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TO THE THEORY OF INTRABAND SINGLE-PHOTON ABSORPTION OF LIGHT IN SEMICONDUCTORS WITH ZINC-BLENDE STRUCTURE

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A theoretical analysis of the frequency-temperature dependence of the coefficient of single-photon absorption of polarized radiation in narrow- and wide-bandgap semiconductors has been conducted, considering intraband optical transitions and the temperature dependence of band parameters. It has been shown that with a fixed frequency, the single-photon absorption coefficient initially increases with temperature, reaches a maximum, and then decreases. The maximum value shifts towards lower frequencies for both narrow- and wide-bandgap semiconductors when considering the temperature dependence of the bandgap width and the effective mass of holes. It was determined that in semiconductors with a zinc-blende lattice structure, the consideration of the temperature dependence of the band parameters leads to a decrease in the amplitude value of the frequency and temperature dependence of the single-photon absorption coefficient. As the temperature increases, the absorption threshold decreases, which is noticeably observed when taking into account the Passler formula. Each type of optical transition contributes differently to the frequency, temperature, and polarization dependencies of $K_{SO,lh}^{(1)}(\omega, \mathrm{T})$.
Keywords: *Temperature dependence of band parameters; Bandgap width; Effective mass of holes; Passler and Varshni formula; Narrow- and wide-bandgap semiconductor; Single-photon absorption coefficient; Coherent saturation effect*
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INTRODUCTION

Intraband light absorption, caused by vertical inter-subband optical transitions in diamond-like semiconductors, has been studied for quite some time [1-3].

In works [4-9], theoretical studies have been conducted on one- and multiphoton absorption associated with both interband and intersubband optical transitions. Specifically, in [4, 6-9], the spectral-temperature dependencies of the multiphoton absorption coefficient and its linear-circular dichroism in semiconductors with cubic symmetry were investigated. In [10, 11], the saturation of photocurrent in topological insulators induced by direct optical transitions in regions of high intensity was discovered. In [12], a quantum-mechanical theory of the intensity-dependent edge photocurrent in graphene was developed; in [13], the polarization dependencies of one- and multiphoton interband transitions in two-dimensional monomolecular transition metal dichalcogenides were calculated.

The analysis of the theoretical calculations of the single-photon absorption coefficient of polarized light presented below indicates that considering the coherent saturation effect will lead to a unique frequency-temperature dependence. Therefore, it is of interest to theoretically study the light absorption caused by single-photon transitions from the branches of heavy and light holes to the spin-orbit split-off subband, taking into account the coherent saturation effect [5-9].

ABSORPTION OF LIGHT CAUSED BY SINGLE-PHOTON TRANSITIONS FROM THE HEAVY AND LIGHT HOLE BRANCHES TO THE SPIN-ORBIT SPLIT-OFF SUBBAND.

The spectral, polarization, and temperature dependencies of the absorption coefficient due to single-photon transitions from the heavy and light hole branches of the valence band to the spin-orbit split-off subband are determined by the expression:

$$K^{(1)} = \frac{2\pi}{\hbar}\frac{\hbar\omega}{I}\sum_{\vec{k}}\left(f_{lh,\vec{k}}^{(1)} - f_{SO,\vec{k}}^{(1)}\right)\left|\sum_{lh,m=\pm1/2;\, SO,m\prime=\pm1/2} M_{lh,m;\, SO,m\prime}^{(2)}\left(\vec{k}\right)\right|^2 \delta\left(E_{SO,\vec{k}} - E_{lh,\vec{k}} - \hbar\omega\right), \quad (1)$$

Considering the coherent saturation effect [5-9, 14], we obtain:

$$K^{(1)} = \frac{2\pi}{\hbar}\hbar\omega\frac{1}{I}\rho(\hbar\omega)f(T,\omega)(\langle\Re_+\rangle + \langle\Re_-\rangle), \quad (2)$$

where

$$\Re_{\pm} = \frac{\left|M_{SO,+1/2,lh,\pm1/2}^{(1)}(\vec{k}) + M_{SO,-1/2,lh,\pm1/2}^{(1)}(\vec{k})\right|^2}{\sqrt{1+4\frac{\alpha_\omega}{\hbar^2\omega^2}\left|M_{SO,+1/2,lh,\pm1/2}^{(1)}(\vec{k}) + M_{SO,-1/2,lh,\pm1/2}^{(1)}(\vec{k})\right|^2}}, \quad (3)$$

