THERMAL AND PLASMA WAVES IN SEMICONDUCTORS

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INTRODUCTION

The absorption of an intensity modulated laser beam results in a modulated temperature profile having the properties of a critically damped wave, i.e., a thermal wave [1]. In a semiconductor such as silicon, if the energy per photon exceeds the band gap energy, then, in addition to the thermal wave, one has a photo-generated electron-hole plasma density that can also be characterized as a critically damped propagating wave, i.e., a plasma wave [2]. In this paper, we present a theoretical description of these two phenomena that shows how they can be used to obtain information about transport and carrier recombination properties of semiconductors. Included in our analysis will be the effects of linear coupling between heat and mass transport (i.e., thermodiffusion) on the propagation of thermal waves and plasma waves.

THEORY

To begin let's consider qualitatively what happens when a laser beam is incident on a semiconductor. If the energy per photon E exceeds the band gap energy E_g then electrons will be excited from the valence band to an energy $E-E_g$ above the conduction band edge. These photoexcited free carriers will, within a fraction of a picosecond, give this excess energy to the lattice through nonradiative transitions to the unoccupied states near the bottom of the conduction band. After a much longer time, typically on the order of microseconds, these photoexcited carriers recombine with holes in the valence band giving up their remaining energy E_g to the lattice. Prior to this recombination there thus exists a plasma of electrons and holes whose density is governed by diffusion in a manner analogous to the flow of heat from a thermal source. Thus, if an incident laser beam is intensity modulated, we would expect to observe, in addition to the thermal wave, a modulated plasma density whose spatial profile is that of a critically damped wave, i.e., a plasma wave.

In order to obtain a quantitative description of these critical wave phenomena, we consider the plasma current density, J_N, and heat current density, J_Q, which we assume are linearly driven by the plasma density

gradient, ∇N, and the temperature gradient, ∇T, according to

$$J_N = -D\nabla N - A\nabla T \tag{1}$$

$$J_Q = -\kappa\nabla T - B\nabla N \tag{2}$$

where D is the ambipolar diffusion coefficient, κ is the thermal conductivity, and A and B are thermodiffusion coefficients. In the absence of any sources, we have the conservation equations

$$\nabla\cdot J_N + \partial N/\partial t = -N/\tau \tag{3}$$

$$\nabla\cdot J_Q + \rho C\partial T/\partial t = NE_g/\tau \tag{4}$$

where ρ is the density, C is the specific heat, and τ is the electron–hole recombination time, all of which are taken to be constants with respect to variations in the temperature and plasma density. In order to keep the equations linear in N and T, we further assume that the transport coefficients are also independent of N and T. Then, by imposing the sinusoidal time dependence, $\exp(-i\omega t)$, we obtain the coupled set of wave equations

$$\nabla^2 N + p^2 N + (A/D)\nabla^2 T = 0 \tag{5}$$

$$\nabla^2 T + q^2 T + (B/\kappa)\nabla^2 N = -NE_g/\kappa\tau \tag{6}$$

where p is the plasma wave vector defined by

$$p^2 = i(\omega\tau + i)/D\tau \tag{7}$$

and q is the thermal wave vector defined by

$$q^2 = i\omega\rho C/\kappa \tag{8}$$

The wave vectors p and q are, respectively, the propagation vectors for thermal waves and plasma waves [2] in the absence of any thermodiffusion effects. To arrive at a general solution for the coupled thermal/plasma wave problem under consideration, we use the plane wave basis functions, $N_k\exp(i k\cdot r)$ and $T_k\exp(i k\cdot r)$, which when substituted into Eqs. (5) and (6) yield the homogeneous pair of algebraic equations

$$(k^2 - p^2)N_k + (A/D)k^2 T_k = 0 \tag{9}$$

$$[(B/\kappa)k^2 - E_g/\kappa\tau]N_k + (k^2 - q^2)T_k = 0 \tag{10}$$

which have nontrivial solutions provided the wave vector k satisfies

$$(1 - \varepsilon)k^4 - [p^2 + q^2 - (A/D)E_g/\kappa\tau]k^2 + p^2 q^2 = 0 \tag{11}$$

where the dimensionless coupling parameter ε is defined as

$$\varepsilon = AB/\kappa D \tag{12}$$

At sufficiently high modulation frequencies where bulk recombination effects are negligible (i.e., $\omega\tau \gg 1$), the thermal and plasma waves are coupled only if ε is nonzero. That is, if either A or B is zero, the wave equations, Eqs. (5) and (6), are uncoupled and can be solved independently with the appropriate propagation vectors being given by Eqs. (7) and (8). However, at low modulation frequencies ($\omega\tau \ll 1$) where the recombination term in Eq. (6) becomes significant, the coupling only depends on A being

nonzero. In this limit we have $p^2 = -1/D\tau$ which corresponds to a purely
diffusive phenomenon that is independent of the modulation frequency.
Since $|q|$ is always a decreasing function of ω, then at low enough
frequencies such that $|q| \ll |p|$, one of the roots of Eq. (11) will also
correspond to a frequency independent and purely diffusive mode.

