Optical heating in semiconductors

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A theory for optical heating in semiconductors has been formulated in terms of the coupled diffusion equations for heat and excess carrier density. The solution for the temperature increase near the surface of the material is given by a general expression which is applicable to a broad range of semiconductors and excitation conditions. The present theory is considerably more comprehensive than previous closed-form results in that the optical and transport properties of the material are allowed to be arbitrary functions of photoexcited-carrier density and temperature.

I. INTRODUCTION

With the relatively recent development of the high-power laser, the generation of dense plasmas of optically excited electrons and holes has become a powerful tool for studying semiconductor properties. Experiments of the last 15 years have shown that many of the basic optical and transport parameters can be highly sensitive to the presence of laser-generated carriers. Examples include the intrinsic¹⁻³ and free-carrier^{4,5} optical absorption, reflectivity,^{6,7} electron and hole mobilities,⁵⁻⁸ ambipolar diffusion coefficient,⁹ and the free-carrier lifetime.¹⁰⁻¹²

When a semiconductor is irradiated by intense laser light, a frequent consequence is the production of heat. Laser heating is a complex process which takes place in a number of steps and involves a variety of semiconductor properties. While the optical properties govern the absorption of laser energy by the material, the free-carrier transport and recombination properties are also relevant since most of the radiation absorbed by a semiconductor goes initially into the system of mobile electrons and holes.¹³

Apart from the general interest in characterizing the temperature within a semiconductor during optical excitation, an accurate determination of laser heating is essential to a number of specific applications, such as laser annealing and laser damage (due to surface melting). As a consequence, several closed-form theoretical models have been proposed in recent years.¹⁴⁻¹⁹ However, these share the important drawback that the carrier density and temperature dependence of the various optical and transport properties have not been taken into account in a comprehensive way. That is, either the dependences are ignored entirely,¹⁴⁻¹⁶ or their inclusion is of limited scope.¹⁷⁻¹⁹ As an alternative to obtaining an approximate closed-form result, calculations have recently appeared in which the coupled partial differential

equations for temperature and excess-carrier density have been solved numerically.^{20,21} Unfortunately, such calculations are tedious, require a great deal of computer time, and offer little physical insight into the heating process.

Derived in the following sections is a first-principles theory for the heating of a semiconductor surface due to laser irradiation. The result is obtained in the form of closed-form expressions which contain no adjustable parameters. The material properties are allowed to depend in a general way on temperature and optically excited carrier density, which means that such nonlinear effects as the dynamic Burstein shift, free-carrier absorption, two-photon carrier generation, carrier diffusion, and radiative and Auger recombination can be accounted for. The inclusion of these "dynamic" processes, particularly at short pulse durations, can have a significant effect on the calculated temperature increase which results from the laser heating.

In Sec. II below the various physical processes involved in the absorption of laser energy and its conversion to heat are discussed. The temperature increase expected to result from the irradiation is considered from a phenomenological standpoint. In Sec. III the problem is rigorously formulated in terms of the coupled diffusion equations for temperature and excess-carrier density. Section IV then deals with the derivation of approximate closed-form solutions to the diffusion equations in the region near the surface of the material. The final result obtained for the laser power density required to increase the surface temperature of the semiconductor by a given amount is general with respect to the dependence of the material parameters on laser-generated carrier density and temperature. In Sec. V this expression is applied to the specific example of surface melting in InSb due to Q-switched CO₂ laser pulses. As a comprehensive test of the theory, a detailed comparison with experimental laser damage

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thresholds of germanium, silicon, InSb, and GaAs for a broad range of laser wavelengths and pulse durations will be dealt with in a future publication. 22

II. PHYSICS OF OPTICAL HEATING

To accurately calculate the temperature increase in a laser-irradiated semiconductor it is necessary to consider in detail the various processes involved in the absorption of optical energy and its conversion to lattice heat. The processes which must be considered include the following: (1) the absorption of photons in the semiconductor, resulting in the creation of electron-hole pairs, carrier heating, or both, (2) thermalization of "hot" electrons and holes to quasiequilibrium with their respective carrier populations, (3) diffusion of the excess electrons and holes, (4) carrier recombination, and possible transfer of the recombination energy in the lattice, and (5) diffusion of the excess lattice heat which is generated at steps (2)and (4).

In order to illustrate the effect of some of these processes on the dynamics of laser heating, we consider a specific example involving the intrinsic absorption of a photon whose energy $h\nu$ is considerably greater than the gap energy E_g . For convenience, a simplified band structure is assumed. Figure 1(a) illustrates the absorption of a photon (A) and subsequent thermalization of the photoexcited carriers (B). Since $h\nu \gg E_g$, the newly created electron and hole have energies E_n and E_p in excess of the quasiequilibrium values E_{Tn} and E_{Tp} , respectively²³ (indicated by the dashed lines). The hot electron and hole rapidly relax to quasiequili-



FIG. 1. (a) Photon absorption (A) and carrier thermalization (B) for a simplified semiconductor band structure. E_i and E_{Ti} represent the newly created carrier energy and the quasiequilibrium energy, respectively. (b) Auger recombination (C) involving transfer of the recombination energy E_R to a second electron (D) and eventual thermalization (E) of the hot electron.

brium with their respective populations, primarily through collisions with phonons and other carriers. Since thermalization typically occurs on a psec time scale, significant carrier diffusion has not yet occurred. The thermalization energy E_T $(=E_n - E_{Tn} + E_p - E_{Tp})$ therefore tends to be converted to lattice heat within one absorption length, α^{-1} , of the surface of the sample. After diffusing through the crystal for some period of time, the electron and hole eventually recombine. The dominant recombination mechanism at high excitation levels is often the Auger process, which is illustrated in Fig. 1(b). In this process, the electronhole recombination energy (C),

$$E_{R} = h\nu - E_{T} = E_{R} + E_{TR} + E_{TP}, \qquad (1)$$

is transferred to a third carrier, in this case an electron (D). The Auger electron then rapidly thermalizes (E), transferring the energy E_R to the lattice. Typically, this occurs within the depth $\alpha^{-1}+L_p$, where L_p is the ambipolar carrier diffusion length. (If recombination occurs by a radiative rather than Auger process, the energy E_R goes into the emission of photons, which must be reabsorbed before heating can occur.) Once the absorbed energy is converted to lattice heat, it is free to diffuse to greater depths via thermal conduction.

