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Effects of energy-band nonparabolicity on the free-carrier absorption in n-type GaP

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The effects of nonparabolicity on the free-carrier absorption in n-type GaP are analyzed on the basis of quantum-mechanical results. It is shown that the absorption coefficient is reduced by about 10–15% in the wavelength range 4-10 μ. The index of wavelength dependence is also somewhat increased.

I. INTRODUCTION

Free-carrier absorption (or, the so-called FCA) in n-type GaP has been studied experimentally by several workers.[1,2] Theoretical values for the absorption coefficient have been obtained by Haga and Kimura[3] and by Wiley and Didomenico.[2] In their analysis, Haga and Kimura considered only acoustic-phonon and polar optical-phonon scattering. As is well-known, the lowest-lying energy-band minima in GaP occurs along the [100] direction away from the zone center, and the constant energy surfaces are ellipsoidal. Wiley and Didomenico extended the analysis of Haga and Kimura by taking into account the ellipsoidal structure of the constant energy surfaces. It was also concluded that experimental results can be explained by considering acoustic-phonon, nonpolar optical phonon and inter-valley scattering. In none of the existing analyses, however, were the effects of nonparabolicity considered. In FCA, the electrons are excited by the incident radiation to fairly high energy levels. For example, for an incident radiation of 2μ wavelength, the energy of an electron may increase by 0.6 eV from the band edge. Even for an energy band gap of 4.5 eV (the theoretically calculated direct band gap[4] corresponding to the conduction-band minima in GaP), the change in electron energy is about $\frac{2}{15}$ of the band gap. The effects of nonparabolicity may thus be significant and for a complete theory of the FCA, its effects should be included in the analysis. In this communication, we have analyzed theoretically the FCA in n-type GaP including the effects of nonparabolicity on the basis of quantum-mechanical results developed by the authors.[5]

II. EXPRESSIONS FOR ABSORPTION COEFFICIENT

We shall assume that the band nonparabolicity is the same for all directions of the wave vector. Since the contribution to FCA is predominantly due to the transverse effective mass which is about one-tenth of the longitudinal effective mass, no significant error should occur even if this assumption is not strictly true.

The E-k relation for the ellipsoidal constant energy surfaces may then be written following Kane[6] as

$$(\hbar^2/2m_0)[(\vec{k}-\vec{k}_0)\cdot\overleftrightarrow{\alpha}\cdot(\vec{k}-\vec{k}_0)] = E(1+E/E_g)\ , \tag{1}$$

where $\vec{k}$ is the electron wave vector, $\vec{k}_0$ is the wave vector corresponding to the energy-band minimum, $\overleftrightarrow{\alpha}$ is the normalized reciprocal effective-mass tensor, and E_g is the energy band gap.

Expressions for the absorption coefficients for the important scattering mechanisms using the above dispersion relation were derived by the present authors in a previous communication.[5] (It may be noted that in Ref. 5, the expression for acoustic-phonon scattering was derived on the assumption that the coupling between free carriers and transverse acoustic phonons is negligible. However, this sort of coupling is important in n-type GaP so that the expression for absorption coefficient applicable to acoustic-phonon scattering has been presented here in a suitably modified form.) These are quoted below for ready reference:

$$\eta_{ac} = \frac{2}{3}\frac{e^2 m_{\parallel} m_{\perp}(k_B T)(L)}{\pi^2\hbar^5 \rho c n \theta^3 K\sqrt{K_1}} \int_0^\infty dP \int_{y_m}^\infty dy\,[f(y)-f(y_0)]\,(\mathrm{I})\,(Q)\ ,$$

$$(L) = \frac{\Xi_d^2}{v_L^2}\left[\tfrac{1}{3}\sqrt{K_1}(2K+1)\right] + \left(\frac{2\,\Xi_d\,\Xi_u}{v_L^2} + \frac{\Xi_u^2}{v_T^2}\right)\left(\frac{K}{K_1}\right)\left[\tfrac{2}{3}\sqrt{K_1}(K+2) - (K+1)\tan^{-1}\sqrt{K_1}\right]$$

