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ON THE THEORY OF INTERBAND TWO-PHOTON ABSORPTION OF LIGHT IN SEMICONDUCTORS. ACCOUNTING ADMIXTURES TO THE STATES OF THE CONDUCTION BAND AND VALENCE STATES, THE RABI EFFECT

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We present a theoretical study of interband two-photon (two-quantum) absorption of polarized light in semiconductors of cubic and tetrahedral symmetry. Our analysis is conducted within a multiband approximation, taking into account the admixture of valence states in the conduction-band states, as well as coherent saturation (Rabi) effects. We use simplified parabolic dispersion laws for both heavy- and light-hole subbands and for the conduction band, and compare two common temperature-dependent band-gap formulas (Varshni and Passler) to illustrate how they alter the spectral–temperature dependence of the total two-photon absorption coefficient. In particular, we show that the interband two-photon absorption first increases with photon frequency, reaches a maximum, and then decreases at a fixed temperature. The amplitude of the absorption for linearly polarized light is found to be larger than that for circularly polarized light, especially at lower temperatures. Our calculations reveal that the admixture of valence states significantly modifies the interband transitions, while the Rabi effect reduces the absorption in the high-intensity regime, especially at elevated temperatures. These findings may be useful for designing optoelectronic and photonic devices that rely on multiphoton interactions in narrow-gap semiconductors.
Keywords: *Two-photon absorption; Rabi effect; Valence–conduction band mixing; Multiband approximation; Kane model; Temperature-dependent band gap; Varshni and Passler formulas; InSb and InAs semiconductors; Nonlinear optics*
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INTRODUCTION

In this paper, we analyze interband two-photon absorption in semiconductors of cubic and tetrahedral symmetry by employing a multiband $\boldsymbol{k}\cdot\boldsymbol{p}$ Kane-type Hamiltonian. Specifically, we consider the conduction band (Γ_6) and the valence bands ((Γ_8) heavy- and light-hole subbands, plus (Γ_7) for spin-orbit split-off). The complete 8×8 Kane model can, in principle, provide non-parabolic dispersion relations for electrons and holes. However, in the moderate energy range relevant to our two-photon absorption processes ($\hbar\omega \lesssim 0.8\,E_g$), higher-order k^4 terms make only small corrections.

Therefore, for simplicity and analytic tractability, we adopt the following parabolic dispersions:

$$E_c(\boldsymbol{k}) = E_g + \frac{\hbar^2 k^2}{2m_c},\ E_L(\boldsymbol{k}) = -\frac{\hbar^2 k^2}{2m_L},$$

where m_c and m_L are effective masses for electrons and holes, respectively. This approximation still incorporates conduction–valence admixture via Kane's matrix elements (including Δ_{SO}), but neglects higher-order nonparabolic terms beyond k^2. Extensive prior studies [see, for instance, Refs. 24–26] confirm that, under these conditions, the simpler parabolic form captures the essential physics of two-photon absorption in InSb and InAs.

The Hamiltonian thus includes admixture between Γ_6, Γ_8, and Γ_7 states, ensuring that valence-band mixing effects are accounted for. The spin-orbit interaction enters via the splitting Δ_{SO}, which modifies the band-coupling strengths and appears explicitly in our transition-matrix elements. In Section 3, we derive the two-photon absorption coefficients $K^{(2)}_{c,m;L,m'}$ under this model and discuss how the Rabi effect further alters the absorption in both low- and high-temperature regimes.

The discovery of powerful quantum generators of coherent laser electromagnetic waves stimulated the development of studies of optical phenomena in semiconductors that are nonlinear in illumination intensity [1-3]. In this aspect, it seems necessary to study the nonlinear optical parameters of both narrow- and wide-bandgap semiconductors. It is associated with the unusualness and complexity of the properties of the effect under consideration, the possibility of obtaining new information about the band parameters of the samples under study, and the prospect of application in optoelectronics and photonics.

Two-photon nonlinear optical phenomena caused by intraband transitions in semiconductors were carried out [1-3], where the calculation of two-photon matrix elements was carried out using perturbation theory for the field of an unpolarized electromagnetic wave in the two-band approximation [2, 3]. In [4-7], two- and three-photon linear-circular dichroism (LCD) were studied, and in [8-23], multiphoton intraband absorption of light of linear and circular polarization in semiconductors with a complex band structure was investigated. In [18], nonlinear single-photon absorption of polarized radiation in topological insulators was investigated.