If we assume the sample to be semi-infinite, all of the laser energy entering the semiconductor in a cross-sectional area A is absorbed in the material. This energy can be written

$$\epsilon = (1 - R) P_0 A t_p, \tag{2}$$

where R is the reflectivity, P_0 the laser power density, and t_i the laser pulse length. If this energy is added uniformly within a depth l of the surface, the temperature increases may be written

$$\Delta T = \epsilon / \rho c A l, \tag{3}$$

where ρ is the mass density of the material and cthe specific heat. This assumes that ΔT is sufficiently small so that all the parameters in Eq. (3) may be considered constant. The temperature increase ΔT depends simply on the density, the specific heat, and the added energy per unit volume ϵ/Al . In general, ϵ may be expressed in terms of the components

$$\epsilon = \epsilon_T + \epsilon_B^{NR} + \epsilon_B^R + \epsilon_S^{NR} + \epsilon_S^R, \tag{4}$$

where ϵ_T represents the thermalization energy of hot electrons and holes which is converted to lattice heat immediately after absorption of the photon, ϵ_B^{NR} is the increase in lattice energy resulting from nonradiative bulk recombination, ϵ_B^R is the radiative bulk recombination energy which appears as emitted photons, and ϵ_S^{NR} and ϵ_S^R represent energy going into nonradiative or radiative surface recombination, respectively. The thermalization energy ϵ_T contains contributions from carriers heated by free-carrier absorption as well as from the relaxation of hot electron-hole pairs. It is assumed that the radiative components ϵ_B^R and ϵ_S^R do not contribute to heating.²⁴

Generally, the lattice heating associated with the various ϵ 's listed in Eq. (4) is distributed over different depths in the material. If we define the thermal diffusion length, L_T , to be the distance heat can diffuse by the end of the laser pulse, then heating which results from the thermalization energy ϵ_T occurs roughly over the depth $l_T \approx \alpha^{-1} + L_T$. Since the excess carriers diffuse before bulk recombination occurs, the energy ϵ_B^{NR} is distributed over a depth $l_B^{NR} \approx \alpha^{-1} + L_D + L_T$. The nonradiative surface recombination energy ϵ_S^{NR} , which originates at the surface, is distributed over a depth $l_S^{NR} \approx L_T$. We see then that $l_S^{NR} < l_T < l_B^{NR}$.

If we consider the three energy components ϵ_T , ϵ_B^{NR} , and ϵ_S^{NR} distributed over their respective depths, Eqs. (2)-(4) can be combined to yield the approximate laser power density needed to increase the surface temperature by ΔT :

$$P_0 = \frac{\rho c \Delta T L_H}{(1-R)t_p},\tag{5}$$

where

$$L_{H} \equiv [\chi_{T} / (\alpha^{-1} + L_{T}) + \chi_{B}^{NR} / (\alpha^{-1} + L_{D} + L_{T}) + \chi_{S}^{NR} / L_{T}]^{-1}, \qquad (6)$$

and $\chi_i \equiv \epsilon_i / \epsilon$ (e.g., χ_B^{NR} is the fraction of the total energy entering the sample which goes into nonradiative bulk recombination, etc.). The quantity L_H may be thought of as a generalized, composite heating depth. Stagni¹⁶ has proposed a similar expression for calculating laser damage thresholds in semiconductors. However, when applied to cases involving large ΔT , Eq. (5) can lead to substantial error because it does not take into account the dependences of the material parameters on temperature and optically excited carrier density. More general expressions which take these dependences into account will be obtained in the sections which follow.

III. MATHEMATICAL FORMULATION

A comprehensive model for optical heating in semiconductors is now formulated in which the material parameters are functionally dependent on temperature and optically generated carrier density. Coupling between the semiconductor and the laser radiation is assumed to occur via three principal absorption mechanisms, so that the total absorption coefficient α can be written

$$\boldsymbol{\alpha} = \boldsymbol{\alpha}_{FC} + \boldsymbol{\alpha}_1 + \boldsymbol{\alpha}_2. \tag{7}$$

The free-carrier absorption coefficient α_{FC} is proportional to the carrier density and absorption cross section for each type of carrier. The one-photon and two-photon band-to-band contributions, α_1 and α_2 , result in the generation of excess electrons and holes. Since α_2 corresponds to the simultaneous absorption of two photons, it is dependent on the power density of the radiation, i.e., $\alpha_2 = \beta(1-R)P_0e^{-\alpha_z}$, where β is the two-photon absorption coefficient and z is the depth into the material.

As shown in Sec. II, the dynamics of laser heating depend on the optical and transport properties of the photoexcited electrons and holes as well as on the thermal properties of the material. Consequently, it is necessary to solve both the excess-carrier and heat diffusion equations, which are coupled, since these equations involve parameters depending on both T and n. A semi-infinite sample thickness and uniform irradiation are assumed, so that the problem can be considered in one dimension. Effects of finite sample thickness and beam diameter have been discussed elsewhere.^{15, 16, 25} We assume pure material, which implies n = p. This causes no appreciable error as long as the photoexcited carrier density is much greater than the extrinsic concentration. Under these conditions, the coupled diffusion equations for temperature and carrier density as functions of time t and depth z can be written

$$\frac{\partial T}{\partial t} - \frac{\partial}{\partial z} \left(k \langle n, T \rangle \frac{\partial T}{\partial z} \right) = \frac{G \langle n, T, z, t \rangle}{\rho c(T)}, \tag{8}$$

$$\frac{\partial n}{\partial t} - \frac{\partial}{\partial z} \left(D(n, T) \frac{\partial n}{\partial z} \right) = g(n, T, z, t) - \frac{n - n_i}{\tau_B(n, T)}, \quad (9)$$

with the boundary conditions

$$T(z, t = 0) = T_{0},$$

$$T(z = \infty, t) = T_{0}, \quad K \partial T / \partial z + \Im_{s} |_{z=0} = 0,$$

$$n(z, t = 0) = n_{i}(T_{0}), \quad D \partial n / \partial z - S(n - n_{i}) |_{z=0} = 0,$$

$$n(z = \infty, t) = n_{i}(T_{0}),$$

where $k (=K/\rho c)$ is the thermal diffusion coefficient, K is the thermal conductivity, G is the rate of heat generation in the bulk, D is the ambipolar diffusion coefficient, g is the rate of excess carrier generation, n_i is the intrinsic carrier concentration, τ_B is the bulk free carrier lifetime, T_0 is the initial sample temperature, g_s is the rate of heat generation at the surface, and s is the surface recombination velocity.