$$+\Xi_u^2\left(\frac{1}{v_L^2}-\frac{1}{v_T^2}\right)\left(\frac{K}{K_1}\right)^2\left(\sqrt{K_1}(2K+1) + \frac{1}{3}\frac{\sqrt{K_1}}{K}(-2K^2+14K+3) - (3K+5)\tan^{-1}\sqrt{K_1}\right)\ , \tag{2}$$

$$\eta_{\text{nop},\text{v}} = \frac{2e^2 m_{\parallel} m_{\perp}^2 D^2}{3\pi^2 \hbar^4 \rho c n \beta^2 \theta^3 m_c \omega_l} \sum_{s=+,-} R_s \int_0^\infty dy\,[f(y) - f(y_0)]\,(x x_0^s y y_0^s)^{1/2}$$

$$\times (x+y)(x_0^s + y_0^s)\left[\left(X + \tfrac{1}{3}Z\right)\left(\frac{xy}{(x+y)^2} + \frac{x_0^s y_0^s}{(x_0^s + y_0^s)^2}\right) - \frac{2}{3}\,\frac{Y(x x_0^s y y_0^s)^{1/2}}{(x+y)(x_0^s + y_0^s)}\right], \tag{3}$$

$$\eta_{\text{pop}} = \frac{4}{3}\,\frac{m_{\parallel} e^4 e^{*2}}{M v_a \theta_l \theta^3 \hbar c n (k_B T)^2} \int_0^\infty dP\,\frac{(J)}{P}\left(\sum_{s=+,-} R_s \int_{y_m^s}^\infty dy\,[f(y) - f(y_0^s)](I^s)(Q^s)\right), \tag{4}$$

$$\eta_{\text{imp}} = \frac{8}{3}\,\frac{Z^2 e^6 N_{\text{imp}} K}{\hbar^2 \epsilon_0^2 \theta^3 c n (k_B T)^2} \int_0^\infty dP\,\frac{(M)}{P^2} \int_{y_m}^\infty dy\,[f(y) - f(y_0)]\,(I)(Q) . \tag{5}$$

The symbols ac, nop, v, pop, imp refer to scatterings due to acoustic-phonon, nonpolar optical and intervalley phonon, polar optical-phonon and impurity atom scattering, respectively. In Eqs. (2)–(5), the dimensionless quantities y, y_0, x, x_0, y_0^s, x_0^s, P, θ, θ_l, β are given by

$$\begin{aligned} &y = E_{\vec{k}}/k_B T, && y_0 = y + \theta, \\ &y_0^{\pm} = y + \theta_{\pm}, && \theta_{\pm} = \theta \pm \theta_l, \\ &\theta = \hbar\omega/k_B T, && \theta_l = \hbar\omega_l/k_B T, \\ &x = y + \beta, && x_0^{\pm} = y_0^{\pm} + \beta, \\ &P = \hbar^2(\vec{q}\cdot\overleftrightarrow{\alpha}\cdot\vec{q})/2m_0 k_B T, && \beta = E_g/k_B T. \end{aligned} \tag{6}$$

ω and ω_l being the photon and phonon frequencies, respectively. The meanings of the symbols y_m, $y_m^{\pm}$, $I^{\pm}$, $Q^{\pm}$, $R^{\pm}$, (J), (M), and K are explained as follows:

$$y_m = \tfrac{1}{2}\left\{-\beta + \left[\beta^2 + \frac{\beta^2 P^2 + \beta^2\theta^2 - \theta^4}{\beta P - \theta^2} - 2\left(\frac{\beta P \theta^2(\beta^2 + \beta P - \theta^2)}{\beta P - \theta^2}\right)^{1/2}\right]^{1/2}\right\}$$

$$= \psi(\theta),$$

say,

$$y_m^{\pm} = \psi(\theta_{\pm}),$$

$$Q^{\pm} = \beta\left(\frac{xy}{(x+y)^2} + \frac{x_0^{\pm} y_0^{\pm}}{(x_0^{\pm} + y_0^{\pm})^2} - \frac{xy + x_0^{\pm} y_0^{\pm} - \beta P}{(x+y)(x_0^{\pm} + y_0^{\pm})}\right),$$

$$I^{\pm} = (x+y)(x_0^{\pm} + y_0^{\pm})\, I_{\text{av}}^2(\vec{k}, \vec{q}),$$

$$R^{\pm} = \sinh(\tfrac{1}{2}\theta)/[\sinh(\tfrac{1}{2}\theta_{\pm})\sinh(\tfrac{1}{2}\theta_l)],$$