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In the above-mentioned works, the nonlinearity of the coefficient of single-photon absorption of light is described by the effect of coherent saturation (Rabi) [19] and it is determined both in intra-band [18] and interband [9, 10, 16, 17] optical transitions by the photoinduced addition to the distribution function of electrons, as well as light and heavy holes.

However, in the above-mentioned works, calculations were made of the spectral-polarization dependences of the intraband two-photon, i.e. two-quantum absorption of light (TQAL) and its LCD in semiconductors of tetrahedral symmetry. in Kane's three-zone model [24, 25] , but not taken into account mixing of valence band states with conduction band states. This paper is devoted to filling this gap.

SPECTRAL-TEMPERATURE DEPENDENCES OF THE COEFFICIENT OF INTERBAND TWO-QUANTUM ABSORPTION OF LIGHT

Note that the coefficient of two-photon (quantum) absorption of light for optical transitions from the valence band to the conduction band is determined by the expression [23]

$$K^{(2)} = \sum_{\vec{k},c,\,m=\pm1/2;L_l m'} K^{(2)}_{c,m;L,m'} = \sum_{\vec{k},c,\,m=\pm1/2;lh,m'=\pm1/2} K^{(2)}_{c,m;lh,m'} + \sum_{\vec{k},c,\,m=\pm1/2;lh,m'=\pm3/2} K^{(2)}_{c,m;hh,m'}. \quad (1)$$

Here

$$\sum_{\vec{k},c,\,m=\pm1/2;L,m'} K^{(2)}_{c,m;L,m'} = \frac{2\pi}{\hbar}\frac{2\hbar\omega}{I}\sum_{\vec{k},c,\,m=\pm1/2;L,m'}\left(f^{(2)}_{c\vec{k}} - f^{(2)}_{L,\vec{k}}\right)\left|M^{(2)}_{c,m;L,m'}(\vec{k})\right|^2 \delta\left(E_{c\vec{k}} - E_{L,\vec{k}} - 2\hbar\omega\right) \quad (2)$$

$(L, m' = lh, m' = \pm1/2 (hh, m' = \pm3/2)$-for heavy (light) holes) , where their energy spectrum has the form $E_{L,\vec{k}} = -\frac{\hbar^2 k^2}{(2m_L)}$, and the energy spectrum of electrons in the conduction band: $E_{c,\vec{k}} = E_g + \frac{\hbar^2 k^2}{(2m_c)}$.

If we take into account that the composite matrix of the two-quantum interband optical transition $M^{(2)}_{L,\vec{k};SO,\vec{k}}$in expression (2) depends on the inclusion of valence states Γ8 (valence band) and Γ7 (spin-orbit splitting band) in the states Γ6 (conduction band), then we have the following expression

$$M^{(2)}_{lh,\vec{k};c,\vec{k}} = \frac{1}{3}\left(\frac{eA_0}{c\hbar}\right)^4 \frac{\left|p^*_{c,V}\right|^2\hbar^2k^2}{(\hbar\omega)^2}\left[\left(1-\frac{4}{3}\zeta_g\right)^2 e_z'^4 - \left(\frac{\hbar\omega\zeta_g}{E_{hh}-E_{lh}-\hbar\omega}\right)^2 |e'_\perp|^4\right], \quad (3)$$

$$M^{(2)}_{hh,\vec{k};c,\vec{k}} = 3\left(\frac{eA_0}{c\hbar}\right)^4 \frac{\left|p^*_{c,V}\right|^2\hbar^2k^2}{(\hbar\omega)^2}\left(1+\frac{2}{3}\frac{\hbar\omega\zeta_g}{E_{lh}-E_{hh}-\hbar\omega}\right)^2 e_z'^2 e'^2_\perp, \quad (4)$$

then the coefficient of two-quantum absorption of light caused by optical transitions from the subband of light holes to the conduction band is expressed as:

$$\sum_{\vec{k},c,\,m=\pm1/2;lh,m'=\pm1/2} K^{(2)}_{c,m;lh,m'} = \frac{2}{3}C_I\left(f^{(2)}_{c,k^{(\omega)}_{c,L}} - f^{(2)}_{lh,k^{(\omega)}_{c,L}}\right)\frac{\left|p_{c,V}\right|^2\left(k^{(\omega)}_{c,L}\right)^3}{(\hbar\omega)^5}\mu_+^{(c,lh)}\left[\left(1-\frac{4}{3}\zeta_g\right)^2 e_z'^4 - \left(\frac{\hbar\omega\zeta_g}{E_{hh}-E_{lh}-\hbar\omega}\right)^2 |e'_\perp|^4\right], \quad (5)$$

and for optical transitions from the heavy hole subband to the conduction band:

$$\sum_{\vec{k},c,\,m=\pm1/2;lh,m'=\pm3/2} K^{(2)}_{c,m;hh,m'} = 6C_I\left(f^{(2)}_{c,k^{(\omega)}_{c,hh}} - f^{(2)}_{lh,k^{(\omega)}_{c,hh}}\right)\frac{\left|p_{c,V}\right|^2\left(k^{(\omega)}_{c,hh}\right)^3}{(\hbar\omega)^5}\mu_+^{(c,hh)}\left(1+\frac{2}{3}\frac{\hbar\omega\zeta_g}{E_{lh}-E_{hh}-\hbar\omega}\right)^2, \quad (6)$$

Where $C_I = \frac{1}{\pi\hbar^3}\left(\frac{2\pi e^2}{\hbar n_\omega c}\right)^2 I\left(\frac{\hbar^2}{m_0}\right)^2$, $k^{(\omega)}_{c,L} = \sqrt{\frac{2\mu_+^{(c,L)}}{\hbar^2}\left(2\hbar\omega - E_g\right)}, L, m' = lh, m' = \pm1/2$ $(hh, m' = \pm3/2)$- for heavy (light) holes and took into account that $\left(\frac{eA_0}{c\hbar}\right)^2 = \frac{2\pi e^2}{n_\omega c}\frac{I}{(\hbar\omega)^2}$, $I(\omega)$is the intensity (frequency) of light, $n_\omega$is the refractive index of light at frequency ω,$p_{c,V} = \left(\frac{3Bm_0^2E_g}{\hbar^2}\right)^{1/2}$ is the Kane parameter, $B = \frac{\hbar^2(m_{hh}-m_{lh})}{(4m_{hh}m_{lh})}$, $m_{hh}(m_{lh})$is the effective mass of light (heavy) holes .

Note that if we take into account the contribution of the coherent saturation effect to $K^{(2)}_{c,m;L,m'}$, then it is necessary to replace in expression (2) $\left|M^{(2)}_{c,m;L,m'}(\vec{k})\right|^2$ with $\sum_{nn'\vec{k}}\left|M^{(N=2)}_{n\vec{k},n'\vec{k}}\right|^2\sum_{nn'\vec{k}}\left[1+\frac{\alpha_\omega}{\hbar^2\omega^2}\left|M^{(N=2)}_{n\vec{k},n'\vec{k}}\right|\right]^{-1/2}$. Then the square of the composite matrix element caused by two-photon optical transitions from the light hole subband to the conduction band consists of two terms, which are determined by the relations:

$$\frac{\alpha_\omega}{\hbar^2\omega^2}\left|M^{(2)}_{lh,\vec{k};c\vec{k}}\right|^2 = \xi^{(2)}\frac{|p^*_{c,V}|^2k^2}{m_0\Delta_{SO}k_\Delta^2\left(\frac{\hbar\omega}{\Delta_{SO}}\right)^6}\left[\left(1-\frac{4}{3}\zeta_g\right)^2 e_z'^4 - \left(\frac{\hbar\omega\zeta_g}{E_{hh}-E_{lh}-\hbar\omega}\right)^2|e_\perp'|^4\right]. \quad (7)$$

$$\frac{\alpha_\omega}{\hbar^2\omega^2}\left|M^{(2)}_{lh,\vec{k};c\vec{k}}\right|^2 = 3\xi^{(2)}\frac{|p^*_{c,V}|^2k^2}{m_0\Delta_{SO}k_\Delta^2\left(\frac{\hbar\omega}{\Delta_{SO}}\right)^6}\left(1+\frac{2}{3}\frac{\hbar\omega\zeta_g}{E_{lh}-E_{hh}-\hbar\omega}\right)^2 e_z'^2e_\perp'^2. \quad (8)$$