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$\rho(\hbar\omega) = \mu_- k_\omega^{(1)}/(\pi^2\hbar^2)$ is the density of states, $k_\omega^{(1)} = (2\mu_-[\hbar\omega - \Delta_{SO}]/\hbar^2)^{1/2}$, $\left\langle \left| M_{n'k',nk}^{(1)} \right|^2 \right\rangle$ is the square of the matrix element of the optical transition type $M_{n'\vec{k}',n\vec{k}}^{(1)}$is the optical transition matrix element for the transition of type $|n\vec{k}\rangle \to |n'\vec{k}'\rangle$ averaged over the solid angles of the wave vector $\vec{k}$. The parameter $\alpha_\omega = 6\omega^2 T_1^{(1)} T_2^{(1)} \frac{I}{I_0}$, where $I_0 = \frac{cn_\omega \hbar^3 \omega^3}{2\pi|B|}$, and $I(\omega)$ is the intensity (frequency) of the light. The functions $f_{L\vec{k}}^{(1)}$ represent the distribution functions of charge carriers (where L=1 (*hh*) corresponds to heavy holes, L=2 (*lh*) corresponds to light holes, and L=SO corresponds to holes in the spin-orbit split-off subband). The energy dispersion of holes in branch L is given by $E_{L\vec{k}} = -\hbar^2 k^2/2m_L$[15,16]. The parametrs $e'_\pm = e_{x'} \pm e_{y'}, e_{x'}, e_{y'}$ are the projections of the polarization vector $\vec{e}$ onto the Ox' and Oy' axes, perpendicular to the wave vector $\vec{k}$ of the holes. The reduced effective mass of the holes is $\mu_-^{(SO,L)} = m_{SO}m_L/(m_{SO} - m_L)$.
In particular, for single-photon transitions from the light hole branch to the spin-orbit split-off subband, the value $\Re_\pm$ is written as:

$$\Re_+ = 3\left(\frac{eA_0}{c\hbar}\right)^2 B^2k^2|e'_-|^2\left[1 + 4\frac{\alpha_\omega}{\hbar^2\omega^2}\left(\frac{eA_0}{c\hbar}\right)^2 B^2k^2 3|e'_-|^2\right]^{-1/2}, \tag{4}$$

$$\Re_- = \left(\frac{eA_0}{c\hbar}\right)^2 B^2k^2(9e'^2_\perp + 4e'^2_z)\left[1 + 4\frac{\alpha_\omega}{\hbar^2\omega^2}\left(\frac{eA_0}{c\hbar}\right)^2 B^2k^2(9e'^2_\perp + 4e'^2_z)\right]^{-1/2}, \tag{5}$$

where $4B = \hbar^2 m_{lh}m_{hh}/(m_{hh} - m_{lh})$. If the contribution of the coherent saturation effect to light absorption is neglected ($\alpha_\omega = 0$) and averaging is performed over the solid angles of $\vec{k}$ from (4, 5), then the expression becomes polarization-independent:

$$\left\langle \Re_+^{(0)} \right\rangle + \left\langle \Re_-^{(0)} \right\rangle = \left(\frac{eA_0}{c\hbar}\right)^2 B^2k^2\langle 9e'^2_\perp + 4e'^2_z\rangle = \frac{22}{3}\left(\frac{eA_0}{c\hbar}\right)^2 B^2k^2. \tag{6}$$

Then (1) takes the form:

$$K^{(1)} = \frac{44\pi}{3\hbar}\left(\frac{eA_0}{c\hbar}\right)^2 \frac{\hbar\omega}{I}\rho(\hbar\omega)f(\beta,\omega)B^2k^2. \tag{7}$$

From Table 1, it can be seen that the reduced effective mass of holes $\mu_-^{(SO,hh)} = \frac{m_{SO}m_{hh}}{m_{SO}-m_{hh}}$, involved in optical transitions from the heavy hole branch to the spin-orbit split-off subband takes a negative value for several A3B5 semiconductors. This, in turn, leads to the wave vector of the charge carriers $k_{SO,hh}^{(1\omega)} = \left[2\mu_-^{(SO,hh)}\hbar^{-2}(\hbar\omega - \Delta_{SO})\right]^{1/2}$ involved in such optical transitions becoming an imaginary quantity. For this reason, unlike the optical transitions from the light hole branch, transitions from the heavy hole branch to the spin-orbit split-off subband are forbidden.

