, achieve the highest possible lasing temperature.

The energies and wave functions of electron states in a QW were calculated using the envelope function method in the Burt–Foreman approximation [5,6] with the 8×8 Kane Hamiltonian [7]. The wave functions of particles were represented as an expansion over a set of periodic basis functions $u_n(\mathbf{r})$ with envelope coefficients $F_n(\mathbf{r})$ depending smoothly on coordinates:

$$\psi(\mathbf{r}) = \sum_n F_n(\mathbf{r}) u_n(\mathbf{r}).$$

The steady-state Schrödinger equation then takes the following form:

$$\hat{\mathbf{H}}\mathbf{F}(\mathbf{r}) = E\mathbf{F}(\mathbf{r}), \tag{1}$$

where Hamiltonian $\hat{\mathbf{H}}$ is a matrix of operators acting on the envelopes. The structures (described in detail in [4]) grown on (013) GaAs substrates were characterized with a corrected Hamiltonian [8] obtained by rotating the coordinate system in accordance with [9]. The calculation model included built-in strain, assuming a fully strained structure that inherits the lattice parameter of the CdTe buffer layer (with a lattice cell size of 6.48 Å). Owing to translational invariance in the QW plane, the projection of quasi-momentum $\mathbf{k}_\parallel$ onto this plane is preserved, which allows one to separate variables and reduce the form of envelope functions $\mathbf{F}(\mathbf{r})$ and Eq. (1) to the following:

$$\mathbf{F}(\mathbf{r}) = e^{i\mathbf{k}_\parallel \mathbf{r}_\parallel}\mathbf{f}(z),$$

$$\hat{\mathbf{H}}(\mathbf{k}_\parallel)\mathbf{f}(z) = E\mathbf{f}(z), \tag{2}$$

where axis z is the direction of QW growth. To calculate localized states in QWs, we consider a virtual superlattice consisting of such QWs separated by sufficiently wide barriers (excluding tunneling between adjacent wells). The unknown part of envelope functions $\mathbf{f}(z)$ is expanded into a Fourier series, and Eq. (2) is reduced to the eigenvalue problem of the Hamiltonian matrix

$$\mathbf{f}(z) = \sum_k \mathbf{c}_k e^{ikz},$$

$$\sum_{k'} \langle e^{i\mathbf{k}_\parallel \mathbf{r}_\parallel + ikz} | \hat{\mathbf{H}} | e^{i\mathbf{k}_\parallel \mathbf{r}_\parallel + ik'z} \rangle \mathbf{c}_{k'} = E\mathbf{c}_k.$$

The following expressions for the dependences of band gap width E_g and shift E_v of the valence band of ternary solution $Cd_xHg_{1-x}Te$ (relative to pure HgTe) on the composition and temperature were used in calculations [10,11]:

$$E_g(x, T)[\text{meV}] = -303(1-x) + 1606x - 132x(1-x)$$
$$+ \frac{\big(0.63(1-x) - 0.325x - 0.592x(1-x)\big)T^2}{11(1-x) + 78.7x + T},$$
$$E_v(x, T)[\text{meV}] = (0.4T - 570)x.$$

The values of other parameters of the Hamiltonian were taken from [7], and the elastic moduli were taken from [8]. We assume that these values are interpolated linearly between HgTe and CdTe and do not change with temperature.

The scattering matrix method [12,13] was used to calculate delocalized states in the energy region below the valence band top of the barriers. With this aim in view, the heterostructure was divided into segments along the z axis, and all linearly independent particular solutions of Eq. (2) were calculated at each segment. The overall wave function was obtained by stitching together linear combinations of these solutions at the boundaries of segments based on the continuity of envelopes and the flow of probability. In the valence band, we obtain four linearly independent solutions corresponding to different types of holes (light or heavy) and directions of their motion (along and opposite the z axis); each of these solutions is also doubly degenerate in spin. Correct sorting of particular solutions with separation into waves propagating in directions $z+$ and $z-$ ensures the stability of this method.