Here $k_\Delta^2=\frac{2m_0}{\hbar^2}\Delta_{SO}$, $\xi^{(2)}=2T_c^{(1)}T_{lh}^{(1)}\left(\frac{2\pi e^2}{n_\omega c\hbar}\right)^2\frac{\hbar^4k_\Delta^2}{m_0\Delta_{SO}^5}I^2$, $T_c^{(1)}\left(T_{lh}^{(1)}\right)$is the time of exit from the final state of photoexcited electrons in the conduction band (light holes in the valence band).

Results of calculation of spectral and temperature dependence of the resulting absorption coefficient $K^{(2)}_{c,m;L,m'}$ of linear (line 1) and circular (line 2) polarization light produced according to (1) and (2) taking into account (3) and (4) and caused by vertical optical transitions from the subband of light and heavy holes of the valence band to the conduction band in InSb (a) and InAs (b) crystals are shown in (Fig. 1). In numerical calculations, the maximum value of the absorption coefficient of linearly polarized light was taken as unity, where the temperature dependence of the band gap and the contribution of the coherent saturation effect were not taken into account. Fig. 1 shows that in the region of low frequencies and temperatures, the value increases with increasing frequency and reaches a maximum, and then decreases. Also, the amplitude of the coefficient of two-quantum absorption of $K^{(2)}_{c,m;L,m'}(\omega,T)$linearly polarized light is approximately 5 times greater than the amplitude of $K^{(2)}_{c,m;L,m'}(\omega,T)$ circular polarization both in InSb (a) and and in InAs (b).

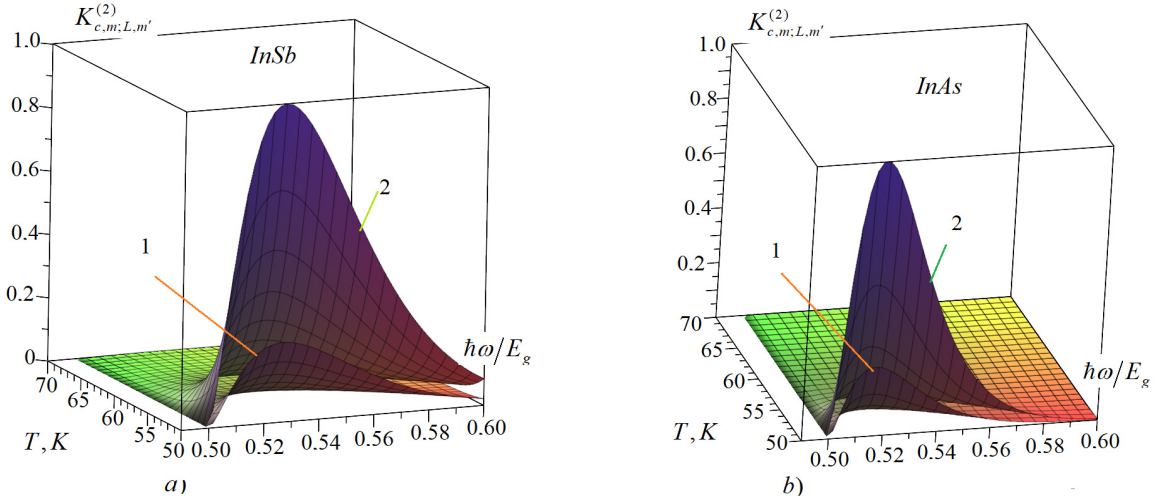

Figure 1. Spectral - temperature dependence $K^{(2)}_{c,m;L,m'}$for light of linear (line 1) and circular (line 2) polarization in InSb (a) and InAs (b) crystals. In the calculations, the maximum value of the absorption coefficient of linearly polarized light $K^{(2)}_{c,m;L,m'}$was taken as unity. In the numerical calculations, the temperature dependence of the band gap and the contribution of the coherent saturation effect were not taken into account.

