# Simple theory of the optical absorption coefficient in nonparabolic semiconductors

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A simple theory is developed of the optical absorption coefficient (OAC) in nonparabolic semiconductors on the basis of the three-band model of Kane, by considering the wave-vector ($\vec{k}$) dependence of the optical matrix element. It has been found that the OAC is proportional to $[(\hbar\omega)^2-E_g^2]^{1/2}$ ($\hbar\omega$ and $E_g$ are the energy of the incident radiation and the bandgap, respectively) instead of $[(\hbar\omega)-E_g]^{1/2}$, the conventional form. It has been demonstrated, by taking $n$-InAs, $n$-InSb, $Hg_{1-x}Cd_xTe$, and $In_{1-x}Ga_xAs_{1-y}P_{1-y}$ lattice matched to InP as examples, that the OAC increases with increasing photon energy and the value of the same coefficient in the three band model of Kane is greater than that in parabolic energy bands in all the cases. The well-known result for wide gap materials having parabolic energy bands has also been obtained from our generalized formulation under certain limiting condition. © *2004 American Institute of Physics.*
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## I. INTRODUCTION

The optical absorption coefficient (OAC) in semiconductor is related to various physical features of semiconducting materials. This property was extensively investigated both theoretically[1–6] and experimentally[4] neglecting the wave-vector ($\vec{k}$) dependence of the optical matrix element (OME). In this article, we focus on the OAC because of the long-standing interest in it in optoelectronics for the last three decades. Incidentally, it appears from the literature that the OAC in $III-V$, ternary and quaternary compounds has yet to be investigated in detail by considering the $\vec{k}$-dependence of the OME on the basis of the three-band model of Kane,[5] which is the most valid description of the dispersion relation of the conduction electrons of the said compounds.[7] This will make our analysis a generalized one since one can obtain the corresponding well-known result for relatively wide-gap materials under certain limiting conditions.

For the purpose of the numerical computations, we shall take InAs and InSb as examples of $III-V$ semiconductors and $Hg_{1-x}Cd_xTe$ and $In_{1-x}Ga_xAs_yP_{1-y}$ lattice matched to InP as examples of ternary and quaternary materials, respectively. The $III-V$ compounds find extensive applications in Bragg reflectors, distributed feedback lasers,[8] passive filter devices,[9] photo reflective materials,[10] and integrated optoelectronics.[11] In this context, it is worth remarking that the ternary alloy $Hg_{1-x}Cd_xTe$ is a classic narrow gap compound and is an important optoelectronics material. The band gap of this ternary alloy can be varied to cover the spectral range from 0.8 to over 30 $\mu$m by adjusting the alloy composition.[12] $Hg_{1-x}Cd_xTe$ finds extensive use in infrared detector materials and photovoltaic detector arrays in the 8–12 $\mu$m wave bands.[13] The above uses have spurred a $Hg_{1-x}Cd_xTe$ technology for the production of high mobility single crystals with specially prepared surfaces and the same material is ideally suited for narrow sub-band physics because the relevant material constants are within easy experimental reach.[14] Moreover the quaternary alloy $In_{1-x}Ga_xAs_yP_{1-y}$ lattice matched to InP, also finds extensive applications in the fabrication of photo detectors,[15] heterojunction lasers,[16] light emitting diodes,[17] avalanche photodiodes,[18] field effect transistors, detectors, and other devices. In addition, other types of integrated optical devices such as switches, modulators, solar cells, and filters are made from the quaternary systems.[19–21]

In what follows, in Sec. II A, of theoretical background, we shall derive the OAC small-gap semiconductors in accordance with the three-band model of Kane. In Sec. II B we shall formulate the corresponding well-known result for isotropic parabolic energy bands. In Sec. III, we shall study the photon energy dependence of the OAC, taking the above mentioned materials for the purpose of numerical computations.