To complete the solution of Eqs. (5) and (6) we note that for any
given k the corresponding wave amplitudes N_k and T_k are not independent.
From Eq. (5) we have

$$T_k = -\frac{B}{\kappa}\left[\frac{k^2 - (\kappa/B)E_g/\kappa\tau}{k^2 - q^2}\right] N_k \qquad (13)$$

or equivalently from Eq. (6)

$$N_k = -\frac{A}{D}\left[\frac{k^2}{k^2 - p^2}\right] T_k \qquad (14)$$

The solution to any particular problem is now straightforward. For
problems in which the thermal and plasma sources are localized at a
boundary, say $z = 0$ for example, then a linear combination of the basis
functions that satisfies the boundary conditions (including the source
terms) will yield the solution. On the other hand, when the sources are
spatially extended, one must first find the particular solutions of the
wave equations (Eqs. (5) and (6) augmented with the proper source terms)
and then to those particular solutions add the appropriate linear
combination of basis functions needed to satisfy the boundary conditions.

DISCUSSION

Before solving any particular examples, let's examine the weak
coupling limit ($\varepsilon \ll 1$ and $AE_g/\kappa \ll 1$) where the solutions of
Eq. (11), k_1 and k_2, are to a good approximation given by

$$k_1^2 = p^2\left[1 - \frac{\varepsilon p^2 - (A/D)E_g/\kappa\tau}{q^2 - p^2}\right] \qquad (15)$$

$$k_2^2 = q^2\left[1 + \frac{\varepsilon q^2 - (A/D)E_g/\kappa\tau}{q^2 - p^2}\right] \qquad (16)$$

In pure silicon with $D = 15$ cm^2/sec, $\kappa = 1.42$ W/cm $^\circ$C, $\rho C = 1.7$ J/cm^3 $^\circ$C
and at sufficiently high modulation frequencies where $\omega\tau \gg 1$, we have
$|q| > |p|$ which means that with increasing ε, $|k_1|$ decreases and $|k_2|$
increases. That is, the spatial extent of the k_1 (plasma-like) mode
increases while that of the k_2 (thermal-like) mode decreases with
increasing ε.

In the low frequency limit ($\omega\tau \ll 1$), the k_1 mode is purely
diffusive and frequency independent as discussed earlier with k_1 increasing
or decreasing in magnitude depending on the sign of A. In this limit we
have,

$$k_1^2 = -\frac{1}{D\tau}[1 + \varepsilon + AE_g/\kappa] \qquad (17)$$

The k_2 mode, however, retains its wavelike properties with the magnitude of k_2 also linearly dependent on A. For k_2 we have

$$k_2^2 = q^2[\ 1 + \varepsilon q^2 D\tau - AE\mathfrak{g}/\kappa\ ] \tag{18}$$

In contrast to the uncoupled problem in which the wave vectors are monotonically decreasing with increasing frequency, recombination effects in the presence of coupling can lead to dispersion in the wave vectors that is non-monotonic with frequency. Of practical importance, however, is the effect of coupling on the plasma density and temperature, particularly at the surface where the excitation occurs and a measurement is most easily made.

As an example, we consider an infinite half-space with a plasma source, P_o, and a thermal source, Q_o, both of which we take to be localized at the surface $z = 0$ and infinite in x and y. Then in terms of our plane wave basis functions, we have for this 1-dimensional problem

$$N(z) = N_1 e^{ik_1 z} + N_2 e^{ik_2 z} \tag{19}$$

$$T(z) = T_1 e^{ik_1 z} + T_2 e^{ik_2 z} \tag{20}$$

with the unknown amplitudes N_i and T_i determined by applying the boundary conditions. For the half-space problem the boundary conditions are that the currents defined by Eqs. (1) and (2) be equal to the sources, P_o and Q_o, respectively. That is, $J_N(z=0)=P_o$ and $J_Q(z=0)=Q_o$. Applying these boundary conditions we obtain for the plasma density and temperature at $z = 0$,

$$N(0) = \frac{1}{M}[\ iP_o\kappa(k_2 - k_1 C_1 C_2)(1 - \alpha) - iQ_o DC_2(k_2 - k_1)(1 - \beta)\ ] \tag{21}$$