In further calculations of the frequency-temperature dependence of the two-photon absorption coefficient, we assume that the temperature dependence of the band gap width is determined by the Varshni formula [26]

$$E_g(T)=E_g(T=0)-\gamma_T\frac{T^2}{T+T_V} \quad (9)$$

here constants γ_T and T_V are material-dependent empirical parameters. Specifically, γ_T controls the rate at which the band gap decreases with increasing temperature, while T_V is a characteristic offset temperature that fine-tunes the shape of the denominator in the $T^2/(T+T_V)$ term. Passler's formula [27]

$$E_g(T)=E_g(T=0)-\frac{\alpha\Theta_p}{2}\left[\left(1+\left(\frac{2T}{\Theta_p}\right)^p\right)^{1/p}-1\right]. \quad (10)$$

Here, α is an empirical coefficient controlling the band-gap shrinkage rate, Θ_p is a characteristic phonon-like temperature scale, and p is an exponent that shapes the functional form of the band-gap temperature dependence. Their values can be found through experimental data or taken from the literature for specific materials such as InSb and InAs [26,27]. The temperature dependences of the effective masses of electrons $m_c(T)$ in the conduction band and holes $m_{SO}(T)$ in the spin-orbit splitting zone can be represented as [26]:

$$\frac{m_0}{m_{SO}(\mathrm{T})} = \gamma_1 - \frac{E_P \Delta_{SO}}{3E_g(E_g+\Delta_{SO})}, \frac{m_0}{m_c(\mathrm{T})} = 1 + 2F + \frac{E_P(E_g+2\Delta_{SO}/3)}{3E_g(E_g+\Delta_{SO})} \quad (11)$$

here F is a dimensionless parameter linked to higher-order non-parabolic corrections in the conduction band; it modifies the usual parabolic dispersion to more accurately reflect the influence of strong band coupling at higher energies. Along with these parameters, the Kane energy E_p and the spin-orbit splitting Δ_{SO} play central roles in describing the band structure within the Kane model. The Kane energy, E_P, originates from the momentum-matrix element between conduction and valence bands; it quantifies the degree of band mixing in narrow-gap semiconductors. A larger E_p generally signals stronger coupling between conduction and valence states, thereby affecting both the effective masses and optical transition probabilities. Meanwhile, the spin-orbit splitting Δ_{SO} represents the energy separation between the topmost valence-band states (often labeled Γ_8) and the spin-orbit split-off band (Γ_7), which arises from relativistic spin-orbit coupling in the crystal. In narrow-gap materials such as InSb and InAs, Δ_{SO} can significantly influence the valence-band structure and, consequently, the optical absorption processes. Numerical values for E_p, Δ_{SO}, F, γ_T and T_V relevant to InSb and InAs are provided in Refs. [25, 26].