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## II. THEORETICAL BACKGROUND

### A. Formulation of the generalized OAC in accordance with the three-band model of Kane

The OAC ($\alpha$) can, in general, be written as[1]

$$\alpha = 2\hbar[\omega n \varepsilon_o C A_o^2]^{-1} W(\omega), \tag{1}$$

where $\hbar = h/2\pi$, $h$ is the Planck constant, $\omega$ is the angular frequency of the incident radiation, $n$ is the refractive of the semiconducting materials, $\varepsilon_o$ is the permittivity of the free space, $C$ is the velocity of light in free space, $A_o$ is the amplitude of the incident light wave, and $W(\omega)$ is the interband optical transition probability per unit time per unit volume which can, in turn, be expressed as

$$W(\omega) = \frac{2\pi}{\hbar}\left(\frac{eA_o}{m}\right)^2 \int \frac{dv}{(2\pi)^3} \langle |\hat{a}.OME|^2 \rangle_{av} . \delta(E_c(\vec{k}) - E_v(\vec{k}) - \hbar\omega), \tag{2}$$

where $m$ is the free electron mass, $dv$ the differential volume element of $\vec{k}$-space and is given by $dv = 4\pi k^2 \cdot dk$, $\hat{a}$ is the polarization vector of the incident radiation, $\delta$ denotes the Dirac delta function, $E_c(\vec{k})$ is the $\vec{k}$-dependent energy of the conduction band (CB), $E_v(\vec{k})$ is the $\vec{k}$-dependent energy of the heavy hole valence band (VB) and $E_c(\vec{k}) - E_v(\vec{k}) = \xi(\vec{k})$ represents the energy difference between the CB and the VB, respectively. It appears that the determination of the OAC requires an expression of the OME which can be derived as follows:

For the arbitrary direction of the wave-vector, the doubly degenerate wave functions, $u_1(\vec{k},\vec{r})$ and $u_2(\vec{k},\vec{r})$ can, respectively, be written as[6,22,23]

$$u_1(\vec{k},\vec{r}) = [(is)\downarrow,]a_{k+} + \left[\frac{X' - iY'}{\sqrt{2}}\uparrow'\right] b_{k+} + [Z'\downarrow,]c_{k+} \tag{3}$$

and

$$u_2(\vec{k},\vec{r}) = [(is)\uparrow']a_{k-} - \left[\frac{X' + iY'}{\sqrt{2}}\downarrow,\right] b_{k-} + [Z'\uparrow']c_{k-} \tag{4}$$

where $\vec{r}$ is the position vector, $a_{k\pm} \equiv \beta[E_g - (\gamma_{k\pm})^2(E_g - \delta')/(E_g + \delta')]^{1/2}$, $\beta \equiv [6(E_g + 2\Delta/3)(E_g + \Delta)/\chi]^{1/2}$, $E_g$ is the direct band-gap of the semiconductor, $\Delta$ is the spin-orbit splitting of the valence band, $\chi \equiv (6E_g^2 + 9E_g\Delta + 4\Delta^2)$, $\gamma_{k\pm} \equiv [\xi(\vec{k}) \mp E_g/2(\xi(\vec{k}) + \delta')]^{1/2}$, $\delta' \equiv E_g^2\Delta/\chi$, $i = \sqrt{-1}$, $s$ is the $s$-type atomic orbital in both unprimed and primed coordinates, $\downarrow,$ indicates the spin down function in the primed coordinates, $b_{k\pm} \equiv \rho\gamma_{k\pm}$, $\rho \equiv (4\Delta^2/3\chi)^{1/2}$; $X'$, $Y'$, and $Z'$ are the $p$-type atomic orbitals in the primed coordinates, $\uparrow'$ indicates the spin-up function in the primed coordinates, $c_{k\pm} \equiv t.\gamma_{k\pm}$, $t \equiv [6(E_g + 2/3\Delta)^2/\chi]^{1/2}$, $\xi(\vec{k}) \equiv [E_g^2 + E_g\hbar^2k^2/m_r]^{1/2}$ and $m_r$ is the reduced effective mass.