Since optical transitions are allowed from the light hole branch to the spin-orbit split-off subband of the valence band, we will further analyze the frequency and temperature dependencies of the single-photon absorption coefficient. Then, according to the law of energy conservation: $\frac{\hbar^2k^2}{2m_{SO}} + \Delta_{SO} - \frac{\hbar^2k^2}{2m_L} - \hbar\omega = 0$ the wave vector is determined by the expression $k_{SO,L}^{(1\omega)} = \left[2\mu_-^{(SO,L)}\hbar^{-2}(\hbar\omega - \Delta_{SO})\right]^{1/2}$.

From (6) and (7), it can be seen that the single-photon absorption coefficient does not depend on the degree of light polarization; therefore, linear-circular dichroism is not observed during single-photon absorption. To account for the effect of coherent saturation on absorption, it is necessary to perform calculations based on (2) and (3).

Table 1. Numerical values of band parameters for some semiconductors [17]

Quantities	*GaAs*	*InSb*	*InAs*
E_g, eV	1.519	0.235	0.417
Δ_{SO}, eV	0.341	0.81	0.39
m_c/m_0	0.067	0 0135	0 026
m_{SO}/m_0	0.172	0.11	0.14
Δ_{SO}/E_g	0.24b	4.65	1.1
m_{lh}/m_0	0.09009	0.0152	0.027027
m_{hh}/m_0	0.34965	0.26316	0.33333
$\alpha_T, meV/K$	0.5405	0 32	0 276
β_T, K	204	170	93
F	-1.94	-0.23	-2.90

Now, we will calculate the frequency-temperature dependencies of the single-photon absorption coefficient using the following expression for the single-photon absorption coefficient, associated with optical transitions from the light hole branch to the spin-orbit split-off subband:

$$K^{(1)} = \frac{4\pi e^2}{c\omega m_0^2 n_\omega}\sum_{nn'\vec{k}}\left|\vec{e}\vec{p}_{SO,lh}(\vec{k})\right|^2\left(f_{lh,\vec{k}} - f_{SO,\vec{k}}\right)\delta\left(E_{SO}(\vec{k}) - E_{lh}(\vec{k}) - \hbar\omega\right). \tag{8}$$

Next, we assume the energy dispersion of light and heavy holes as $E_{lh}(\vec{k}) = -\hbar^2k^2/(2m_{lh})$ and $E_{hh}(\vec{k}) = -\hbar^2k^2/(2m_{hh})$, while in the spin-orbit split-off subband it is $E_{SO}(\vec{k}) = -\Delta_{SO} - \hbar^2k^2/(2m_{SO})$, where m_{lh} (m_{hh}) are the effective masses of light and heavy holes, respectively, and, Δ_{SO}- is the spin-orbit splitting energy, with numerical values for various semiconductors provided in [17]. Then, from (8), we obtain:

$$K_{SO,lh}^{(1)} = \frac{22}{3}\frac{e^2}{c\hbar n_\omega \hbar\omega}\frac{\mu_-}{\hbar^2}B^2\left(k_\omega^{(1)}\right)^3 f_{lh,k_\omega^{(1)}}[1-\exp(-\hbar\omega/k_BT)]$$

or

$$K_{SO,lh}^{(1)} = \frac{11}{12}\frac{e^2}{c\hbar n_\omega}\left(\frac{m_{hh}-m_{lh}}{m_{SO}-m_{lh}}\frac{m_{SO}}{m_{lh}}\right)^2\frac{\hbar\omega-\Delta_{SO}}{\hbar\omega}\left(\frac{m_{hh}-m_{lh}}{m_{hh}}\right)^2 k_\omega^{(1)} f_{lh,k_\omega^{(1)}}\left(1-e^{-\hbar\omega/k_BT}\right), \tag{9}$$

where $k_\omega^{(1)} = \left[2\mu_-^{(SO,lh)}\hbar^{-2}(\hbar\omega-\Delta_{SO})\right]^{1/2}$, $f_{lh,k_\omega^{(1)}} = \exp\left(\frac{E_F}{k_BT}\right)\cdot\exp\left[-\frac{m_{SO}}{m_{SO}-m_{lh}}\frac{\hbar\omega-\Delta_{SO}}{k_BT}\right]$ (see Fig. 1).