The excess carrier generation rate g contains terms due to both one- and two-photon absorption, i.e., $g=g_1+g_2$, where

$$g_{1} = [\eta_{0}(1-R)P_{0}\alpha_{1}/h\nu]e^{-\alpha \varepsilon}, \qquad (10a)$$

$$g_2 = [(1 - R)^2 P_0^2 \beta / 2h\nu] e^{-2\alpha z}, \qquad (10b)$$

and η_Q is the quantum efficiency for one-photon carrier generation. If $h\nu \gg E_g$, then $\eta_Q > 1$, since more than one electron-hole pair per photon can be produced owing to impact ionization.

The inverse lifetime for bulk recombination of excess carriers, τ_B^{-1} , can be separated into the components²⁶

$$\tau_{B}^{-1} = \tau_{SR}^{-1} + \tau_{R}^{-1} + \tau_{A}^{-1} = \tau_{SR}^{-1} + \gamma_{2}(n+n_{i}) + \gamma_{3}n(n+n_{i}), \quad (11)$$

where $\tau_{\rm SR}$, τ_R , and τ_A are the Shockley-Read, radiative, and Auger recombination lifetimes. Because of the dependences of τ_A and τ_R on carrier density, Auger or radiative recombination usually dominates at high optical flux levels.

The rate of heat generation in the bulk is given by

$$G = (1 - R) P_0 \alpha_{FC} e^{-\alpha x} + (h\nu/\eta_Q - E_R) g_1 + (2h\nu - E_R) g_2 + E_R (n - n_i) / \tau_B^{NR}.$$
(12)

The first term of Eq. (12) represents heating due to free-carrier absorption, while the second and third terms correspond to the thermalization energy which results from the relaxation of optically excited electron-hole pairs to quasiequilibrium. The fourth term corresponds to energy which is converted into lattice heat only after the electronhole pairs recombine nonradiatively (τ_B^{NR} is the nonradiative component of the bulk lifetime). The average electron-hole recombination energy E_R is given by Eq. (1).

Finally, the rate of heat generation at the surface is

$$S_{s} = S_{NR} [n(z=0, t) - n_{i}] E_{R},$$

where s_{NR} is the part of the total surface recombination velocity which is due to nonradiative processes.

IV. SOLUTION TO THE DIFFUSION EQUATIONS

The coupled diffusion equations (8) and (9) represent a general formulation of the optical heating problem within the restrictions outlined at the beginning of Sec. III. Although an analytic solution is not possible, the introduction below of certain simplifications allows us to obtain a closed-form result for the temperature increase near the surface of the material which closely approximates the exact solution for most cases of interest. The approach consists of first obtaining expressions which are valid in the short pulse regime and which do not take heat conduction into account. It is for these short times that processes which depend on optically excited carrier density and temperature have their greatest effect. Thermal diffusion is then incorporated phenomenologically using the results of Sec. II as a guide. Similarly, surface recombination is initially assumed to be radiative, and later the effects of surface heating are incorporated phenomenologically.

We therefore proceed by setting k=0 and $9_s=0$ in Eqs. (8) and (9). We also note that for high carrier densities the free-carrier lifetimes due to Auger and radiative recombination are usually much shorter than the laser pulse durations considered here.²⁷ Hence we can set $\partial n/\partial t = 0$ since, at a particular depth, the carrier density reaches a steady state value at each temperature. With these simplifications, Eqs. (8) and (9) become

$$\frac{\partial T}{\partial t} = \frac{G}{\rho c},\tag{13}$$

$$-D\frac{\partial^2 n}{\partial z^2} - \frac{\partial D}{\partial n} \left(\frac{\partial n}{\partial z}\right)^2 - \frac{\partial D}{\partial T}\frac{\partial T}{\partial z}\frac{\partial n}{\partial z} = g - \frac{n - n_i}{\tau_B}.$$
 (14)

Owing to the temperature and carrier density dependences of the various parameters, Eqs. (13) and (14) still represent a complex mathematical problem which must be simplified further in order to obtain a closed-form result. Since we are primarily interested in the behavior near the surface, we proceed by approximating T(z) in Eq. (14) by T(z=0). This effectively decouples the two equations and allows Eq. (14) to be solved for the carrier density at the surface n(z=0, t) for each value of T(z=0). The error introduced by this approach is usually small, as is discussed in the Appendix.

To solve the decoupled form of Eq. (14), we note that when carrier diffusion is unimportant $(L_D\alpha \ll 1)$, terms involving *D* can be ignored and the solution is $n(z=0, t) = n_i + g(z=0)\tau_B$. The effects of surface recombination can be accounted for by replacing τ_B with the composite lifetime τ due to both bulk and surface recombination $(\tau^{-1}=\tau_B^{-1}+\tau_S^{-1})$, where $\tau_S^{-1} \equiv s/L_D$. When carrier diffusion is significant, its effect is to redistribute the excess carriers over the depth $\alpha^{-1}+L_D$, which results in a decrease of the concentration near the surface by a factor of about $L_D\alpha+1$. In this case n(z=0,T)is approximated by

$$n(z=0, T) = n_i + g(z=0)\tau / (L_D \alpha + 1)|^{T=T(z=0)}, \quad (15)$$

where L_p is given by the usual expression L_D = $(D\tau_B)^{1/2}$. In order to test the accuracy of Eq. (15), Eq. (14) was solved numerically by computer to obtain *n* as a function of *z* for various representative forms of T(z) and for various dependences of the lifetime, diffusion coefficient, and absorption coefficient on *n*. The results, discussed in the Appendix, indicate that the approxima-

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tions made in decoupling Eqs. (13) and (14) are usually quite reasonable and that the n(z=0, T) obtained using Eq. (15) agrees with the numerical result to better than 20% for a very broad range of experimental conditions.²⁸ It should be remembered that g, τ , L_D , and α can all depend on carrier density, so that n appears on both sides of Eq. (15).