We can, therefore, write the expression for the OME as

$$\text{OME} = \langle u_1(\vec{k},\vec{r})|\hat{p}|u_2(\vec{k},\vec{r})\rangle \tag{5}$$

in which $\hat{p}$ is the momentum operator. Since the photon vector has no interaction in the same band for the study of interband optical transition, we can therefore write

$$\langle S|p|S\rangle = \langle X|p|X\rangle = \langle Y|p|Y\rangle = \langle Z|p|Z\rangle = 0 \tag{6}$$

and

$$\langle X|p|Y\rangle = \langle Y|p|Z\rangle = \langle Z|p|X\rangle = 0. \tag{7}$$

It is worth remarking to note that

$$\langle S|p|X\rangle = \langle S|p|Y\rangle = \langle S|p|Z\rangle = \frac{m}{\hbar}P \tag{8}$$

in which $P$ is the optical matrix element at $\vec{k} = 0$ and is given by

$$P = \left\{ h^2 E_g(E_g + \Delta) \Big/ \left[ 2m_c\left(E_g + \frac{2}{3}\Delta\right)\right]\right\}^2, \tag{9}$$

where $m_c$ is the effective electron mass at the edge of the CB.

In this context, we can write that

$$\uparrow' = \exp(-i\phi/2)\cos(\theta/2)\uparrow + \exp(i\phi/2)\sin(\theta/2)\downarrow, \tag{10}$$

$$\downarrow, = -\exp(-i\phi/2)\sin(\theta/2)\uparrow + \exp(i\phi/2)\cos(\theta/2)\downarrow, \tag{11}$$

$$|X'\rangle = \cos\theta\cos\phi|X\rangle + \cos\theta\sin\phi|Y\rangle - \sin\theta|Z\rangle, \tag{12}$$

$$|Y'\rangle = -\sin\phi|X\rangle + \cos\phi|Y\rangle, \tag{13}$$

$$|Z'\rangle = \sin\theta\cos\phi|X\rangle + \sin\theta\sin\phi|Y\rangle + \cos\theta|Z\rangle, \tag{14}$$

$$\hat{r}_1 = \hat{i}\cos\theta\cos\phi + \hat{j}\cos\theta\sin\phi - \hat{k}\sin\theta, \tag{15}$$

$$\hat{r}_2 = -\hat{i}\sin\phi + \hat{j}\cos\phi, \tag{16}$$

$$\hat{r}_3 = \hat{i}\sin\theta\cos\phi + \hat{j}\sin\theta\sin\phi + \hat{k}\cos\theta, \tag{17}$$

$$\text{Spin-vector} = \frac{h}{2}\overline{\sigma}, \tag{18}$$

in which $\theta$ and $\phi$ are defined in spherical polar coordinates where the primed and the unprimed axes are described elsewhere;[6] $\hat{r}_1$, $\hat{r}_2$, and $\hat{r}_3$ are the unit vectors in primed axes; and $\hat{i}$, $\hat{j}$, and $\hat{k}$ are the unit vectors along $x$, $y$, and $z$ axes respectively,

$$\sigma_x \equiv \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma_y \equiv \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \text{ and } \sigma_z \equiv \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.$$

Using Eqs. (5)–(17) and after performing tedious operator algebra, we can write that

$$\text{OME} = \frac{P}{\sqrt{2}}(i\hat{r}_1 - \hat{r}_2) \times \{(b_{k+}a_{k-})\langle\uparrow'|\uparrow'\rangle + (b_{k-}a_{k+}) \times \langle\downarrow,|\downarrow,\rangle\} + iP\hat{r}_3(c_{k+}a_{k-} + c_{k-}a_{k+})\langle\downarrow,|\uparrow'\rangle. \tag{19}$$