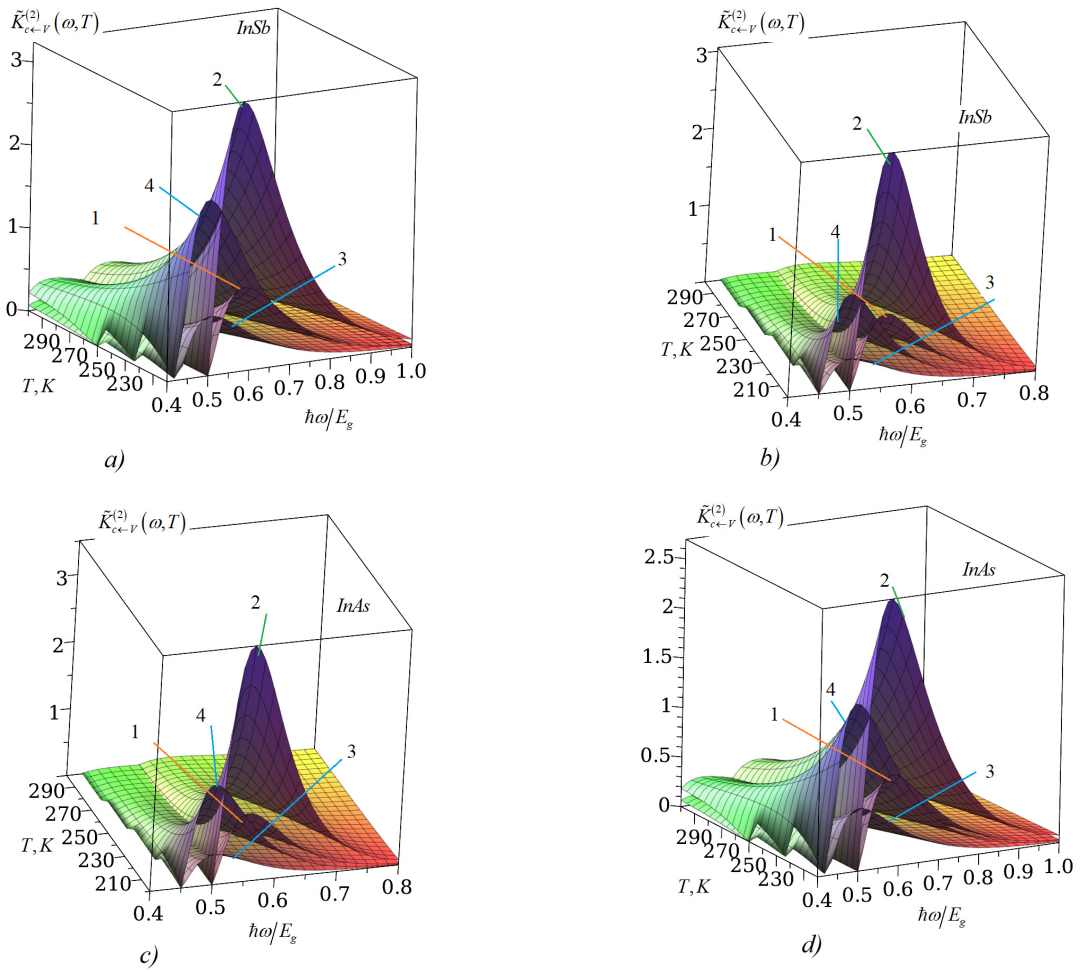

Figure 2. Spectral - temperature dependence of the total coefficient of two-quantum absorption $\tilde{K}^{(2)}_{c,\pm1/2;hh,\pm3/2}(\omega,T)$of light of linear (lines 1 and 3) and circular (lines 2 and 4) polarization, caused by transitions of the heavy-hole subband of the valence band to the conduction band in In Sb (a, b) and InAs (c, d). In Fig. (a and c) the Rabi coefficient is 0.5, and in Fig. (b) and (d) is equal to 0.7

Figure 2 shows the spectral-temperature dependence of the total coefficient of two-quantum absorption of light $\tilde{K}^{(2)}_{c,\pm1/2;hh,\pm3/2}(\omega,T)$of linear (lines 1 and 3) and circular (lines 2 and 4) polarization , caused by transitions from the subbands of light and heavy holes of the valence band to the conduction band in InAs (a,b) and InAs (c,d). Here $\tilde{K}^{(2)}_{c,\pm1/2;hh,\pm3/2}(\omega,T)$ $\left(K^{(2)}_{c,\pm1/2;hh,\pm3/2}(\omega,T)\right)$ - the coefficient of two-photon absorption in the case when the temperature dependence of the band parameters is taken into account (not taken into account). In the calculations, the maximum value $\tilde{K}^{(2)}_{c,\pm1/2;hh,\pm3/2}(\omega,T)$for linearly polarized light was taken as one unit. In Fig. 2 (a and c), the Rabi coefficient is equal to 0.5, and in Fig. 2 (b and d) is equal to 0.7. Graphs 1 and 2 are calculated using formula (9), and 3 and 4 using (10), respectively. From Fig. 2 it is evident that dependence (9) significantly affects the amplitude value of the temperature

dependence $\widetilde{K}^{(2)}_{c,\pm1/2;hh,\pm3/2}(\omega,T)$than (10), and the light absorption edge shifts by frequency $\omega_T^{(V)}(T)=\frac{\gamma_T}{\hbar}\frac{T^2}{T+T_V}$when choosing (9), by $\omega_T^{(P)}(T)=\frac{\alpha\Theta_p}{2\hbar}\left[\left(1+\left(\frac{2T}{\Theta_p}\right)^p\right)^{1/p}-1\right]$when choosing (10). Note also that regardless of the frequency of light, with an increase in the Rabi coefficient $\widetilde{K}^{(2)}_{c,\pm1/2;hh,\pm3/2}(\omega,T)$in InSb it is unnoticeable, but in InAs it decreases noticeably in the high temperature region, and in the low temperature region it is the opposite, which is associated with the complexity of the temperature dependence $\widetilde{K}^{(2)}_{c,\pm1/2;hh,\pm3/2}(\omega,T)$.