Applying the two approaches discussed above, we may calculate the energies and wave functions of any carrier states (both localized and delocalized) in a heterostructure with QWs. Let us first consider the above-barrier states of holes. The results of calculations of the probability density as a function of growth coordinate z for different values of particle energy are shown in Fig. 2. Since a symmetric QW is being examined, symmetric and antisymmetric states, wherein two holes move towards each other in phase or out of phase, are of our main interest; accordingly, these are the solutions that may yield resonant states near the well. It is evident that the probability of hole localization inside a QW is lower than outside of it for states near the top of the valence band of barriers (the effect of above-barrier reflection is observed). This is the reason why the wave functions of above-barrier states are unlikely to have a significant overlap integral with localized states in a QW; therefore, the resonant behavior of the Auger recombination coefficient observed in the experiment is hardly attributable to the ejection of holes directly into the continuum of barrier layers. Note also that according to the results of calculations, resonant above-barrier states (largely localized in a QW) in the examined energy region exist only for light holes, but they are also positioned approximately 200 meV away from the top of the valence band and, consequently, may be neglected.

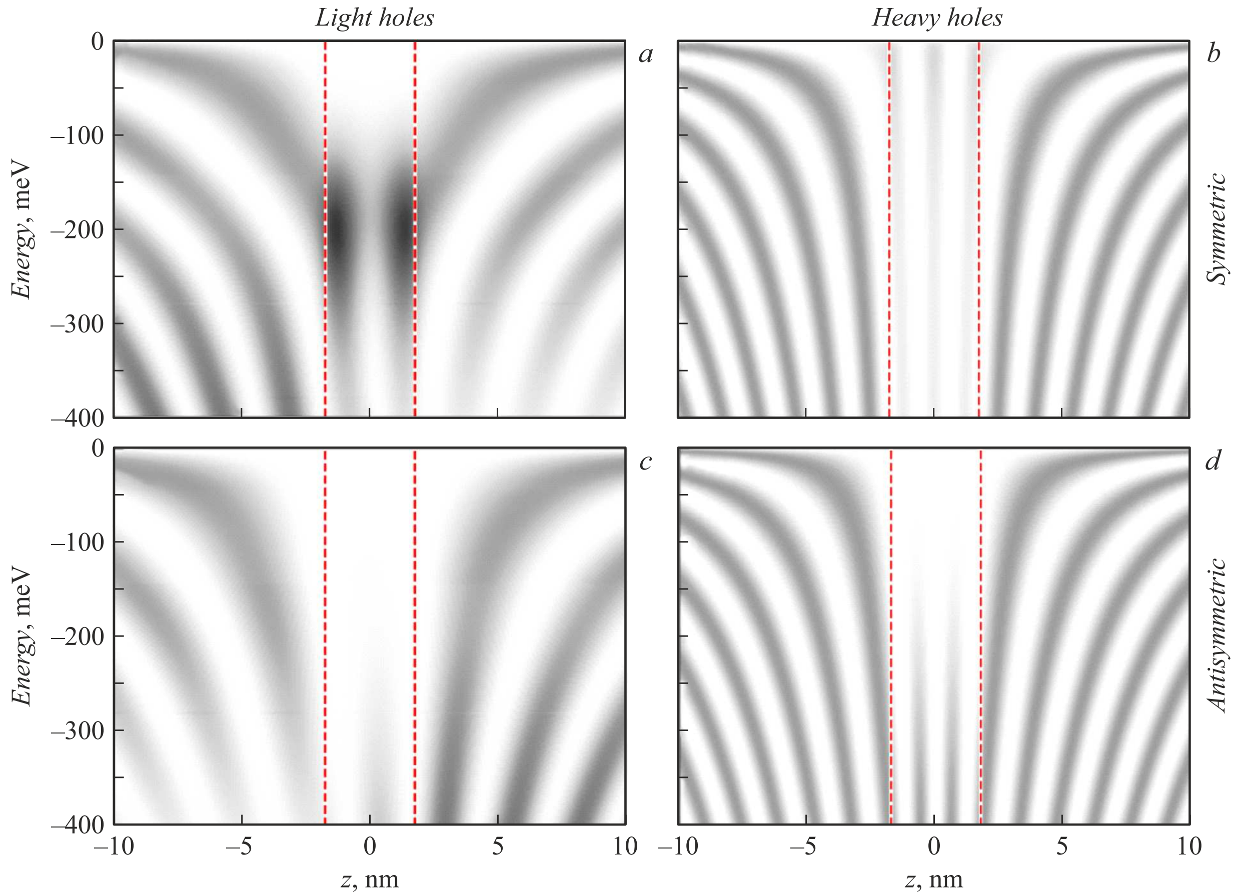

Figure 2. Probability density distribution for above-barrier hole states in the valence band continuum of heterostructures with $Hg_{0.89}Cd_{0.11}Te/Cd_{0.85}Hg_{0.15}Te$ QWs (QW width $d_{QW} = 3.5$ nm). The profiles for even (*symmetric*) (*a* and *b*) and odd (*antisymmetric*) (*c* and *d*) states of light (*a*, *c*) and heavy (*b*, *d*) holes are presented. Calculations were performed for temperature $T = 125$ K. The energy is measured from the top of the valence band of barriers; vertical dashed lines correspond to the boundaries of a QW (centered at $z = 0$).