Using Eqs. (10)–(18), we can write

$$\langle\downarrow,|\uparrow'\rangle = \frac{1}{2}[\hat{r}_1 + i\hat{r}_2], \tag{20}$$

$$\langle\uparrow'|\uparrow'\rangle=\frac{1}{2}\hat{r}_3, \tag{21}$$

$$\langle\downarrow,|\downarrow,\rangle=-\frac{1}{2}\hat{r}_3. \tag{22}$$

Using Eqs. (19)–(22), we get

$$\mathrm{OME}=\frac{1}{2}P\hat{r}_3(i\hat{r}_1-\hat{r}_2)\times[A(\vec{k})+B(\vec{k})] \tag{23}$$

in which

$$A(\vec{k})=\beta\left(t+\frac{\rho}{\sqrt{2}}\right)\times\left\{\left(\frac{E_g}{E_g+\delta'}\right)\gamma_{k+}^2-\gamma_{k+}^2\gamma_{k-}^2\left(\frac{E_g-\delta'}{E_g+\delta'}\right)\right\}^{1/2} \tag{24}$$

and

$$B(\vec{k})=\beta\left(t+\frac{\rho}{\sqrt{2}}\right)\times\left\{\left(\frac{E_g}{E_g+\delta'}\right)\gamma_{k-}^2-\gamma_{k+}^2\gamma_{k-}^2\left(\frac{E_g-\delta'}{E_g+\delta'}\right)\right\}^{1/2}. \tag{25}$$

Substituting $\gamma_{k\pm}^2=[\xi(\vec{k})\mp E_g/2(\xi(\vec{k})+\delta')]$ into Eqs. (24) and (25) and performing further calculations we get

$$A(\vec{k})=\frac{\beta}{2}\left(t+\frac{\rho}{\sqrt{2}}\right)\times(E_g-\delta')\times\left\{\frac{1}{\xi(\vec{k})+\delta'}-\frac{1}{E_g+\delta'}\right\}^{1/2}\times\left\{\frac{1}{\xi(\vec{k})+\delta'}-\frac{E_g+\delta'}{(E_g-\delta')^2}\right\}^{1/2} \tag{26}$$

and

$$B(\vec{k})=\frac{\beta}{2}\left(t+\frac{\rho}{\sqrt{2}}\right)\times\left[1+\frac{E_g-\delta'}{\xi(\vec{k})+\delta'}\right]. \tag{27}$$

For the plane polarized light, with the direction of polarization $\hat{a}=\hat{k}$, we can write

$$\langle|\hat{a}.\mathrm{OME}|^2\rangle_{av}=\frac{2P_z^2}{4}[A(\vec{k})+B(\vec{k})]^2\int_0^{2\pi}d\phi\int_0^{\pi}\cos^2\theta\sin\theta d\theta=\frac{2\pi}{3}|\hat{a}.P_{cv}(0)|^2\times[A(\vec{k})+B(\vec{k})]^2 \tag{28}$$

in which $|P_z|^2=|\hat{a}.P_{cv}(0)|^2$ and $P_{cv}(0)=\int u_c^*(0,\vec{r}).p.u_v(0,\vec{r})d^3r$.
Therefore Eq. (28) can be expressed as

$$\langle|\hat{a}.\mathrm{OME}|^2\rangle_{av}=\frac{2\pi}{3}|\hat{a}P_{cv}(0)|^2\times\left(\frac{\beta^2}{4}\right)\times\left(t+\frac{\rho}{\sqrt{2}}\right)^2\times\left\{\left[1+\frac{E_g+\delta'}{\hbar\omega+\delta'}\right]-(E_g-\delta')\left[\frac{1}{E_g+\delta'}-\frac{1}{\hbar\omega+\delta'}\right]^{1/2}\times\left[\frac{E_g+\delta'}{(E_g-\delta')^2}-\frac{1}{\hbar\omega+\delta'}\right]^{1/2}\right\}^2. \tag{29}$$

