

Near-infrared free-carrier optical absorption in silicon: Effect of first-order phonon-assisted scattering in a nonparabolic conduction band

G. N. Koskowich

IBM—General Technology Division, Route 52, Hopewell Junction, New York 12533

M. Soma and R. B. Darling

Department of Electrical Engineering, University of Washington, Seattle, Washington 98195

(Received 1 September 1989)

The scattering rate and free-carrier optical-absorption coefficient for nonpolar dispersionless intervalley phonon scattering are determined for interaction matrix elements of first order in the phonon wave vector. Analytic expressions are derived which include the effect of band nonparabolicity on this contribution to the scattering rate, which was previously demonstrated as the dominant mechanism for free-carrier absorption of near-infrared light in silicon. Comparison with experimental data for *n*-type Si shows improved correlation with the absorption coefficient in the near infrared, using deformation potentials which are consistent with the electron transport properties.

I. INTRODUCTION

The absorption coefficient of semiconductors for photon energies near to but below the band-gap energy is primarily caused by the presence of free carriers. The Drude-Zener theory of free-carrier absorption¹ was one of the earliest treatments of this phenomenon, while others have derived the classical expression based on a solution to the Boltzmann transport equation.² Implicit in these results is the assumption that the photon energy ($\hbar\omega_v$) is small compared with the thermal energy of the electrons ($k_B T$), which yields good agreement with experimental data only for photon energies in the far infrared.

The absorption coefficient for these materials has also been described theoretically using a quantum-mechanical formulation by quantizing the electron states and determining the scattering rates between states due to phonons.³ Expressions for electron scattering due to acoustic, nonpolar optical, and polar optical phonons have been determined and excellent summaries of these results are available.^{1,4} The effect of a nonparabolic band has been derived rigorously for these scattering mechanisms by Das and Nag,⁵ but the resulting expressions require numerical integration. Previously, the authors have calculated the scattering rate and absorption coefficient due to nonpolar dispersionless phonon scattering.⁶ In this paper, new expressions are derived which include band nonparabolicity and result in an improved match between the predicted and observed dispersion of the absorption coefficient of silicon in the near infrared. In addition, the deformation potential which describes the strength of this optical interaction is now nearly equal to the value used by Ferry⁷ to describe the electron transport properties.

Electron scattering in Si has been studied by Ferry⁷ and Long,⁸ who achieved good agreement between the theoretical predictions of a quantum-mechanical treatment and experimental data. Acoustic-phonon and

optical-phonon (630 K) scattering have been used to describe electron transport in Si.⁸ In addition to the scattering processes discussed by Long,⁸ Ferry⁷ used a first-order interaction with a 190-K dispersionless phonon to accurately predict the transport properties of Si at high temperatures. A new analytic expression for this first-order interaction which includes band nonparabolicity is presented in this paper and is used to predict the absorption coefficient of *n*-type Si in the near infrared. The increase in the density of final states for the scattered carriers due to the higher *X* valleys in the Si band structure is included as described by Ridley⁹ for hot-electron transport.

II. ACOUSTIC-PHONON AND NONPOLAR OPTICAL-PHONON ABSORPTION PROCESSES

To predict the absorption coefficient of Si in the near infrared, all the scattering processes which contribute must be included. Expressions for the contributions due to acoustic phonons and optical phonons have been derived elsewhere⁴ and are used in this calculation of the absorption coefficient. The contribution of acoustic-phonon scattering to the absorption coefficient (K_{vac}) as defined by Ridley⁴ is

$$K_{\text{vac}} = \frac{8\alpha_f (2m^* k_B T)^{1/2} \Xi^2 n}{3\pi^{1/2} \eta_r \hbar^2 \omega_v c_L} \sinh \left[\frac{\hbar\omega_v}{2k_B T} \right] K_2 \left[\frac{\hbar\omega_v}{2k_B T} \right], \quad (1)$$

where α_f is the fine-structure constant, m^* is the low-energy (parabolic band) carrier effective mass, k_B is Boltzmann's constant, T is the lattice temperature, Ξ is the effective deformation potential,⁴ n is the carrier concentration, η_r is the index of refraction, \hbar is Planck's constant divided by 2π , ω_v is the photon energy, c_L is the longitudinal phonon velocity, and K_2 is a modified Bessel function of the second kind.

