Effect of first-order phonon-assisted scattering on near-infrared free-carrier optical absorption in silicon

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The scattering rate and free-carrier optical-absorption coefficient for nonpolar dispersionless intervalley scattering is determined for interaction matrix elements of first order in the phonon wave vector. This scattering mechanism is known to be significant at high electron temperatures in Si and its effect on the optical properties is discussed. Comparison with experimental data for n-type Si shows improved correlation with the absorption coefficient in the near infrared, with use of 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. One of the earliest treatments of this phenomenon resulted in the Drude-Zener theory of free-carrier absorption.[1] This is a classical treatment which can also be derived based on a solution to the Boltzmann transport equation.[2] Good agreement between this result and experimental data occurs for photon energies in the far infrared where the photon energy $(\hbar\omega_v)$ is small compared with the thermal energy of the electrons $(k_B T)$.

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] Piezoelectric and charged impurity scattering may also be present,[4] and contribute to the absorption coefficient. Piezoelectric scattering does not occur in Si and will not be considered here although it may be important for III-V and II-VI compound materials.

Recently there has been a renewed interest in the optical properties of crystalline silicon (Si) at near infrared energies for integrated optics applications[5] and optical voltage measurement in integrated circuits.[6,7] The Drude-Zener theory with an appropriate carrier effective mass has been used to describe the optical properties in this region.[5] This leads to an inaccurate description of the energy dependence of the absorption coefficient at these energies. In order to maintain good agreement with the free-carrier absorption data in the far infrared, the Drude-Zener theory underestimates the absorption coefficient in the near infrared.

Electron scattering in Si has been studied by Long[8] and Ferry,[9] 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] Ferry[9] used a first-order interaction with a 190-K dispersionless phonon to accurately predict the transport properties of Si at high lattice temperatures. This process has thus far been omitted in the calculation of the free-carrier absorption coefficient. An analytic expression for this first-order interaction is presented in this paper and is used to predict the absorption coefficient of n-type Si in the near infrared. In addition, the effect of higher X valleys in the Si band structure is included as described by the hot-electron transport theory of Ridley.[10] An adjusted value of the deformation potential for the first-order interaction Si is calculated which is consistent with both the experimentally measured mobility characteristics and the absorption coefficient.

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 elsewhere[4] 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 Ridley[4] is

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

$$\text{(1)}$$

where α 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 scattering[4] is given by the expression

$$K_{\text{vop}} = \frac{4\alpha(2m^*)^{1/2}D_o^2 n\{n(\omega_o)[n(\omega_o)+1]\}^{1/2}}{3\pi^{1/2}\eta_r\hbar^3\omega_v^3\omega_o\rho_m(k_BT)^{1/2}}$$

$$\times \sinh\left[\frac{\hbar\omega_v}{2k_BT}\right]\left[(\hbar\omega_+)^2 K_2\left[\frac{\hbar\omega_+}{2k_BT}\right]\right.$$

$$\left. + (\hbar\omega_-)^2 K_2\left[\frac{|\hbar\omega_-|}{2k_BT}\right]\right], \quad (2)$$

where D_o is the deformation potential, $n(\omega_o)$ is the Bose-Einstein phonon occupation factor, ω_o is the optical-phonon frequency, ρ_m is the mass density, $\omega_+ = \omega_v + \omega_o$, and $\omega_- = \omega_v - \omega_o$. These expressions were derived assuming spherical constant energy surfaces and parabolic bands.[4] The six Δ valleys in Si form the conduction band and higher-lying X and L valleys[4] 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.[10]

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 Ferry[9] 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 as[9]

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

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, 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.[4,9] This simplification allows the derivation of analytic expressions for the absorption coefficient and will be used. Assuming a spherical constant energy surface and a parabolic band the transition rate between electron states is given by[4]

$$W_\pm(\mathbf{k}) = \frac{e^2\hbar^3 n_v}{8\pi^2\epsilon_v(\hbar\omega_v)^3 m^{*2}}\int |\langle \mathbf{k}\pm\mathbf{q}|H'|\mathbf{k}\rangle|^2(\mathbf{a}\cdot\mathbf{q})^2$$

$$\times \delta(E_f - E_i)d\mathbf{q}, \quad (4)$$

where $\pm$ refers to the phonon absorption $(+)$ and emission $(-)$ processes, e is the electronic charge, n_v is the number of photons, ϵ_v is the permittivity, $\mathbf{a}$ is the vector magnetic potential, and δ is the Dirac δ 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

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

$$\times [\tfrac{16}{3}E^2 + \tfrac{16}{3}(\hbar\omega_\pm)E + (\hbar\omega_\pm)^2], \quad (5)$$

where $\omega_\pm = \omega_v \pm \omega_o$.

Further assuming no orientational dependence of the scattering processes and Boltzmann statistics, the photon absorption rate can then be calculated using the expression[4]

$$W_{v\pm} = \int_0^\infty W_\pm(\mathbf{k})f(E_k)(2V)N(E_k)dE_k, \quad (6)$$

where $f(E_k)$ is the Fermi-Dirac distribution function, $N(E_k)$ is the density of states, and E_k is the electron energy. Performing the integration yields the result

$$W_{v\pm}^{\text{abs}} = \frac{2nV}{\pi^{1/2}(k_BT)^{3/2}}\frac{e^2\hbar n_v A_{S\pm}(\hbar\omega_\pm)^4}{72\pi\epsilon_v(\hbar\omega_v)^3 m^*}\left[\frac{2m^*}{\hbar^2}\right]^{5/2}$$

$$\times \exp\left[\frac{\hbar\omega_\pm}{2k_BT}\right]\left[K_4\left[\frac{\hbar\omega_\pm}{2k_BT}\right] - K_2\left[\frac{\hbar\omega_\pm}{2k_BT}\right]\right] \quad (7)$$

for photon absorption. The emission process is described by changing the sign of $\hbar\omega_v$ in (7).