Now that an expression for n(z=0, T) has been obtained, Eq. (13) can be solved by separation of variables for the region near z=0. While the laser pulse can in general have an arbitrary time profile, we assume for convenience a single square pulse of the form $P_0[U(t) - U(t - t_p)]$, where U(t) is the unit step function. The solution to Eq. (13) can then be written

$$t_{p} = \int_{T_{0}}^{T_{f}} \frac{\rho c \, dT}{G(z \approx 0)},\tag{16}$$

where T_f is the final surface temperature at the end of the laser pulse. Since ρ is not very temperature dependent it can be assumed a constant in most cases and taken out of the integral. On the other hand, the temperature dependence of cmay be appreciable and should not be neglected. From Eqs. (12) and (15) the heat generation rate at $z \approx 0$ is

$$G(z \approx 0) = (1 - R) P_0 \alpha [\chi_T + \chi_B^{NR} / (L_D \alpha + 1)], \qquad (17)$$

where, as in Sec. II, χ_T is the fraction of the total laser energy entering the material which thermalizes with the lattice before carrier diffusion can occur:

$$\chi_T = [(1 - \eta_Q E_R / h\nu)\alpha_1 + (1 - E_R / 2h\nu)\alpha_2 + \alpha_{FC}]/\alpha, \qquad (18)$$

and χ_B^{NR} is that fraction transferred to the lattice following nonradiative bulk recombination:

$$\chi_B^{NR} = (\tau/\tau_B^{NR})[(\eta_Q E_R/h\nu)\alpha_1 + (E_R/2h\nu)\alpha_2]/\alpha$$
$$= (\tau/\tau_B^{NR})(1-\chi_T).$$
(19)

Using Eq. (17), Eq. (16) can be inverted to obtain P_0 , the power density required to increase the surface temperature from T_0 to T_f , as a function of t_p :

$$P_{0} = \frac{\rho c_{0} \Delta T L_{H}}{(1 - R_{0}) t_{p}},$$
(20)

where $c_0 = c(T_0)$, $R_0 = R(T_0)$, and

$$L_{H}|^{K} \cdot \mathbf{g}_{s} = \mathbf{0} = \frac{1 - R_{0}}{c_{0} \Delta T} \int_{T_{0}}^{T_{f}} \frac{dT c(T) \alpha^{-1}}{1 - R(T)} [\chi_{T} + \chi_{B}^{NR} / (L_{D} \alpha + 1)]^{-1}$$
(21)

Equations (20) and (21) represent a solution to the laser heating problem for short laser pulses where thermal diffusion may be neglected. It was also assumed in obtaining this solution that any surface recombination is radiative and therefore does not contribute to heating. The solution can be generalized to incorporate thermal conduction and surface heating by making use of phenomenological arguments discussed in Sec. II. Using Eq. (6) as a guide, L_H can be written

$$L_{H} = \frac{1 - R_{0}}{c_{0} \Delta T} \int_{T_{0}}^{T_{f}} \frac{dT c \alpha^{-1}}{1 - R} \times [\chi_{T} / (L_{T} \alpha + 1) + \chi_{B}^{NR} / (L_{T} \alpha + L_{D} \alpha + 1) + \chi_{S}^{NR} / L_{T} \alpha]^{-1}.$$
(22)

 χ_{s}^{NR} is the fraction which is converted to heat via nonradiative surface recombination:

$$\chi_{S}^{NR} = (\tau / \tau_{S}^{NR})(1 - \chi_{T}) L_{D} \alpha / (L_{D} \alpha + 1), \qquad (23)$$

The factor $L_D \alpha/(L_D \alpha + 1)$ in Eq. (23) represents that fraction of the excess carriers which are close enough to the surface to take part in surface recombination. The dependence of the thermal diffusion length on temperature can be estimated by using the usual relation $L_T \approx (kt)^{1/2}$ with the approximation²⁹ $T(z=0) - T_0 \approx \Delta T (t/t_p)^{1/2}$. One then obtains³⁰

$$L_{T}(T) \approx \pi^{1/2} [k(T)t_{p}]^{1/2} (T - T_{0}) / \Delta T.$$
 (24)

It should be remembered that the integral of Eq. (22) contains several terms which can depend on P_0 , indicating that Eqs. (20) and (22) must be solved self-consistently.

Our final result for the laser power density required to heat the surface of a semiconductor from an initial temperature T_0 to a final temperature T_f is thus represented by Eq. (20), where L_H is given by Eq. (22). As in Sec. II, L_H may be thought of as a generalized composite heating depth, while the χ_i represent those fractions of the laser energy entering the sample which go into the various thermalization and recombination processes ($\chi_T + \chi_B^{NR} + \chi_B^R + \chi_S^{NR} + \chi_S^R = 1$). In Eq. (22) χ_B^R and χ_S^R do not appear because radiative recombination does not contribute directly to lattice heating.

Each of the three terms within brackets in Eq. (22) can dominate depending upon the experimental conditions. The first term usually dominates when the photon energy is well above the bandgap or when free carrier absorption is very large, since most of the laser energy is then immediate-ly transferred to the lattice due to the thermalization of hot electrons and holes. The second term has its greatest effect when the photon energy is only slightly above the bandgap and the intrinsic absorption is stronger than the free-carrier absorption. In this case, most of the laser energy

reaches the lattice only after electron-hole recombination. The third term is important in materials with a high surface recombination velocity and may dominate in the short pulse regime where the thermal diffusion length L_T is small. When the surface recombination velocity is small this term may usually be neglected. In general, the relative importance of the three terms depends not only on the magnitude of the χ_i , but also the depth over which each energy component is distributed, as given by the denominator of each term. For pulse durations sufficiently long that $L_T \gg \alpha^{-1} + L_p$, the separation of the laser energy into fractional parts is unnecessary (unless χ^R_B or χ_s^R is large), since all three components will have diffused over the same depth L_{τ} .

The simplifications required to obtain the closed form solution Eq. (20) follow primarily from three approximations:

(1) The carrier density reaches a quasiequilibrium at times short compared to the laser pulse duration $[\partial n/\partial t \rightarrow 0 \text{ in Eq. (9)}]$. Owing to the short lifetimes for Auger and radiative recombination, this assumption is almost always valid in the nsec pulse regime. It may break down for psec pulses.

(2) The carrier density near the surface is given by Eq. (15). It is shown in the Appendix that Eq. (15) approximates the exact solution of Eq. (14) to within 20% for a wide range of experimental conditions. Only for certain cases (specified in the Appendix) where surface recombination or surface heating dominates is caution required, and even then Eq. (15) represents a good order-of-magnitude approximation.