Let us turn to localized states in a QW. Figure 3 presents the calculated energies of localized states of electrons (E_c) and holes (E_{v1}, E_{v2}, E_{v3}, E_{v4}) in a QW as functions of temperature. The temperature dependence of the probability density of finding a hole in the above-barrier QW region, which allows one to determine the energy of the resonant state, is also shown for comparison. Assuming that the interband recombination (both radiative and non-radiative) involves electrons and holes located at the edges of the corresponding bands (the recombination energy is approximately equal to $E_g \equiv E_{c1} - E_{v1}$), one may estimate the energy $(E_{v1} - E_g)$ of the final state of a second hole in *ehh* Auger recombination; this quantity is represented by the dash-and-dot line in Fig. 3. It can be seen that the distance between the ground (E_{v1}) and excited (E_{v4}) subbands of size quantization is approximately the same as E_g at $T \sim 120{-}130$ K (i.e., at temperatures close to the maximum of the experimentally measured dependence of Auger coefficient $C_A^{eff}(T)$ in Fig. 3). This is the reason why the resonance in $C_A(T)$ is logically associated with the contribution of *ehh* Auger processes, wherein a second hole passes from the ground state in a QW to the upper excited state with an energy close to the energy of the valence band top of barrier layers. In fact, the energy of recombination of an electron and a hole exceeds the band gap width due to the presence of a finite non-zero thermal energy of particles. This provides an explanation for the fact that resonant Auger recombination in the experiment is „activated" at temperatures somewhat lower than those derived from calculated data.

The obtained results suggest an approach to suppressing this type of resonant Auger processes: apparently, this may be done by „ejecting" the „resonant" excited subband into the continuous spectrum region with a reduction in QW width (while preserving the energy of radiative transitions through a reduction in cadmium content x_{Cd}^{QW} in a QW). Specifically, the E_{v4} level becomes delocalized in transition from a QW with width $d_{QW} = 3.5$ nm and $x_{Cd}^{QW} \sim 8{-}10\,\%$ to a QW with width $d_{QW} = 3$ nm and $x_{Cd}^{QW} \sim 5{-}7\,\%$, but this does not lead to the emergence of a resonant state of heavy holes near the barrier, and the probability density distribution remains qualitatively similar to that shown in Fig. 2. Such detuning of the energies of intersubband hole transitions (between the ground and