$$T(0) = \frac{1}{M}[\ iQ_o D(k_1 - k_2 C_1 C_2)(1 - \beta) - iP_o \kappa C_1(k_1 - k_2)(1 - \alpha)\ ] \tag{22}$$

where

$$M = k_1 k_2 \kappa D(1 - \varepsilon)(1 - C_1 C_2) \tag{23}$$

and where α and β are dimensionless thermodiffusion coefficients defined by

$$\alpha = AQ_o/\kappa P_o \tag{24}$$

$$\beta = BP_o/DQ_o \tag{25}$$

Also in Eq. (23), C_1 is defined as the numerical factor relating T_1 to N_1 in Eq. (13)

$$C_1 = -\frac{B}{\kappa}\left[\frac{k_1^2 - (\kappa/B)E\mathfrak{g}/\kappa\tau}{k_1^2 - q^2}\right] \tag{26}$$

and C_2 is defined as the numerical factor relating N_2 to T_2 in Eq. (14)

$$C_2 = -\frac{A}{D}\left[\frac{k_2^2}{k_2^2 - p^2}\right] \tag{27}$$

Finally, to be complete, we need to specify the source terms P_o and Q_o. Assuming, as discussed in the introduction, that an intensity modulated

laser beam is incident on the sample, then by letting Q denote the total energy flux absorbed at the surface, we have

$$P_o = Q/E \tag{28}$$

and

$$Q_o = Q(E - E_g)/E \tag{29}$$

where E is the energy per photon and E_g is the band gap energy. In all of the following calculations we will assume an Ar^+ ion laser operating at a wavelength $\lambda = 0.5$ μm, i.e., E = 2.5 eV, incident on silicon which has a band gap energy, $E_g = 1.1$ eV. Thus, slightly more than half of the absorbed energy flux, Q, will go directly into heating the lattice with the remaining portion being carried away from the source region by the photogenerated electron-hole pairs.

In Figs. 1, 2 and 3 we show the calculated surface plasma density and surface temperature in silicon as functions of the modulation frequency and the dimensionless thermodiffusion coefficient, α, for different values of the ratio, β/α, and a fixed bulk recombination time, $\tau = 0.1$ μsec. Setting $\beta = 0$ yields the results shown in Fig. 1.
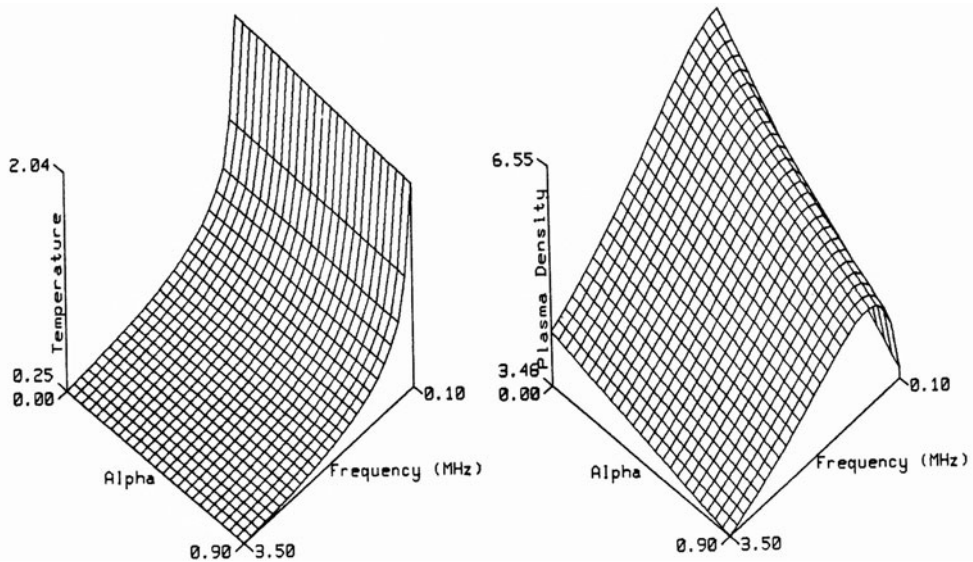

Fig. 1   Surface temperature T(0) (°C) and plasma density N(0) (10^{17}/cm^3) as functions of α and modulation frequency with $\beta/\alpha = 0$, $\tau = 0.1$ μsec, and Q = 3.2 kW/cm^2.