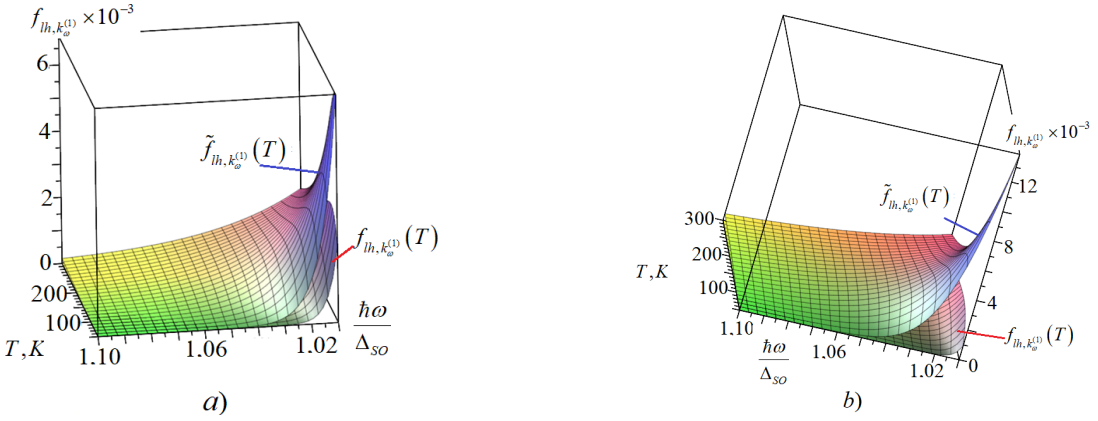

Figure 1. The frequency-temperature dependence of the distribution function of light holes $f_{lh,k_\omega^{(1)}}(\mathrm{T})$, involved in single-photon transitions in GaAs (a) and InAs (b), considering the temperature dependence of the bandgap width $E_g(\mathrm{T})$ and the effective mass of charge carriers using the Varshni formula. The function $\tilde{f}_{lh,k_\omega^{(1)}}(\mathrm{T})$ represents the distribution function of light holes at $E_g(\mathrm{T}=0)$.

The Fermi energy E_F is determined by the relation:

$$e^{\frac{E_F}{k_BT}} = \frac{1}{2}p\left(\frac{k_BT}{2\pi\hbar^2}\right)^{-3/2}\left(m_{hh}^{3/2}+m_{lh}^{3/2}+m_{SO}^{3/2}e^{-\frac{\Delta_{SO}}{k_BT}}\right)^{-1}, \tag{10}$$

where p is the hole concentration. Note that in our case, $\hbar\omega \gg k_BT$, so $e^{-\hbar\omega/k_BT} \ll 1$.

Thus, the frequency ($x = \hbar\omega/\Delta_{SO}$) and temperature ($y = k_BT/\Delta_{SO}$) dependencies of the single-photon absorption coefficient can be written as:

$$K_{SO,lh}^{(1)}(\omega,T) = K_0^{(1)}\frac{x-1}{x}(x-1)^{1/2}\frac{\exp\left[-\frac{m_{SO}}{m_{SO}-m_{lh}}\frac{x-1}{y}\right]}{y^{3/2}\left(m_{hh}^{3/2}+m_{lh}^{3/2}+m_{SO}^{3/2}e^{-1/y}\right)}, \tag{11}$$

where

$$K_0^{(1)} = \frac{11}{6}\frac{\pi^{3/2}e^2}{c\hbar n_\omega}\frac{(m_{hh}-m_{lh})^4}{(m_{SO}-m_{lh})^{5/2}}\frac{m_{SO}^{5/2}}{m_{lh}^{3/2}m_{hh}^2}\frac{\hbar^2p}{\Delta_{SO}}.$$