The contribution of optical-phonon scattering⁴ is given by the expression

$$K_{\text{vop}} = \frac{4\alpha_f(2m^*)^{1/2}D_0^2n\{n(\omega_0)[n(\omega_0)+1]\}^{1/2}}{3\pi^{1/2}\eta_r\hbar^3\omega_v^3\omega_0\rho_m(k_B T)^{1/2}} \\ \times \sinh\left[\frac{\hbar\omega_v}{2k_B T}\right] \left[(\hbar\omega_+)^2 K_2 \left[\frac{\hbar\omega_+}{2k_B T} \right] \right. \\ \left. + (\hbar\omega_-)^2 K_2 \left[\frac{|\hbar\omega_-|}{2k_B T} \right] \right], \quad (2)$$

where D_0 is the deformation potential, $n(\omega_0)$ is the Bose-Einstein phonon occupation factor, ω_0 is the optical-phonon frequency, ρ_m is the mass density, $\omega_+ = \omega_v + \omega_0$, and $\omega_- = \omega_v - \omega_0$. These expressions were derived assuming spherical constant-energy surfaces and parabolic bands.⁴ The six Δ valleys in Si form the lowest-energy conduction-band minima and higher-lying X and L valleys⁴ are present which increase the density of final states for the high photon energies under consideration. The parabolic-band approximation also breaks down at high photon (electron) energies and can be included in an approximate manner akin to the method for hot-electron transport described by Ridley.⁹

III. FIRST-ORDER INTERACTION

The absorption-coefficient formulation based on these processes has given good agreement with experimental results for low photon energies. The necessary inclusion of a first-order interaction by Ferry⁷ to describe the transport characteristics at high electron temperatures suggests that this process also contributes significantly to the absorption coefficient at high photon energies. To allow direct comparison with the results given by Eqs. (1) and (2) the contribution due to the first-order interaction is derived following the procedure outlined by Ridley.⁴

The first-order nonpolar optical matrix element can be written as⁷

$$|\langle \mathbf{k} \pm \mathbf{q} | H' | \mathbf{k} \rangle|^2 = \frac{D_1^2 \hbar q^2}{2V\rho_m\omega_0} [n(\omega_0) + \frac{1}{2} \pm \frac{1}{2}] = A_{S\pm} q^r, \quad (3)$$

where H' is the interaction Hamiltonian, \mathbf{k} is the electron wave vector, \mathbf{q} is the phonon wave vector, D_1 is the first-order deformation potential, and V is the volume of a unit cell. The matrix element is often expressed as a constant $A_{S\pm}$ multiplied by a power of q .^{4,7} This simplification is used as it allows the derivation of analytic expressions for the absorption coefficient. To incorporate the effect of nonparabolicity, we take the usual $\mathbf{k} \cdot \mathbf{p}$ theory approximation of

$$\frac{\hbar^2 k^2}{2m^*} = \gamma(E) \approx E(1 + \alpha E), \quad (4)$$

where α is the nonparabolicity factor with magnitude 0.4 eV⁻¹ taken from Ridley.⁹ Also,

$$v(E) = \frac{1}{\hbar} \frac{dE}{dk} = \left[\frac{2\gamma(E)}{m^*} \right]^{1/2} \left[\frac{d\gamma(E)}{dE} \right]^{-1} \quad (5)$$

and

$$N(E) = \frac{k^2}{2\pi^2} \frac{dk}{dE} = \left[\frac{2m^*}{\hbar^2} \right]^{3/2} \frac{[\gamma(E)]^{1/2}}{4\pi^2} \frac{d\gamma(E)}{dE}, \quad (6)$$

where $v(E)$ is the electron velocity, $N(E)$ is the density of states, and E is the electron energy. Assuming a spherical constant-energy surface, the transition rate between electron states is given by

$$W_{\pm}(\mathbf{k}) = \frac{e^2 \hbar^3 n_v}{8\pi^2 \epsilon_v (\hbar\omega_v)^3 m^{*2} (1 + 2\alpha E)^2} \\ \times \int |\langle \mathbf{k} \pm \mathbf{q} | H' | \mathbf{k} \rangle|^2 (\mathbf{a} \cdot \mathbf{q})^2 \delta(E_f - E_i) d\mathbf{q}, \quad (7)$$