The contribution of the first-order interaction to the absorption coefficient is then calculated by considering the difference between the photon absorption and emission process[4] using the equation

$$K_{v1} = \frac{1}{v_v n_v}(W_{v\pm}^{\text{abs}} - W_{v\pm}^{\text{em}}), \quad (8)$$

where v_v is the velocity of light in the medium, and n_v is the number of photons. This leads directly to an analytic expression for the absorption coefficient due to the first-order interaction,

$$K_{v1} = \frac{\eta_r n e^2 D_1^2 \hbar^2 \{n(\omega_o)[n(\omega_o)+1]\}^{1/2}}{6c\pi^{3/2}(\hbar\omega_v)^3\omega_o m^*\epsilon_v\rho_m(k_BT)^{1/2}}\left[\frac{2m^*}{\hbar^2}\right]^{5/2}$$

$$\times \sinh\left[\frac{\hbar\omega_v}{2k_BT}\right]\left[(\hbar\omega_+)^3 K_3\left[\frac{\hbar\omega_+}{2k_BT}\right]\right.$$

$$\left. + (|\hbar\omega_-|)^3 K_3\left[\frac{|\hbar\omega_-|}{2k_BT}\right]\right], \quad (9)$$

where c is the speed of light.

IV. APPLICATION TO SILICON

Infrared absorption in Si has been measured by Spitzer and Fan[11] who attempted to characterize their data using the Drude-Zener theory. Their data was subsequently analyzed by Basu and Nag[12] 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 consistency with electron transport in Si. Basu and Nag[12] achieved good agreement (< 30% error) for wavelengths greater than 5 μ and suggested that a correction of the effective mass would improve the error to < 15%.

After the work of Basu and Nag[12] and Long,[8] Ferry[9] proposed the inclusion of a low-energy phonon, 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 the transport phenomena has been studied by Ridley[10] who gave a detailed analysis of hot-electron transport which included the effects of nonparabolicity and higher lying X and L valleys. Nonparabolicity induces an energy-dependent effective mass and alters the density of states function. The higher-lying X valleys increase the density of states for energies greater than 0.2 eV. Both these effects were incorporated as corrections to the free-carrier absorption coefficient given by (1), (2), and (9), in the manner described by Ridley.[10] The effect of ellipsoidal energy surfaces on the free-carrier absorption coefficient has been described by Risken[13] and is also included in this analysis.

To illustrate the effect of the first-order phonon interaction we consider the absorption data of Spitzer,[11] with the impurity absorption band removed as described in Ref. 12. The results of Basu and Nag[12] (which used the deformation potential values of Long[8]) are compared with our model which includes the first-order interaction as shown in Fig. 1. We have used the deformation potentials given in Ref. 9 for acoustic and optical phonons, and a slightly stronger coupled first-order interaction. Ferry used 5.6 eV for the first-order deformation potential, while we have used a value of 7.9 eV. The contribution
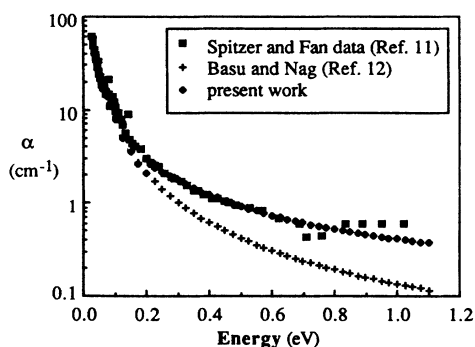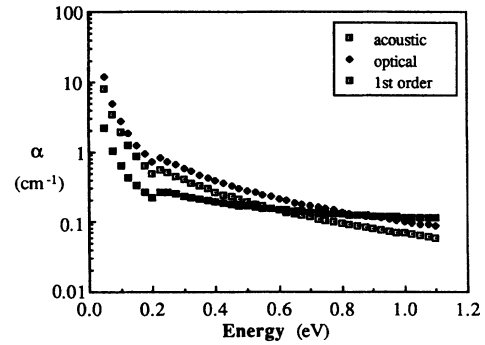

FIG. 2. Contributions to the absorption coefficient from each scattering process.

of the first-order interaction to the electron mobility is small, and using this value maintains the excellent fit to the transport data shown in Ref. 9 while improving agreement of the theory with the experimental data for free-carrier absorption. The relative contributions to the absorption coefficient of acoustic-phonon scattering, optical-phonon scattering, and the first-order interaction are shown in Fig. 2. For photon energies below 0.2 eV the effect of the first-order interaction could be considered negligible, while for the energies of interest for integrated optics (i.e., 0.2–1.0 eV) it is a major component of the total free-carrier absorption.

Existence of the first-order interaction of phonons in Si is further confirmed by this result as the wavelength dependence of the absorption coefficient cannot be described using optical-phonon scattering alone. Incorporating the first-order interaction improves the theoretical dispersion characteristics. The abrupt increase in the theoretical result at 0.2 eV shown in Figs. 1 and 2 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.

V. CONCLUSIONS

Free-carrier absorption due to the phonon scattering via a first-order interaction has been examined and was used to predict the absorption coefficient of silicon in the near infrared. The absorption coefficient using this theory maintains the good fit to the experimental data of Ref. 11 given by Ref. 12, for photon energies less than 0.2 eV. Inclusion of the first-order scattering process results in an improvement in the correlation between theory and experiment for photon energies between 0.2 and 1.1 eV (the band-gap energy), due to the different dispersion characteristics of the first-order interaction.

ACKNOWLEDGMENT

FIG. 1. Comparison of theoretical results and experimental data for free-carrier optical absorption in silicon.

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