In further calculations, we assert that the temperature dependence of the bandgap width is determined by the Varshni formula [17]:

$$E_g(T) = E_g(T=0) - \gamma_T\frac{T^2}{T+T_V}, \tag{12}$$

and by the Passler formula [18]:

$$E_g(T) = E_g(T=0) - \frac{\alpha\Theta_p}{2}\left[\left(1+\left(\frac{2T}{\Theta_p}\right)^p\right)^{1/p}-1\right]. \tag{13}$$

According to the multiband Kane model, the effective masses of electrons in the conduction band (m_c) and holes in the spin-orbit split-off subband (m_{SO}) depend on temperature and are expressed as [17]:

$$m_0/m_c = \left[1+2F+\frac{E_P}{3}\left(E_{g0}-\frac{\alpha T}{\beta+T}+\frac{2}{3}\Delta_{SO}\right)\left(E_{g0}-\frac{\alpha T}{\beta+T}\right)^{-1}\left(E_{g0}-\frac{\alpha T}{\beta+T}+\Delta_{SO}\right)^{-1}\right], \tag{14}$$

$$m_0/m_{SO} = \left[\gamma_1 - \frac{E_P}{3}\Delta_{SO}\left(E_{g0} - \frac{\alpha T}{\beta+T}\right)^{-1}\left(E_{g0} - \frac{\alpha T}{\beta+T} + \Delta_{SO}\right)^{-1}\right], \quad (15)$$

where $E_{g0} = E_g(T=0)$. For quantitative calculations, the numerical values of the parameters γ_T, T_V, α, Θ_p, p are taken from [18].

Using the numerical values of the band parameters for GaAs and InAs (see Table 1), when the temperature changes from 10 K to 300 K, the effective mass of electrons in the conduction band decreases by 0.053% and 0.051%, respectively, and the effective mass of holes in the spin-orbit split-off subband decreases by 0.01% and 0.04%, respectively. Although these changes are minor, considering $E_g(T)$ leads to significant changes in the frequency-temperature dependence of the absorption coefficient.

As seen from equation (8), the temperature dependence of $K_{SO,lh}^{(1)}$ is determined by the temperature dependence of $f_{lh,k_\omega^{(1)}}(\mathrm{T})$, while the frequency dependence is determined by the term $\frac{\hbar\omega-\Delta_{SO}}{\hbar\omega}k_\omega^{(1)}\rho(\hbar\omega)\exp\left(-\frac{m_{SO}}{m_{SO}-m_{lh}}\frac{\hbar\omega-\Delta_{SO}}{k_BT}\right)$, In this context, Figure 1 presents the frequency-temperature dependence of the distribution function of light holes involved in single-photon transitions in GaAs and InAs. It shows that, at a fixed frequency, the distribution function $f_{lh,k_\omega^{(1)}}$ initially increases with temperature, reaches a maximum, and then decreases. Specifically, at $\hbar\omega = 1{,}01\Delta_{SO}$ in GaAs (InAs), the function $f_{lh,k_\omega^{(1)}}$ reaches its maximum at a temperature of 90 K (60 K). Figure 1 also shows that the functions $f_{lh,k_\omega^{(1)}}(\mathrm{T}) = f_{lh,k_\omega^{(1)}}\left(\mathrm{T}, E_g(T)\right)$ and $\tilde{f}_{lh,k_\omega^{(1)}}(\mathrm{T}) = f_{lh,k_\omega^{(1)}}\left(\mathrm{T}, E_g(T)=0\right)$ differ significantly at low frequencies across all temperatures, but converge at high frequencies. Furthermore, the temperature dependence of the band parameters is prominently observed at low frequencies. The calculations do not account for the contribution of the coherent saturation effect in $f_{lh,k_\omega^{(1)}}(\mathrm{T})$ and $\tilde{f}_{lh,k_\omega^{(1)}}(\mathrm{T})$.

The frequency-temperature dependence of the single-photon absorption coefficient $K_{SO,lh}^{(1)}(\omega,\mathrm{T})$ $\left(\tilde{K}_{SO,lh}^{(1)}(\omega,\mathrm{T})\right)$ in InSb (a, b) GaAs (c, d) (see Figure 2) was calculated according to (14), using the Varshni formula (plots a, c) and the Passler formula (plots b, d), where $K_{SO,lh}^{(1)}(\omega,\mathrm{T})$ $\left(\tilde{K}_{SO,lh}^{(1)}(\omega,\mathrm{T})\right)$ is the absorption coefficient with (without) considering the temperature dependence of $E_g(\mathrm{T})$ and the effective masses of holes. The contribution of the coherent saturation effect is not accounted for, and the amplitude value of $\tilde{K}_{SO,lh}^{(1)}(\omega,\mathrm{T})$ was normalized to unity.