$$(J) = \tfrac{1}{2}P^2\left[\frac{1}{P_1 P_2} - \frac{3\sqrt{K_1}\,P_1}{K P^2 P_2} - \frac{3\sqrt{K_1}}{K P_1 P_2} + \left(\frac{1}{P_1} + \frac{\sqrt{K_1}}{KP} + \frac{3P_1}{KP^2}\right) \times \frac{1}{\sqrt{K_1}\,P_3}\tan^{-1}(\sqrt{K_1}\,P_4)\right],$$

$$(M) = \tfrac{1}{2}P^2\left[\frac{1}{P_1 P_2} + \frac{1}{K P_1 P_2} + \left(\frac{1}{P_1} - \frac{1}{KP}\right) \times \frac{1}{\sqrt{K_1}\,P_3}\tan^{-1}(\sqrt{K_1}\,P_4)\right], \tag{7}$$

$$\begin{aligned} &P_1 = P + S, && P_2 = KP + S, \\ &P_3 = (PP_1)^{1/2}, && P_4 = (P/P_1)^{1/2}, \\ &K = m_{\parallel}/m_{\perp}, && S = m_0 X_0 / l_0^2\, m_{\perp}, \\ &X_0 = \hbar^2/2m_0 k_B T . \end{aligned}$$

The quantity $I_{\text{av}}(\vec{k}, \vec{q})$ represents the overlap integral the general form of which has been given by Matz,[7] as

$$I_{\text{av}}^2(\vec{k}, \vec{q}) = x + y\cos\theta + Z\cos^2\theta, \quad \theta = (\vec{k}, \vec{k}'), \tag{8}$$

and D, Ξ_d, Ξ_u are, respectively, the electron-nonpolar optical-phonon coupling constant and the acoustic deformation potential constants.[8]

III. FCA IN GaP

We shall now proceed to calculate the contribution to FCA due to the various scattering mechanisms, and finally to estimate the total FCA coefficient for GaP. We assume the three-ellipsoid model to be valid so that the total FCA coefficient will be given by

$$\eta = \eta_{\text{ac}} + \eta_{\text{nop}} + \eta_{\text{pop}} + \eta_{\text{imp}} + 2\eta_{\text{v}} . \tag{9}$$

It has been found that the optical absorption (due to interband transition) in GaP occurs at 3 μ and free-carrier absorption results are available in the wavelength range of 4–10 μ. We have, therefore, made computations in this wavelength region. To demonstrate the effects of nonparabolicity, and also for the sake of comparison with previous results,[2] we have calculated the FCA coefficients for the three cases of $E_g = \infty$, $E_g = 4.5$, $E_g = 3$, in eV units. While the value of 4.5 eV for E_g is taken from theoretical calculations,[4] the first value corresponds to the parabolic limit. However, there is evidence that the effective forbidden gap may be somewhat lower than 4.5 eV and we have made calculations for $E_g = 3$ eV for comparison purposes.