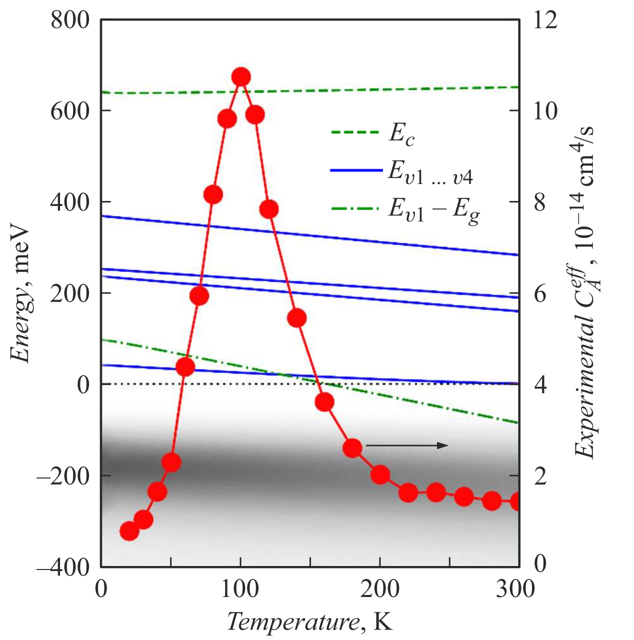

Figure 3. Energies of electron and hole states in the studied QWs calculated as a function of temperature (lines) and experimental temperature dependence of effective Auger recombination coefficient C_A^{eff} from [4] (symbols). In the lower part, the probability density integral over the QW for holes in the above-barrier energy region is shown in grayscale.

excited subbands of size quantization) from the energy of interband recombination may improve significantly the performance of HgCdTe lasers operating in the mid-infrared range.

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Conflict of interest

The authors declare that they have no conflict of interest.

References

[1] Z. Du, S. Zhang, J. Li, N. Gao, K. Tong, Appl. Sci., **9**, 338 (2019). DOI: 10.3390/app9020338
[2] J.R. Meyer, C.L. Canedy, M. Kim, C.S. Kim, C.D. Merritt, W.W. Bewley, I. Vurgaftman, IEEE J. Quantum Electron., **57** (5), 2500110 (2021). DOI: 10.1109/JQE.2021.3096219
[3] T.D. Eales, I.P. Marko, B.A. Ikyo, A.R. Adams, S. Arafin, S. Sprengel, M.-C. Amann, S.J. Sweeney, IEEE J. Select. Top. Quantum Electron., **23** (6), 1500909 (2017). DOI: 10.1109/JSTQE.2017.2687823
[4] K.E. Kudryavtsev, A.A. Yantser, M.A. Fadeev, V.V. Rumyantsev, A.A. Dubinov, V.Ya. Aleshkin, N.N. Mikhailov, S.A. Dvoretsky, V.I. Gavrilenko, S.V. Morozov, Appl. Phys. Lett., **123**, 182102 (2023). DOI: 10.1063/5.0177912
[5] M.G. Burt, J. Phys.: Condens. Matter, **4**, 6651 (1992). DOI: 10.1088/0953-8984/4/32/003
[6] B.A. Foreman, Phys. Rev. B, **48**, 4964 (1993). DOI: 10.1103/PhysRevB.48.4964
[7] E.G. Novik, A. Pfeuffer-Jeschke, T. Jungwirth, V. Latussek, C.R. Becker, G. Landwehr, H. Buhmann, L.W. Molenkamp, Phys. Rev. B, **72**, 035321 (2005). DOI: 10.1103/PhysRevB.72.035321
[8] M. Zholudev, F. Teppe, M. Orlita, C. Consejo, J. Torres, N. Dyakonova, M. Czapkiewicz, J. Wróbel, G. Grabecki, N. Mikhailov, S. Dvoretskii, A. Ikonnikov, K. Spirin, V. Aleshkin, V. Gavrilenko, W. Knap, Phys. Rev. B, **86**, 205420 (2012). DOI: 10.1103/PhysRevB.86.205420
[9] J. Los, A. Fasolino, A. Catellani, Phys. Rev. B, **53**, 4630 (1996). DOI: 10.1103/PhysRevB.53.4630
[10] J.P. Laurenti, J. Camassel, A. Bouhemadou, B. Toulouse, R. Legros, A. Lusson, J. Appl. Phys., **67**, 6454 (1990). DOI: 10.1063/1.345119
[11] C.R. Becker, V. Latussek, A. Pfeuffer-Jeschke, G. Landwehr, L.W. Molenkamp, Phys. Rev. B, **62**, 10353 (2000). DOI: 10.1103/PhysRevB.62.10353
[12] D.Y.K. Ko, J.C. Inkson, Phys. Rev. B, **38**, 9945 (1988). DOI: 10.1103/PhysRevB.38.9945
[13] M.S. Zholudev, O.M. Litovchenko, S.V. Morozov, Semicond. Sci. Technol., **40**, 035001 (2025). DOI: 10.1088/1361-6641/ada9cc

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