(3) Thermal diffusion and surface heating have been incorporated phenomenologically. The correct dependence on pulse length and material properties is obtained when limiting cases are considered, thus demonstrating the reasonableness of this approach.

We conclude that Eq. (18) represents a simple, but accurate description of laser heating near the surface of a semiconductor. It is thus unnecessary in most cases to obtain tedious numerical solutions to the coupled partial differential equations for thermal and carrier diffusion. Physical insight into the nature of the heating process can also be gained from the straightforward phenomenological interpretation of the derived expressions.

V. APPLICATION OF THE THEORY: DAMAGE OF InSb DUE TO 170-nsec PULSES OF 10.6-µm RADIATION

A detailed comparison of the present theory with experiment will be given e^{22} for a broad range of materials, laser wavelengths, and pulse

durations. Here we illustrate the application of the derived expressions by considering InSb irradiated by Q-switched CO₂ pulses. The case of 10.6 μ m laser damage in InSb is particularly interesting because each of the different absorption mechanisms considered in Eq. (7) becomes important at different stages during the laser pulse. Near-room-temperature carriers are generated primarily by two-photon absorption since $h\nu < E_{\sigma}(T)$ $< 2h\nu$. The dominant absorption mechanism in this temperature range is free-carrier absorption since $\alpha_{FC} \gg \alpha_2$ for the power densities involved. At higher temperatures the energy gap decreases sufficiently that $h\nu \approx E_{\rm g}$ and α_1 becomes the dominant carrier generation term. It can be shown that over the entire temperature range of interest α is sufficiently small that $L_T \alpha$, $L_p \alpha \ll 1$, that recombination mechanisms other than the bulk Auger process can be ignored (i.e., $\tau = \tau_A = \tau_B^{NR}$), and that $\chi_T + \chi_B^{NR} \approx 1$. The dependence of the reflectivity on temperature and carrier density is also small and can be ignored. Under these conditions Eq. (22) reduces to the relatively simple form

$$L_{H} \approx (1/c_{0} \Delta T) \int_{T_{0}}^{T_{m}} dT \, c(T) \alpha^{-1}(T), \qquad (25)$$

where the melting temperature T_m of InSb is³¹ 798 °K.

In order to calculate the melting threshold, we must determine the temperature dependence of α , which consists of three components: one-photon and two-photon band-to-band absorption and freecarrier absorption. If the value of α_1 at low excitation intensities is designated α'_1 , we can estimate the temperature dependence by assuming it is due only to the temperature shift of the bandgap (see Ref. 22),

$$\alpha'_{1}(h\nu, T) = \alpha_{1}(h\nu + E_{\sigma}(300^{\circ}\text{K}) - E_{\sigma}(T), 300^{\circ}\text{K}).$$
(26)

When the 300 °K data of Moss *et al.*³² are used in Eq. (26), the resulting $\alpha'_1(T)$ roughly agrees with the limited high temperature data³³ which have been published. At high excitation intensities, the band-to-band absorption is limited by the dynamic Burstein shift³⁴

$$\alpha_1 = \alpha'_1 [1 - f_n(E_n) - f_p(E_p)], \qquad (27)$$

where $f_{n,p}$ are the electron and hole Fermi distribution functions and $E_{n,p}$ are the energies of the particular electron and hole states involved in the absorption process. Since the electron effective mass is quite small in InSb, a large electron Fermi energy can be obtained with relatively few carriers. As a result the decrease in absorption due to the dynamic Burstein shift is quite large in the present example.

The two-photon absorption coefficient at low ex-

citation levels is taken to have the room-temperature value³⁵ $\beta' \approx 0.2 \text{ cm/MW}$. As with one-photon absorption, β is expected to decrease at high excitation levels because of the dynamic Burstein shift. The value of β can be calculated using Eq. (27), where β and β' are substituted for α_1 and α'_1 . The two-photon absorption is then given by α_2 = $(1-R)P_0\beta$.

The free-carrier absorption is dependent on the density of electrons and holes, and is given by

$$\alpha_{FC} = \sigma_n n + \sigma_p p \approx \sigma_{FC} n, \qquad (28)$$

where $\sigma_{FC}(T) = \sigma_n(T) + \sigma_p(T)$ is the sum of electron and hole free-carrier absorption cross sections, which can be estimated from Ref. 36. The carrier density is given by Eq. (15) which, when Auger recombination is dominant and $L_p \alpha \ll 1$, reduces to

$$n(z=0,T) \approx_{n \gg n_{1}} (g/\gamma_{3})^{1/3}$$
$$\approx \left(\frac{(1-R)^{2}P_{0}^{2}\beta}{2h\nu\gamma_{2}} + \frac{\eta_{0}(1-R)P_{0}\alpha_{1}}{h\nu\gamma_{2}}\right)^{1/3}, \quad (29)$$

where we can assume $\eta_Q \approx 1$ and $\gamma_3(T)$ can be obtained from the Beattie-Landsberg result.³⁷ It must be remembered that α_1 and β are functions of *n*, since, from Eq. (27) they depend on the electron and hole Fermi energies.

The calculated variations of n, α , and T as functions of time during the laser pulse are illustrated in Fig. 2. In the first ≈ 0.1 nsec of the pulse, the carrier density increases rapidly due to two-photon absorption from the intrinsic thermal value $n_i(300 \,^{\circ}\text{K}) \approx 2 \times 10^{16} \text{ cm}^{-3}$ to the optically excited val-



FIG. 2. Calculated behavior of the carrier density n, total absorption coefficient α , and temperature T vs time during the laser pulse for irradiation of InSb by a Q-switched CO₂ laser (10.6 μ m).

ue $\approx 1.9 \times 10^{17} \text{ cm}^{-3}$ (which is limited by the dynamic Burstein shift). At the same time, α_{FC} increases from³⁶ 16 cm⁻¹ to \approx 150 cm⁻¹, due to the increasing photoexcited carrier density. Since the elapsed time is so short, no significant heating has taken place. On a longer time scale the temperature rises, causing the carrier density to gradually increase because the degeneracy of the electrons is lifted somewhat, making the dynamic Burstein shift less effective. Once T reaches \approx 450 °K, *n* (and therefore α_{FC}) begins to rise sharply due to one-photon absorption. Because of this increased optical absorption, the temperature rises rapidly to the melting point, which is reached at the end of the 170 nsec laser pulse. The importance of accounting for the "dynamic" nature of the material parameters during the heating process is illustrated by this example.