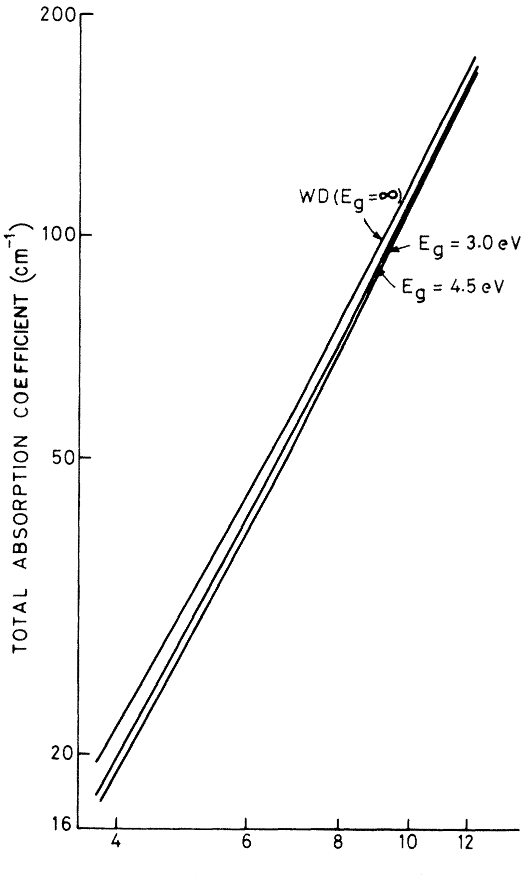

FIG. 1. Effects of nonparabolicity on the total absorption coefficient are shown here. The effects of polar optical-phonon and impurity atom scattering are neglected. The uppermost curve corresponds to the case of infinite band gap and was obtained by Wiley and Didomenico (WD). The central and lowermost curves correspond respectively to band gaps of 4.5 and 3.0 eV.

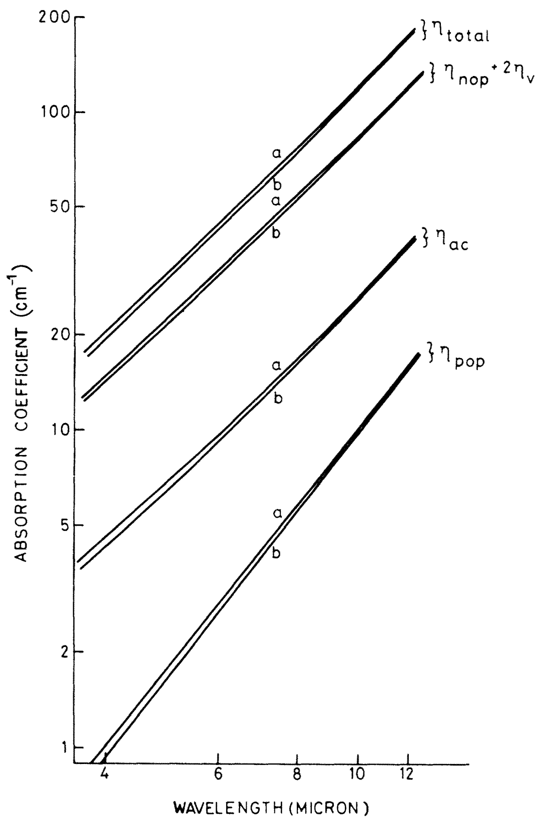

FIG. 2. The contributions of the different scattering mechanisms to the total absorption coefficient. The curves labeled "a" and "b" are, respectively, obtained by using the values 4.5 and 3.0 eV and the band-gap energy. The total absorption coefficients shown here include the effect of polar optical scattering.

The values of the parameters employed for calculations are the same as quoted in Ref. 2.

Our results are shown graphically in Figs. 1 and 2. The effects of nonparabolicity are found to be twofold. One of these is to increase the index of wavelength dependence for each of the different scattering mechanisms. This is illustrated in Table I. The other effect of nonparabolicity is to reduce the absorption coefficient. This fact is evident from the graphs.

In Fig. 2, we have plotted the magnitude of the FCA coefficient for the different scattering mechanisms. We conclude that the effect of ionized impurity scattering is indeed negligible for the con-

TABLE I. Effect of nonparabolicity on the index of wavelength dependence of the absorption coefficients due to the different scattering mechanisms.

Type of scattering	Acoustic			Nonpolar and intervalley			Polar			Ionized impurity		
Value of E_g	∞	4.5	3.0	∞	4.5	3.0	∞	4.5	3.0	∞	4.5	3.0
Index of wavelength dependence	1.87	1.92	1.94	1.84	1.91	1.93	2.42	2.51	2.55	2.76	2.92	3.01

centration range of the experiment[9] (i.e., 3×10^{17}/c.c.). On the other hand, if the polar optical scattering is neglected and the effects of nonparabolicity are included, the theoretical results are about 10% less on the higher-wavelength side and about 5% less on the lower-wavelength side. The contribution of the polar optical scattering (which was neglected in the analysis of Wiley and Didomenico) however makes up for this decrease at large wavelengths and approximate agreement between theory and experiment is obtained when this contribution is taken into account.

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[9]It may be noted that Eq. (5) of the text gives $\eta_{\mathrm{imp}} \cong 0.4$ cm^{-1} at $\lambda = 10\mu$ (assuming $N_{\mathrm{imp}} = N_e$) which is much less than the estimate made in Ref. 3.