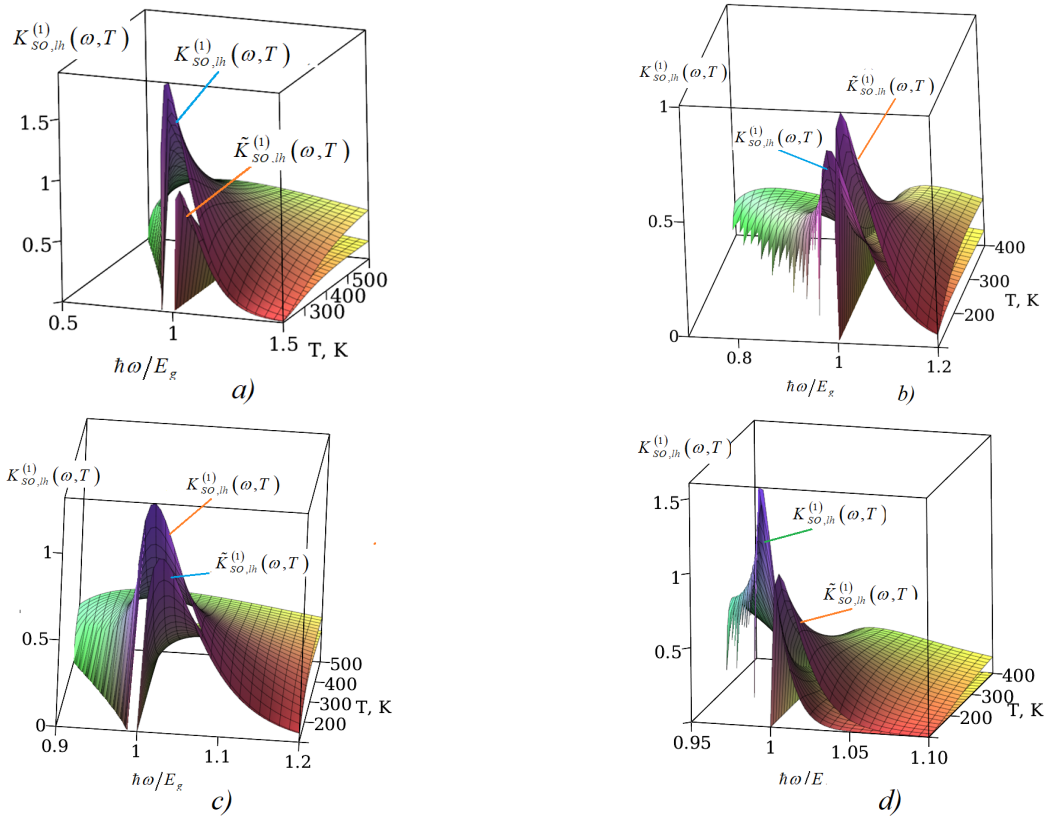

Figure 2. Frequency-temperature dependence of $K_{SO,lh}^{(1)}(\omega,\mathrm{T})$ in InSb (a, b) and GaAs (c, d), where $K_{SO,lh}^{(1)}(\omega,\mathrm{T})$ was calculated using the Varshni (plots a, c) and Passler (plots b, d) formulas. $K_{SO,lh}^{(1)}(\omega,\mathrm{T})$ $(\tilde{K}_{SO,lh}^{(1)}(\omega,\mathrm{T}))$ is the absorption coefficient with (without) accounting for the temperature dependence of $E_g(\mathrm{T})$ and the effective masses of holes.