Using the above expressions for α_1 , α_2 , and α_{FC} as functions of temperature in conjunction with c(T) from the literature,³⁸ Eq. (25) was integrated numerically to give $L_H \approx 39 \ \mu$ m. The value of L_H^{-1} is compared to α in Fig. 2. Substituting L_H into Eq. (20) yields for the damage threshold $P_0 \approx 2.2$ $\times 10^7$ W/cm². The agreement with the experimental value 4×10^7 W/cm² obtained by Kruer *et al.*³⁹ for the same pulse length is quite good when one considers the number of "nonlinear" physical processes which were taken into account. Current uncertainty in the high temperature and carrier density behavior of σ_{FC} , γ_3 , β , and α_1 is probably responsible for most of the disagreement between experiment and theory. The agreement should improve as more extensive experiments are performed involving the various parameters which appear in the calculations.

In order to more thoroughly test the present theory, melting damage thresholds calculated using Eq. (20) are compared in Ref. 22 with the available experimental results for Ge, Si, InSb, and GaAs over a wide variety of laser wavelengths and pulse durations. Agreement is within a factor of two for all cases considered, and is often much better. In contrast to any previous formulation, the present theory is seen to give a reliable description of laser heating for a broad spectrum of materials and experimental conditions.

VI. CONCLUSIONS

The physical processes involved in the conversion of high intensity optical energy to lattice heat have been considered in a theory for optical heating in semiconductors. The problem has been formulated in terms of the coupled diffusion equations for temperature and excess carrier density. For the first time, closed-form solutions valid near

$$-\frac{D\partial^{2}n}{\partial z^{2}} - \left(\frac{\partial D}{\partial n}\frac{\partial n}{\partial z}\right)^{2} - \frac{\partial D}{\partial T}\frac{\partial T}{\partial z}\frac{\partial n}{\partial z} = \frac{\eta_{Q}(1-R)P_{0}\alpha e^{-\alpha z}}{h\nu} - \frac{n}{\tau_{B}},$$
$$\frac{D\partial n}{\partial z} - sn|^{z=0} = 0. \quad (A2)$$

We wish to solve Eq. (A2) for the most general c case in which τ_B , D, and α depend on carrier density, and a thermal gradient exists. It is impractical to solve Eq. (A2) for every possible functional form of these quantities. Rather, we choose representative dependences which reflect the nature of the variations observed experimentally, but which require a minimum number of independent parameters. For example, we assume the carrier density dependence of the ambipolar diffusion coefficient D to be $D(n) \equiv D(n/\tilde{n})^a$. The parameter a can be either negative due to electronhole scattering or positive due to free-carrier screening or degeneracy. The temperature dependence of D can be assumed to follow an inverse power law.

Since the optical absorption is intrinsic $(\alpha = \alpha_1)$, the absorption coefficient in Eq. (A2) depends on the carrier density primarily through the dynamic Burstein shift. If we consider for simplicity a case where the holes are nondegenerate but the electrons are degenerate, we have from Eq. (27), $\alpha(n) = \alpha' [1 - f_n(E_n)]$. For a "worst case" test of Eqs. (15), we consider the limit $E_n, k_BT \ll E_{F_n}$ since the variation of α with *n* is much smaller if either E_n or $k_B T$ is comparable to or larger than the electron Fermi energy. For this case $\alpha(n)$ becomes $\alpha' \exp[(E_n - E_{F_n})/k_B T]$. Introducing the reduced Fermi energies $\eta_n = \tilde{E}_{Fn}/k_B T$ and $\tilde{\eta}_n$ $=\tilde{E}_{F_n}/k_BT$, $\alpha(n)$ can be rewritten $\tilde{\alpha} \exp(\tilde{\eta}_n - \eta_n)$. If we assume that the electron Fermi energy varies approximately as the two-thirds power of the electron density, the expression for $\alpha(n)$ becomes

$$\alpha(n) = \tilde{\alpha} \exp\{ \tilde{\eta}_n [1 - (n/\tilde{n})^{2/3}] \}.$$
 (A3)

The dynamic Burstein shift can be ignored by setting the parameter $\tilde{\eta}_n$ equal to zero.

Finally, we model the temperature gradient term $(\partial D/\partial T)(\partial T/\partial z)$ of Eq. (A2). If surface heating is dominant, $\partial T/\partial z]^{z=0}$ depends on the rate of nonradiative surface recombination. The temperature gradient varies with depth approximately as $e^{-z/L}r$, where L_T is the thermal diffusion length. If surface heating is unimportant, the thermal gradient is governed by the optical absorption depth and the carrier and thermal diffusion distances. In this case the gradient varies roughly as $\exp(-\alpha z/\gamma_1)$, where $1 \leq \gamma_1 \leq L_T \alpha + L_D \alpha + 1$. In order to account for both cases, we assume a general temperature gradient of the form $\exp(-\tilde{\alpha} z/\gamma)$.

the surface of the material have been obtained for the general case where the optical and transport properties vary with carrier density and temperature. The problem was made tractable through the use of several assumptions which are reasonable for a very wide range of experimental conditions. This permitted the differential equations to be decoupled and solved independently. The solutions give physical insight into the roles various mechanisms play in the heating process.

The importance of accounting for such nonlinear processes as two-photon absorption, free-carrier absorption, the dynamic Burstein shift, Auger recombination, and the temperature shift of the energy gap has been illustrated by considering melting in InSb due to Q-switched CO₂ laser pulses. Good agreement between theory and experiment is obtained. More generally, uniformly good agreement is obtained when melting damage thresholds calculated from the present theory are compared to experimental results for a wide variety of materials, laser wavelengths, and pulse durations. This agreement is expected to become even better as the parameters used in these calculations are measured more exactly at high carrier densities and temperatures.