CONCLUSIONS

We have presented a theoretical study of interband two-photon (two-quantum) absorption in cubic and tetrahedral semiconductors by incorporating valence-band admixture to conduction-band states and the coherent saturation (Rabi) effect within a multiband approximation. By employing parabolic dispersion laws that emerge from the full 8×8 Kane-type Hamiltonian (truncated to second order in $\boldsymbol{k}$ for moderate photon energies $\hbar\omega\lesssim0.8\,E_g$), we have derived analytic expressions for the two-photon absorption coefficients of both linearly and circularly polarized light. To capture the material's temperature dependence, we have implemented both the Varshni and Passler formulas for the band-gap evolution, showing how these choices shift the absorption edges and alter amplitude values in InSb and InAs. The interplay between valence admixture and the spin-orbit-split $\boldsymbol{\Gamma_7}$ band leads to nontrivial differences in the relative contributions from heavy- and light-hole subbands, while the Rabi effect suppresses absorption at high intensities, especially at elevated temperatures.

The novelty of this study lies in the combined treatment of valence–conduction admixture and coherent saturation in narrow-gap semiconductors, highlighting how each mechanism modifies the spectral–temperature dependence of two-photon absorption. Our results reveal that, under low-temperature conditions, the amplitude of two-photon absorption can be substantially enhanced for linearly polarized radiation compared to circular polarization, whereas at higher temperatures, the suppression from the Rabi effect becomes more pronounced. We further find that the choice of temperature-dependent gap formula (Varshni or Passler) significantly influences absorption peaks in the photon-frequency domain. These findings may guide future experimental work on multiphoton processes in narrow-gap materials and aid in the design of optoelectronic or photonic devices where higher-order absorption processes are crucial.

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ДО ТЕОРІЇ МІЖЗОННОГО ДВОФОТОННОГО ПОГЛИНАННЯ СВІТЛА В НАПІВПРОВІДНИКАХ: ВРАХУВАННЯ ЗМІШАННЯ СТАНІВ ПРОВІДНОСТІ ТА ВАЛЕНТНИХ СТАНІВ, ЕФЕКТ РАБІ

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Ми представляємо теоретичне дослідження міжзонного двофотонного (двоквантового) поглинання поляризованого світла в напівпровідниках з кубічною та тетраедричною симетрією. Наш аналіз здійснюється в рамках багатозонного наближення з урахуванням змішування валентних станів у станах зони провідності, а також когерентних насичувальних (ефект Рабі) процесів. Ми використовуємо спрощені параболічні закони дисперсії для важких та легких дірок, а також для зони провідності, і порівнюємо дві поширені температурно-залежні формули ширини забороненої зони (Варшні та Песслера), щоб показати, як вони змінюють спектрально-температурну залежність загального коефіцієнта двофотонного поглинання. Зокрема, показано, що міжзонне двофотонне поглинання спочатку зростає з частотою фотона, досягає максимуму, а потім зменшується при фіксованій температурі. Встановлено, що амплітуда поглинання для лінійно поляризованого світла вища, ніж для кругової поляризації, особливо при низьких температурах. Наші розрахунки показують, що змішування валентних станів суттєво змінює міжзонні переходи, у той час як ефект Рабі зменшує поглинання в режимі високої інтенсивності, особливо при підвищених температурах. Отримані результати можуть бути корисними при проєктуванні оптоелектронних та фотонних пристроїв, що базуються на багатофотонній взаємодії в вузькозонних напівпровідниках.

Ключові слова: *двофотонне поглинання; ефект Рабі; змішування валентної та провідної зон; багатозонне наближення; модель Кейна; температурно-залежна ширина забороненої зони; формули Варшні та Песслера; напівпровідники InSb та InAs; нелінійна оптика*