Using Eqs. (2) and (29), we get

$$W(\omega)=\left[\frac{1}{\pi}\left(\frac{eA_o}{m}\right)^2\cdot\frac{m_r^{3/2}}{E_g^{3/2}\hbar^4}\hbar\omega((\hbar\omega)^2-E_g^2)^{1/2}\right]\times\left[\frac{2\pi}{3}|\hat{a}.P_{cv}(0)|^2.f_p(\hbar\omega,E_g,\Delta)\right] \tag{30}$$

in which

$$f_p(\hbar\omega,E_g,\Delta)\equiv\frac{\beta^2}{4}\left(t+\frac{\rho}{\sqrt{2}}\right)^2\cdot\left\{\left[1+\frac{E_g+\delta'}{\hbar\omega+\delta'}\right]-(E_g-\delta')\left[\frac{1}{E_g+\delta'}-\frac{1}{\hbar\omega+\delta'}\right]^{1/2}\times\left[\frac{E_g+\delta'}{(E_g-\delta')^2}-\frac{1}{\hbar\omega+\delta'}\right]^{1/2}\right\}^2.$$

Using Eqs. (1) and (30), we finally arrive at the expression of the OAC as

$$\alpha=V\left(\frac{\pi}{3\sqrt{2}}\right)\left(\frac{2m_r}{E_g}\right)^{3/2}\sqrt{(\hbar\omega)^2-E_g^2}\times[f_p(\hbar\omega,E_g,\Delta)], \tag{31}$$

TABLE I. The values of the energy band constants for (a) InSb, (b) InAs, (c) $Hg_{1-x}Cd_xTe$, and (d) $In_{1-x}Ga_xAs_yP_{1-y}$ lattice matched to InP.[25,26]

| | |
|---|---|
| (a) | InSb: $E_g=0.235$ eV, $\Delta=0.803$ eV, $m_c=0.0145\,m_o$, $m_v=0.43\,m_o$ and $n=3.5$; |
| (b) | InAs: $E_g=0.418$ eV, $\Delta=0.38$ eV, $m_c=0.026\,m_o$, $m_v=0.45\,m_o$ and $n=3.96$ |
| (c) | $Hg_{1-x}Cd_xTe$: $E_g=[-0.302+1.93x+5.35(10)^{-4}(1-2x)T-0.810x^2+0.832x^3]$ eV, $\Delta=(0.63+0.24x-0.27x^2)$ eV, $m_c=3\hbar^2E_g(x)[4p^2(x)]^{-1}$, $x=0.2$, $p(x)=[(\hbar^2/2m_o)(18+3x)]^{1/2}$, $m_v=0.4\,m_o$ and $n=3.56$ |
| (d) | $In_{1-x}Ga_xAs_yP_{1-y}$ lattice matched to InP: $E_g=[1.337-0.73y+0.13y^2]$ eV, $\Delta=(0.114+0.26y-0.22y^2)$ eV, $m_c=(0.080-0.039y)m_o$, $y=0.5$, $m_v=0.724\,m_o$ and $n=3.26$ |

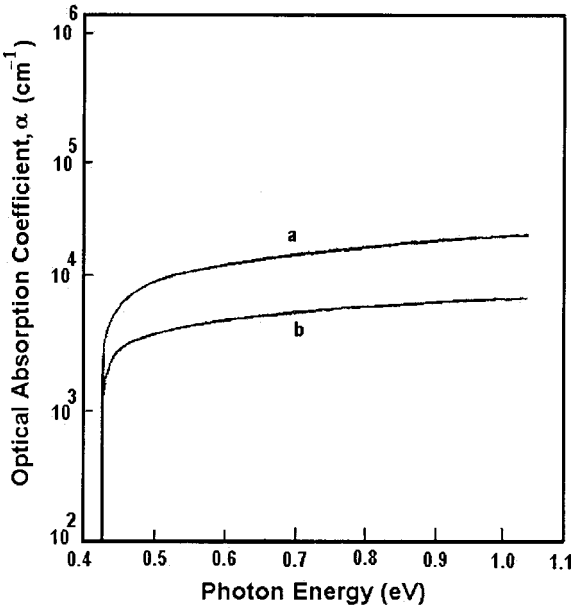


FIG. 1. The plot **a** represents the dependence of the OAC for *n*-InAs as a function of incident photon energy $\hbar\omega$ (in electron volts) in accordance with the three models of Kane while plot **b** exhibits the same dependence for the corresponding isotropic parabolic bands.