APPENDIX: NUMERICAL SOLUTION OF THE CARRIER DIFFUSION EQUATION

To determine the accuracy of Eq. (15) as an expression for the carrier density at the surface of an optically excited semiconductor, the general carrier diffusion equation is solved numerically. The numerical result n is then compared to the approximate result (which we denote \tilde{n}) given by Eq. (15). For convenience, the carrier density is assumed to be much greater than n_i for the high optical flux levels involved. Two-photon carrier generation and free-carrier absorption are also neglected, since these effects are only important when $L_p \alpha \ll 1$, the regime for which Eq. (15) is expected to be most accurate. Under these conditions, Eq. (15) may be written

(A1)

 $\tilde{n} = \frac{\eta_{Q} (1 - R) P_{0} \tilde{\alpha} (\tilde{\tau}_{B}^{-1} + \tilde{\tau}_{S}^{-1})^{-1}}{h \nu (\tilde{L}_{D} \tilde{\alpha} + 1)},$

where

$$\tilde{L}_{D} = (\tilde{D}\tilde{\tau}_{B})^{1/2}, \ \tilde{\tau}_{B}^{-1} = \gamma_{r}\tilde{n}^{r-1},$$

and

$$\tilde{\tau}_{s}^{-1} = s/\tilde{L}_{p}$$

A tilde over a parameter indicates the value of that parameter for $n=\tilde{n}$ and T=T(z=0). Here r= 2,3 corresponds to radiative and Auger recombination, respectively.

With the simplifications specified above, the car-

The coefficient of $\partial n/\partial z$ in Eq. (A2) can then be written:

$$\frac{\partial D}{\partial T} \frac{\partial T}{\partial z} = \tilde{\alpha} \tilde{D} \Gamma e^{-\tilde{\alpha}_{z}/\gamma}, \qquad (A4)$$

where Γ and γ are adjustable parameters. When surface heating is unimportant, neither Γ nor the product Γ_{γ} should exceed 0.5.

We now introduce the variables $x = \tilde{\alpha}z$ and $y = n/\tilde{n}$. With the models for *D*, α , and $\partial T/\partial z$ given above, Eq. (A2) becomes

$$-y^{a+1}\frac{\partial^{2}y}{\partial x^{2}} - ay^{a}\left(\frac{\partial y}{\partial x}\right)^{2} - \Gamma e^{-x/\gamma}y^{a+1}\frac{\partial y}{\partial x}$$
$$= \frac{1}{(\tilde{L}_{D}\tilde{\alpha})^{2}}\left(\frac{\alpha(y)}{\tilde{\alpha}}(1+R_{S})(\tilde{L}_{D}\tilde{\alpha}+1)e^{-[\alpha(y)/\tilde{\alpha}]_{x}} - y^{r}\right),$$
with the boundary condition (A5)

with the boundary condition

$$\frac{\partial y}{\partial x} - \frac{R_s}{\tilde{L}_D \tilde{\alpha}} y^{1-a} \bigg|^{x=0} = 0,$$

where $R_s \equiv \tilde{\tau}_s^{-1}/\tilde{\tau}_B^{-1}$ and $\alpha(y)/\tilde{\alpha}$ is given by Eq. (A3).

Equation (A5) was solved numerically by computer for the ranges of the seven independent parameters given in Table I. These ranges should adequately cover most conditions likely to be encountered for real semiconductors at high excitation levels.

The results of the numerical solutions indicate

TABLE I. Ranges for the various parameters for which Eq. (A5) was solved numerically.

 r=2,3	
$\begin{array}{ll} 0.01 & \leqslant \tilde{L}_D \tilde{\alpha} \leqslant 100 \\ -0.3 & \leqslant a \leqslant 1.0 \\ 0 & \leqslant \tilde{\eta}_n \leqslant 15 \\ 0 & \leqslant R_s \leqslant 10 \\ 0 & \leqslant \Gamma \leqslant 50 \\ 0.002 \leqslant \gamma \leqslant 10 \end{array}$	

that for $R_{s} \leq 1$ and $\Gamma \leq 0.5$ and $\Gamma_{\gamma} \leq 0.5$, or $\Gamma \leq 50$ and $\Gamma_{\gamma} \leq 0.1$, the value of y at x=0 is between 0.8 and 1.2 for all values of the other parameters within the range tested. Hence Eq. (15) approximates the exact solution to the carrier diffusion equation to within 20%, unless either a large carrier density gradient or a large thermal gradient is present due to surface recombination. It was further found that for R_s as large as 10 and $\Gamma \leq 0.5$ and Γ_{γ} \leq 0.5, Eq. (15) agrees with the numerical solution to within a factor of 2. This indicates that Eq. (15) is qualitatively reasonable even when surface recombination is highly predominant. These results demonstrate that Eq. (15) satisfactorily describes the carrier density at the surface of an optically excited semiconductor for a broad range of physical parameters and excitation conditions.

- ¹J. Shah, R. F. Leheny, and C. Lin, Solid State Commun. <u>18</u>, 1035 (1976); J. Shah, R. F. Leheny, and W. Wiegmann, Phys. Rev. B <u>16</u>, 1577 (1977).
- ²A. V. Nurmikko, Opt. Commun. <u>16</u>, 365 (1976); <u>18</u>, 522 (1976).
- ³P. Lavallard, R. Bichard, and C. Benoit à la Guillaume, Phys. Rev. B <u>16</u>, 2804 (1977).
- ⁴L. M. Blinov, E. A. Bobrova, V. S. Vavilov, and G. N. Galkin, Fiz. Tverd. Tela (Leningrad) <u>9</u>, 3221 (1967) [Sov. Phys.-Solid State 9, 2537 (1968)].
- ⁵J. R. Meyer and M. Glicksman, Phys. Rev. B <u>17</u>, 3227 (1978).
- ⁶G. N. Galkin, L. M. Blinov, V. S. Vavilov, and A. G. Golovashkin, Pis'ma Zh. Eksp. Teor. Fiz. <u>7</u>, 93 (1968) [JETP Lett. <u>7</u>, 69 (1968)].
- ⁷S. A. Jamison, A. V. Nurmikko, and H. J. Gerritsen, Appl. Phys. Lett. <u>29</u>, 640 (1976).
- ⁸R. Baltramiejūnas, A. Sakalas, J. Vaitkus, and J. Viščakas, Phys. Status Solidi A <u>3</u>, K277 (1970).
- ⁹D. H. Auston and C. V. Shank, Phys. Rev. Lett. <u>32</u>, 1120 (1974).
- ¹⁰D. H. Auston, C. V. Shank, and P. LeFur, Phys. Rev. Lett. 35, 1022 (1975).
- ¹¹M. S. Epifanov, G. N. Galkin, E. A. Bobrova, V. S. Vavilov, and L. D. Sabanova, Fiz. Tekh. Poluprov. <u>10</u>, 889 (1976) [Sov. Phys.-Semicond. <u>10</u>, 526 (1976)].
- ¹²A. Haug, Solid State Commun. <u>28</u>, 291 (1978).