From Fig. 2, it is evident that at a fixed frequency, $K_{SO,lh}^{(1)}(\mathrm{T})$ increases with temperature, reaches a maximum, and then decreases. This temperature-dependent behavior of $K_{SO,lh}^{(1)}(\omega,\mathrm{T})$ $\left(\widetilde{K}_{SO,lh}^{(1)}(\omega,\mathrm{T})\right)$ is described by the analogous behavior of the corresponding distribution function. It is noted that in the frequency range $\Delta_{SO} \leq \hbar\omega \leq 1{,}3\Delta_{SO}$ the absorption coefficient $K_{SO,lh}^{(1)}(\omega,\mathrm{T})$ is greater then $\widetilde{K}_{SO,lh}^{(1)}(\omega,\mathrm{T})$, whereas for $\hbar\omega > 1{,}3\Delta_{SO}$ the plots of $K_{SO,lh}^{(1)}(\omega,\mathrm{T})$ and $\widetilde{K}_{SO,lh}^{(1)}(\omega,\mathrm{T})$ merge.

It is worth noting that in narrow-gap crystals, if the dependencies $E_g(\mathrm{T})$, $m_{SO}(\mathrm{T})$, $m_c(\mathrm{T})$, are considered, the dependence $K_{SO,lh}^{(1)}(\omega,\mathrm{T})$ increases sharply (see Fig. 2). This can be explained by the sharp increase in the quantity $\left(\frac{m_{hh}-m_{lh}}{m_{SO}-m_{lh}}\right)^2\left(\frac{m_{hh}-m_{lh}}{m_{hh}}\right)^2\left(\frac{m_{SO}\cdot m_{lh}}{m_{SO}-m_{lh}}\cdot\Delta_{SO}\right)^{1/2}$ with increasing temperature (particularly in InSb, this quantity increases up to 10 times).

3. CONCLUSIONS

From the above-mentioned results and Figures 1-2, it is evident that, at a fixed frequency, the coefficient of one-photon absorption in the semiconductors GaAs and InAs initially increases with temperature, reaches a maximum, and then decreases. The maximum value, considering the temperature dependence of $E_g(\mathrm{T})$, $m_{SO}(\mathrm{T})$, $m_c(\mathrm{T})$ shifts towards lower frequencies, and this shift is sensitive when accounting for (13) for both narrow-gap and wide-gap semiconductors.

It is also noted that considering the temperature dependence of band parameters leads to a reduction in the frequency and temperature dependence of the one-photon absorption coefficient $K_{SO,lh}^{(1)}(\omega,\mathrm{T})$.

As the temperature increases, the absorption threshold (edge) decreases, which is noticeably observed when considering the Passler formula. It has been shown that each type of optical transition contributes differently to the frequency, temperature, and polarization dependencies of $K_{SO,lh}^{(1)}(\omega,\mathrm{T})$, as some optical transitions are forbidden.

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ДО ТЕОРІЇ ВНУТРІШНЬОГО ОДНОФОТОННОГО ПОГЛИНАННЯ СВІТЛА У НАПІВПРОВІДНИКАХ ІЗ СТРУКТУРОЮ ЦИНКОВОЇ ОБМАНКИ

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Проведено теоретичний аналіз частотно-температурної залежності коефіцієнта однофотонного поглинання поляризованого випромінювання у вузько- та широкозонних напівпровідниках з урахуванням внутрішньозонних оптичних переходів та температурної залежності зонних параметрів. Показано, що при фіксованій частоті коефіцієнт однофотонного поглинання спочатку зростає з температурою, досягає максимуму, а потім зменшується. Максимальне значення зміщується в бік нижчих частот як для вузькозонних, так і для широкозонних напівпровідників при розгляді температурної залежності ширини забороненої зони та ефективної маси дірок. Визначено, що в напівпровідниках зі структурою гратки цинкової обманки врахування температурної залежності параметрів зони призводить до зменшення амплітудного значення частотної та температурної залежності коефіцієнта однофотонного поглинання. З підвищенням температури поріг поглинання знижується, що помітно спостерігається при врахуванні формули Пасслера. Кожен тип оптичного переходу по-різному впливає на частоту, температуру та поляризаційні залежності $K^{(1)}_{SO,lh}(\omega, \mathrm{T})$.

Ключові слова: *температурна залежність параметрів зони; ширина забороненої зони; ефективна маса дірок; формула Пасслера та Варшні; вузько- та широкозонний напівпровідник; коефіцієнт однофотонного поглинання; ефект когерентного насичення*