where \pm refers to the phonon absorption (+) and emission (-) processes, e is the electronic charge, n_v is the photon density, ϵ_v is the permittivity, \mathbf{a} is the vector magnetic potential, and δ is the Dirac delta function which implies energy conservation between the initial electron energy (E_i) and the final electron energy (E_f). The transition rate for this first-order process ($r=2$) is given by

$$W_{\pm}(\mathbf{k}) = \frac{e^2 \hbar n_v A_{S\pm}}{6\pi \epsilon_v (\hbar\omega_v)^3 m^{*2} (1 + 2\alpha E)} \left[\frac{2m^*}{\hbar^2} \right]^{5/2} \\ \times (E + \hbar\omega_{\pm})^{1/2} \left[\frac{16}{3} E^2 + \frac{16}{3} (\hbar\omega_{\pm}) E + (\hbar\omega_{\pm})^2 \right], \quad (8)$$

where $\omega_{\pm} = \omega_v \pm \omega_0$.

Further assuming no orientational dependence of the scattering processes and Boltzmann statistics, the photon-absorption rate can then be calculated using the expression⁴

$$W_{v\pm} = \int_0^{\infty} W_{\pm}(\mathbf{k}) f(E) 2V N(E) dE, \quad (9)$$

where $f(E)$ is the Fermi-Dirac distribution function. Performing the integration yields the result

$$W_{v\pm}^{\text{abs}} = \frac{2nV}{\pi^{1/2} (k_B T)^{3/2}} \frac{e^2 \hbar n_v A_{S\pm} (\hbar\omega_{\pm})^4}{72\pi \epsilon_v (\hbar\omega_v)^3 m^*} \\ \times \left[\frac{2m^*}{\hbar^2} \right]^{5/2} \beta(\hbar\omega_{\pm}) \exp\left[\frac{\hbar\omega_{\pm}}{2k_B T} \right] \\ \times \left[K_4 \left[\frac{\hbar\omega_{\pm}}{2k_B T} \right] - K_2 \left[\frac{\hbar\omega_{\pm}}{2k_B T} \right] \right] \quad (10)$$

for photon absorption, where

$$\begin{aligned}
\beta(\hbar\omega_{\pm}) = & \left\{ 1 + \alpha(\hbar\omega_{\pm}) \left[\frac{2}{z} K_4 \left(\frac{z}{2} \right) - \frac{3}{z} K_3 \left(\frac{z}{2} \right) + \frac{1}{z} K_2 \left(\frac{z}{2} \right) + \frac{3}{4} K_0 \left(\frac{z}{2} \right) \right] \right. \\
& + (\alpha\hbar\omega_{\pm})^2 \left[\frac{1}{32} K_6 \left(\frac{z}{2} \right) - \frac{2}{z} K_4 \left(\frac{z}{2} \right) + \frac{15}{8z} K_3 \left(\frac{z}{2} \right) - \frac{1}{z} K_2 \left(\frac{z}{2} \right) + \frac{71}{32} K_0 \left(\frac{z}{2} \right) \right] \\
& + \frac{(\alpha\hbar\omega_{\pm})^3}{192} \left[\frac{1}{2} K_7 \left(\frac{z}{2} \right) - K_6 \left(\frac{z}{2} \right) + 2K_5 \left(\frac{z}{2} \right) - 7K_4 \left(\frac{z}{2} \right) \right. \\
& \left. \left. + 47K_2 \left(\frac{z}{2} \right) - \frac{15}{2} K_1 \left(\frac{z}{2} \right) + 30K_0 \left(\frac{z}{2} \right) \right] \right\} \left[\frac{3}{z} K_3 \left(\frac{z}{2} \right) \right]^{-1}
\end{aligned} \tag{11}$$

describes the effect of the nonparabolic bands on the absorption (and emission) rate and $z = \hbar\omega_{\pm}/k_B T$. The emission process is described by changing the sign of $\hbar\omega_{\pm}$ in (10).