- ¹³We will consider only cases for which the laser photon energy $h\nu$ is at least half the bandgap E_g , for which excess carriers will be generated due to one or two photon band-to-band absorption. When $h\nu << E_g$, heating may involve effects such as electric field induced breakdown or absorption by extrinsic defects, which are beyond the scope of this paper.
- ¹⁴A. A. Grinberg, R. F. Mekhtiev, S. M. Ryvkin, V. M. Salmanov, and I. D. Yaroshetskii, Fiz. Tverd. Tela (Leningrad) <u>9</u>, 1390 (1967) [Sov. Phys.-Solid State <u>9</u>, 1085 (1967)].
- ¹⁵F. Bartoli, L. Esterowitz, M. Kruer, and R. Allen, J. Appl. Phys. <u>46</u>, 4519 (1975).
- ¹⁶L. Stagni, Appl. Phys. <u>12</u>, 31 (1977).
- ¹⁷M. Lax, J. Appl. Phys. <u>48</u>, 3919 (1977); Appl. Phys. Lett. <u>33</u>, 786 (1978).
- ¹⁸K. T. Yang, J. Appl. Mech. <u>25</u>, 146 (1958); K. T. Yang and A. Szevczyk, ASMD Trans. C81, 251 (1959).
- ¹⁹I. P. Dobrovol'skii and A. A. Uglov, Kvant. Elektron. (Moscow) <u>1</u>, 1423 (1974) [Sov. J. Quantum Electron. <u>4</u>, 788 (1974)].
- ²⁰A. Lietoila and J. F. Gibbons, Appl. Phys. Lett. <u>34</u>, 332 (1979).
- ²¹J. C. Schultz and R. J. Collins, Appl. Phys. Lett. <u>34</u>, 84 (1979); P. Baeri, S. U. Campisano, G. Foti, and E. Rimini, J. Appl. Phys. <u>50</u>, 788 (1979). In these two papers the heat diffusion equation was solved, but

coupling to the carrier diffusion was ignored.

²²J. R. Meyer, M. R. Kruer, and F. J. Bartoli (unpublished).

²³In general,

$$E_{T1} = \frac{k_B T \int_0^\infty x^{3/2} f_0 (1 - f_0) B(x) dx}{\int_0^\infty x^{1/2} f_0 (1 - f_0) B(x) dx}$$

where $f_0 [=(e^{x-\eta}+1)^{-1}]$ is the Fermi distribution function, B(x) is a weighting factor which reduces to unity for parabolic bands (see the Appendix of Ref. 22), and $\eta [\equiv E_F/k_BT]$ is the reduced Fermi energy. For parabolic bands, $E_T = E_F$ in the degenerate limit and $E_T = \frac{3}{2}k_BT$ in the nondegenerate limit.

- ²⁴It² can be shown that this assumption is valid in most cases of interest.
- ²⁵F. Bartoli, L. Esterowitz, R. Allen, and M. Kruer, J. Appl. Phys. 47, 2867 (1976); 47, 2875 (1976).
- ²⁶J. S. Blakemore, Semiconductor Statistics (Pergamon, New York, 1962).
- ²⁷This assumption is usually valid for pulse lengths in the nsec regime, although it is often questionable for psec pulses.
- 28 In Ref. 22 the present theory is applied to the calculation of laser damage thresholds in Ge, Si, InSb, and GaAs for several laser wavelengths and for pulse durations between 10^{-9} and 10^{-3} sec. Of these cases, only for GaAs under certain excitation conditions should the error exceed 20% (because of the high surface recombination velocity), and then not by a great deal.
- ²⁹H. Carslaw and T. Jaeger, Conduction of Heat in Solids, (Oxford University Press, New York, 1959), Chap. 2. This functional dependence of $T(z=0) - T_0$ on time is exact when k is independent of T and L_T

 $>>L_{D}+\alpha^{-1}$.

³⁰The factor $\pi^{1/2}$ in Eq. (24) is necessary to ensure that when $\chi_T + \chi_N^{R} + \chi_N^{NR} = 1$ and k is not a function of T, then

$$L_{H} \rightarrow \frac{1}{\Delta T} \int_{T_{0}}^{T_{f}} L_{T}(T) dT$$
$$L_{T} >> L_{D} + \alpha^{-1}$$

should reduce to the exact result (see Ref. 25)

$$L_{H} = \frac{\pi^{1/2}}{2} \left(kt_{p}\right)^{1/2}.$$

It can be shown that even when k depends on T, L_H is proportional to $t_p^{1/2}$ in the limit $L_T >> L_D + \alpha^{-1}$.

- ³¹ M. Neuberger, *Handbook of Electronic Materials*, (IFI/Plenum, New York, 1970), Vol. 2.
- ³²T. S. Moss, E. D. Smith, and T. D. F. Hawkins, Proc. Phys. Soc., London, Sect. B 70, 776 (1957).
- ³³M. Kaiser and H. Y. Fan, Phys. Rev. <u>98</u>, 966 (1955).
 ³⁴E. J. Johnson, *Semiconductors and Semimetals*, edited by R. K. Willardson and A. C. Beer (Academic, New York, 1967), Vol. 3, p. 153.
- ³⁵A. F. Gibson, C. B. Hatch, P. N. D. Maggs, D. R. Tilley, and A. C. Walker, J. Phys. C <u>9</u>, 3259 (1976).
- ³⁶S. W. Kurnick and J. M. Powell, Phys. Rev. <u>116</u>, 597 (1959).
- ³⁷ À. R. Beattie and P. T. Landsberg, Proc. Roy. Soc., London, Ser. A <u>249</u>, 216 (1959).
- ³⁸Y. S. Touloukian and E. H. Buyco, *Thermophysical Properties of Matter* (IFI/Plenum, New York, 1970), Vol. 5.
- ³⁹M. Kruer, L. Esterowitz, F. Bartoli, and R. Allen, in *Laser Induced Damage in Optical Materials: 1977*, edited by A. J. Glass and A. H. Guenther (NBS Special Publication No. 509, Washington, D.C., 1977), p. 473.