where $V \equiv \dfrac{e^2 E_g(E_g+\Delta)}{2,\pi,\hbar^2,n,\varepsilon_o C,m_r\left(E_g+\dfrac{2}{3}\Delta\right)}$.

Equation (31) shows that the OAC is proportional to $\sqrt{(\hbar\omega)^2-E_g^2}$ instead of $\sqrt{(\hbar\omega)-E_g}$ as is well-known in the literature.[1]

### B. Special case

In the limit, as $\Delta \to 0$, Eq. (31) gets transformed as

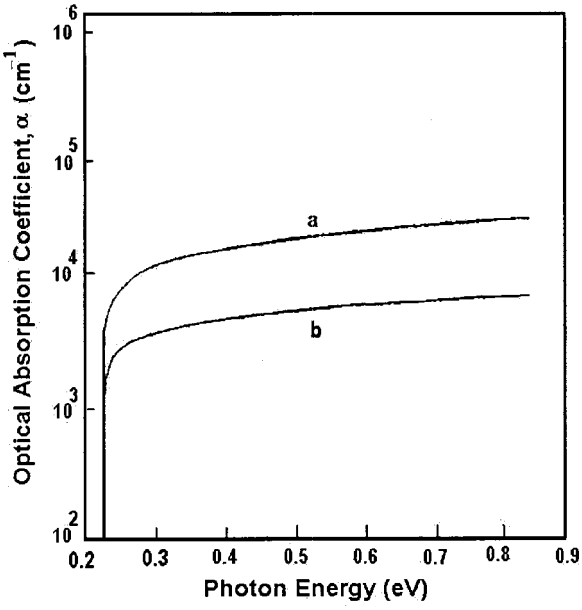


FIG. 2. All cases of Fig. 1 have been plotted for *n*-InSb.

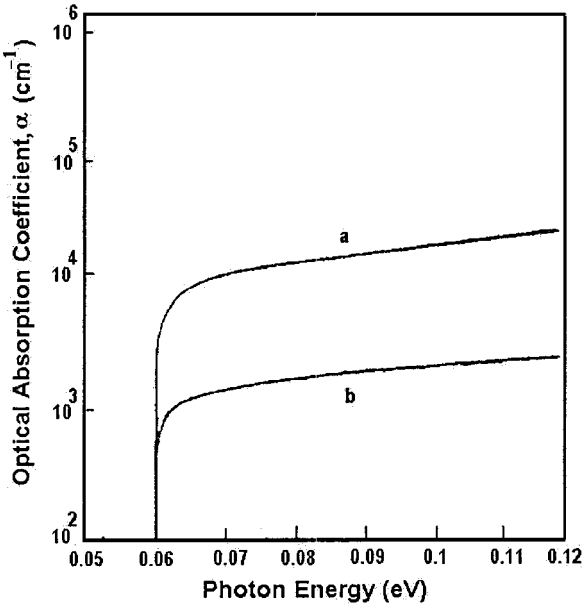


FIG. 3. All cases of Fig. 1 have been plotted for $Hg_{1-x}Cd_xTe$.

$$\alpha = S_o \frac{\pi}{3\sqrt{2}} \cdot \frac{(2m_r)^{3/2} E_g^{1/2}}{(\hbar\omega)^2} \sqrt{(\hbar\omega)^2 - E_g^2};$$
$$S_o = (e^2 E_g/(2,\pi,n,C,\varepsilon_o,m_r,\hbar^2)). \tag{32}$$