The contribution of the first-order interaction to the absorption coefficient is then calculated by considering the difference between the photon absorption and emission processes⁴ using

$$K_{\nu 1} = \frac{1}{v_{\nu} n_{\nu}} (W_{\nu_{\pm}}^{\text{abs}} - W_{\nu_{\pm}}^{\text{em}}), \tag{12}$$

where v_{ν} is the velocity of light in the medium. This leads directly to an analytic expression for the absorption coefficient due to the first-order interaction,

$$\begin{aligned}
K_{\nu 1} = & \frac{\eta_r n e^2 D_1^2 \hbar^2 \{n(\omega_0)[n(\omega_0+1)]\}^{1/2}}{6c \pi^{3/2} (\hbar\omega_{\nu})^3 \omega_0 m^* \epsilon_{\nu} \rho_m (k_B T)^{1/2}} \left[\frac{2m^*}{\hbar^2} \right]^{5/2} \sinh \left[\frac{\hbar\omega_{\nu}}{2k_B T} \right] \\
& \times \left[(\hbar\omega_{+})^3 K_3 \left[\frac{\hbar\omega_{+}}{2k_B T} \right] \beta(\hbar\omega_{+}) + (|\hbar\omega_{-}|)^3 K_3 \left[\frac{|\hbar\omega_{-}|}{2k_B T} \right] \beta(|\hbar\omega_{-}|) \right],
\end{aligned} \tag{13}$$

where c is the speed of light.

IV. APPLICATION TO SILICON

Infrared absorption in Si has been measured by Spitzer and Fan,¹⁰ who attempted to characterize their data using the Drude-Zener theory. Their data was subsequently analyzed by Basu and Nag¹¹ using a deformation-potential description for acoustic-phonon and nonpolar optical-phonon-scattering processes. The deformation-potential values were taken from Long,⁸ to maintain con-

sistency with electron transport in Si. Basu and Nag¹¹ achieved good agreement (<30% error) for wavelengths greater than 5 μm and suggested that a correction of the effective mass would improve the error to <15%.

After the work of Basu and Nag¹¹ and Long,⁸ Ferry⁷ proposed the inclusion of a low-energy phonon (190 K), which induced electron scattering via a first-order interaction, to account for the discrepancies between the theory and data presented by Long for electron transport. The transport theory described by Ferry is accurate for energies up to 50 meV. Beyond this energy, Ridley⁹ has

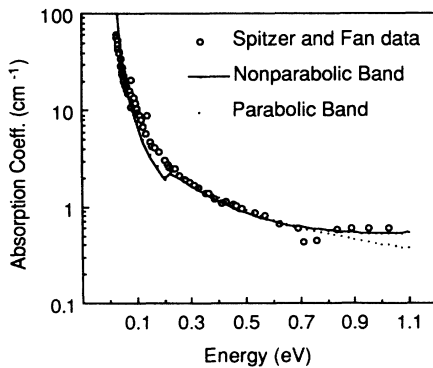


FIG. 1. Free-carrier absorption calculated using nonparabolic-band and parabolic-band first-order scattering theory compared with experimental data.

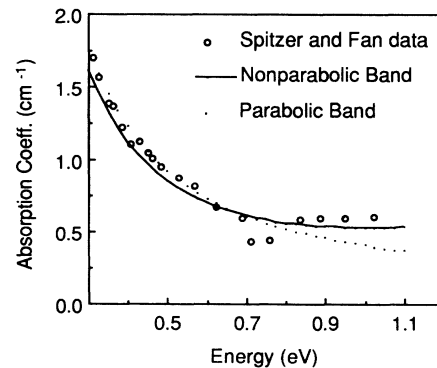


FIG. 2. Expanded view illustrating improved dispersion characteristics of the nonparabolic-band first-order scattering result.

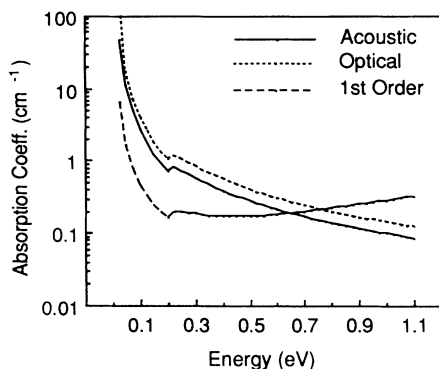


FIG. 3. Contribution of each scattering process to the absorption coefficient.

given a detailed analysis of hot-electron transport which included the effects of nonparabolicity and the higher-lying X and L valleys. The higher-lying X valleys increase the density of states for energies greater than 0.2 eV. This effect was incorporated as a correction to the free-carrier absorption coefficient, in the manner described by Ridley.⁹ The effect of ellipsoidal energy surfaces on the free-carrier absorption coefficient has been derived by Risken¹² and is also included in an approximate manner as suggested therein.

To illustrate the effect of the first-order phonon interaction we consider the absorption data of Spitzer,¹⁰ with the impurity absorption band removed as described in Ref. 11. The results of Basu and Nag¹¹ (which used the deformation-potential values of Long⁸ are compared with our model which includes the first-order interaction as shown in Figs. 1 and 2. We have used the deformation potentials given in Ref. 7 for acoustic and optical phonons. Ferry used 5.6 eV for the first-order deformation potential in his description of the electron transport properties. The new result given by Eqs. (11) and (13) gives a best fit with a deformation potential of 5.9 eV, well within the margin given by Ferry⁷ for his results describing the electron mobility. This close match of the resulting deformation-potential values (5.6 versus 5.9 eV) is a significant improvement over our prior result, which required a value of 7.4 eV to attain similar agreement with the experimental data. The relative contributions to the absorption coefficient of acoustic-phonon scattering, optical-phonon scattering, and the first-order interaction are shown in Fig. 3. For photon energies below 0.1 eV the effect of the first-order interaction can be considered

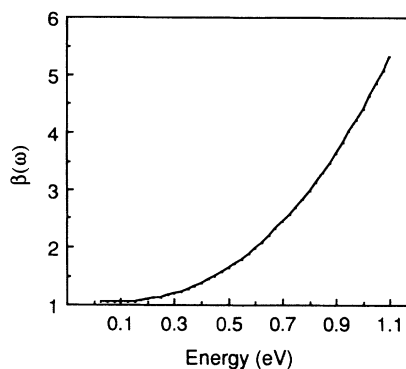


FIG. 4. Energy dependence of the nonparabolic-band correction factor.

negligible, while for the energies of interest for integrated optoelectronics (i.e., 0.4–1.0 eV) it is the largest component of the total free-carrier absorption. Incorporating this new result for the first-order interaction further improves the theoretical dispersion characteristics in the near infrared, and has a smaller magnitude than our previous result⁸ over the energy range (<0.1 eV) which is well described by classical techniques. The abrupt increase in the theoretical result at 0.2 eV shown in Figs. 1 and 3 is due to the density-of-states increase caused by the presence of the higher-lying X valleys. The absence of similar structure in the experimental data may be due to thermal broadening. The effect of band nonparabolicity described by $\beta(\omega)$ is shown for the silicon conduction band in Fig. 4.

V. CONCLUSIONS

Free-carrier absorption due to first-order phonon scattering has been reexamined using an analytic expression for the conduction-band nonparabolicity and was used to predict the absorption coefficient of silicon in the near infrared. The absorption coefficient using this new result utilizes a deformation potential which is nearly equal to the value proposed by Ferry to describe the electron transport properties. Inclusion of the new first-order scattering result improves the correlation between theory and experiment for photon absorption at energies between 0.2 and 1.1 eV (the band-gap energy) while maintaining the fit using classical expressions for lower energies.

¹K. Seeger, *Semiconductor Physics*, 2nd ed. (Springer-Verlag, New York, 1982), pp. 343–355.

²H. Y. Fan, W. Spitzer, and R. J. Collins, *Phys. Rev.* **101**, 566 (1956).

³W. P. Dumke, *Phys. Rev.* **124**, 1813 (1963).

⁴B. K. Ridley, *Quantum Processes in Semiconductors* (Oxford University Press, New York, 1982), pp. 217–226.

⁵A. K. Das and B. R. Nag, *Phys. Status Solidi B* **69**, 329 (1975).

⁶G. N. Koskovich, R. B. Darling, and M. Soma, *Phys. Rev. B*

38, 1281 (1989).

⁷D. K. Ferry, *Phys. Rev. B* **14**, 1605 (1976).

⁸D. Long, *Phys. Rev.* **120**, 2024 (1960).

⁹B. K. Ridley, *Solid-State Electron.* **24**, 147 (1981).

¹⁰W. Spitzer and H. Y. Fan, *Phys. Rev.* **108**, 268 (1957).

¹¹P. K. Basu and B. R. Nag, *Phys. Status Solidi B* **53**, K61 (1972).

¹²H. Risken and H. J. C. Meyer, *Phys. Rev.* **123**, 416 (1961).