Finally, it may be noted that Eq. (32) is valid for semiconductors having parabolic energy bands.[24]

## III. RESULTS AND DISCUSSION

Using Eq. (31) together with parameters as given in Table I, we have plotted in Fig. 1, the OAC for *n*-InAs as function of $\hbar\omega$ (in eV) where the curve (a) represents the three-band model of Kane and curve (b) exhibits the same

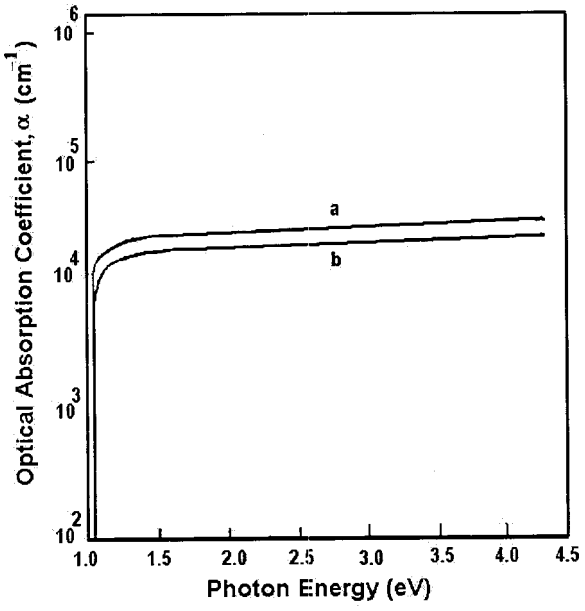


FIG. 4. All cases of Fig. 1 have been plotted for $In_{1-x}Ga_xAs_yP_{1-y}$ lattice matched to InP.

dependence for isotropic parabolic energy bands. In Figs. 2, 3, and 4 and using parameters of Table I, we have plotted all the cases of Fig. 1 for InSb, $Hg_{1-x}Cd_xTe$, and $In_{1-x}Ga_xAs_yP_{1-y}$ lattice matched to InP, respectively.

It appears from Fig. 1 that the OAC is numerically higher for the three-model Kane as compared with the parabolic energy bands. This is due to the fact that $f_p(\hbar\omega, E_g, \Delta)$ is greater than one for the three-model Kane and is equal to one for parabolic energy bands. Besides, $\alpha$ increases as $\hbar\omega$ increases. From Figs. 1 and 2, it appears that the separation between the OAC in accordance with the two models is wider for InSb as compared with that of InAs. From Figs. 3 and 4 we observe that the separation is greatest for $Hg_{1-x}Cd_xTe$ and the least for $In_{1-x}Ga_xAs_yP_{1-y}$ lattice matched to InP, respectively. For greater separation, the low values of $E_g$ and the high values of $\Delta$ are needed. $Hg_{1-x}Cd_xTe$ satisfies this condition whereas for $In_{1-x}Ga_xAs_yP_{1-y}$ lattice matched to InP, the opposite inequalities are applicable for the band constants.

Our formulation is valid for all types of $III-V$, ternary and quaternary materials. For the purpose of condensed presentation, only InSb, InAs, $Hg_{1-x}Cd_xTe$, and $In_{1-x}Ga_xAs_yP_{1-y}$ lattice matched to InP have been considered for the purpose of numerical computations. The influence of energy band constants on the OAC is also apparent from Figs. 1 to 4.

From our generalized results, we have obtained the expression of the OAC for the isotropic parabolic energy bands, which indirectly exhibits the compatibility of our formulation. Finally, it may be noted that the OAC is proportional to $\sqrt{(\hbar\omega)^2 - E_g^2}$, a phenomena which is valid for all types of semiconductors having arbitrary band structures, instead of $\sqrt{(\hbar\omega) - E_g}$ which, in turn, reflects the conventional result.[1]


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