As one might anticipate for this case, the dependence of T on α is weak even at the lowest frequencies where recombination is significant. The effects of recombination, incidentally, on the surface temperature are evident in the figure as the dependence on frequency is much stronger than $1/\sqrt{\omega}$. That is, at the lowest frequency shown, 0.1 MHz, recombination heating is most significant (raising the temperature from 1.46°C to 2.04°C) while at the highest frequency shown, recombination heating is a negligible effect constituting about 2% of the total heating. More interesting, however, are the results for the surface plasma density. As

expected in the absence of coupling (i.e., $\alpha = 0$), the plasma density tends toward saturation at the lower frequencies as the recombination becomes more significant. The effect of coupling in this frequency regime is quite dramatic, reducing the plasma density by nearly a factor of two as α increases from 0 to 0.9. As we go to higher frequencies the coupling effect decreases substantially thereby giving rise to a plasma density whose dependence on frequency is non-monotonic for fixed non-zero values of α. To get some idea of the origin of this latter effect, let's consider Eq. (21) assuming that the coupling has no effect on the wave vectors, i.e., set $k_1 = p$ and $k_2 = q$, and that the product, $C_1 C_2$, can be neglected. Under these assumptions we obtain for the surface plasma density

$$N(0) = \frac{iP}{pD}o \left[1 - \alpha \left[\frac{p}{p + q} \right] \right] \tag{30}$$

At the 0.1 MHz modulation frequency where $p = -1/D\tau$ and $|p| \sim |q|$, the dependence of $N(0)$ on the coupling is approximately $[1 - .5\alpha]$ which is consistent with the results shown in Fig. 1. Going to higher frequencies where the recombination effects become negligible, $|p| \sim .25|q|$ and the dependence of $N(0)$ on α predicted by Eq. (30) approaches $[1 - .2\alpha]$, which is also consistent with the complete calculations shown in Fig. 1.

In Fig. 2 we show results for $N(0)$ and $T(0)$ obtained with $\beta/\alpha = 1$. Here we see that the effect of β on $N(0)$ opposes that of α reducing the amount by which $N(0)$ decreases with increasing α as compared to the results shown in Fig. 1.
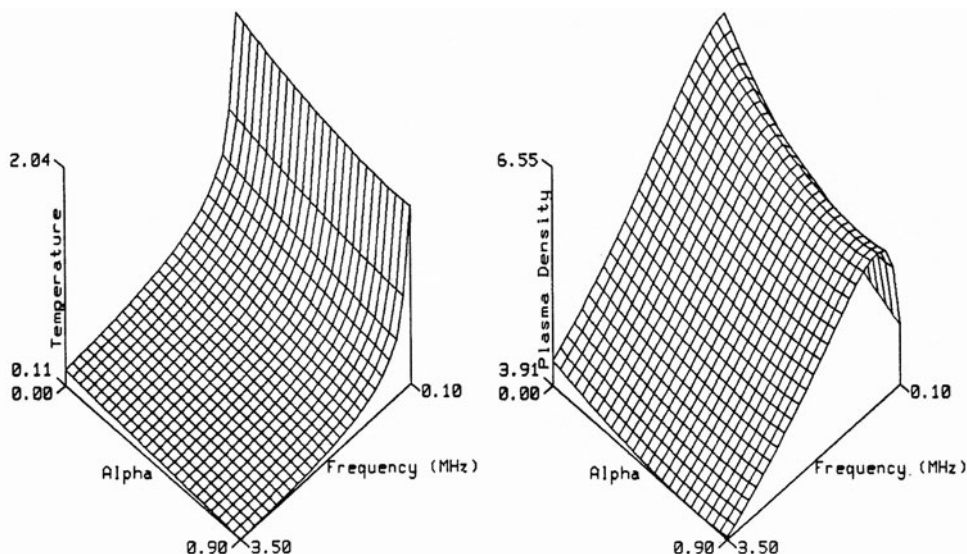

Fig. 2   Surface temperature $T(0)$ (°C) and plasma density $N(0)$ (10^{17}/cm^3) as functions of α and modulation frequency with $\beta/\alpha = 1, \tau = 0.1$ μsec, and $Q = 3.2$ kW/cm^2.

The surface temperature now shows a dependence on coupling which is most pronounced at the higher modulation frequencies. Specifically, as α increases from 0 to 0.9, $T(0)$ decreases from 2.04°C to 168°C at 0.1 MHz compared with a drop from 0.25°C to 0.11°C at 3.5 MHz. Here, the

increased recombination at the lower frequencies reduces the effect of the coupling on T(0) compared with the higher frequency results where the recombination is negligible. This is even more significant when we set $\beta/\alpha = 10$ and allow α to vary from 0 to 0.09 as shown in Fig. 3. Essentially α is no longer playing any role and the effects are due almost entirely to β, which in that figure is varying from 0 to 0.9. The plasma density is unaffected by this coupling while the variation in T(0) with β is more significant than in the previous figure.
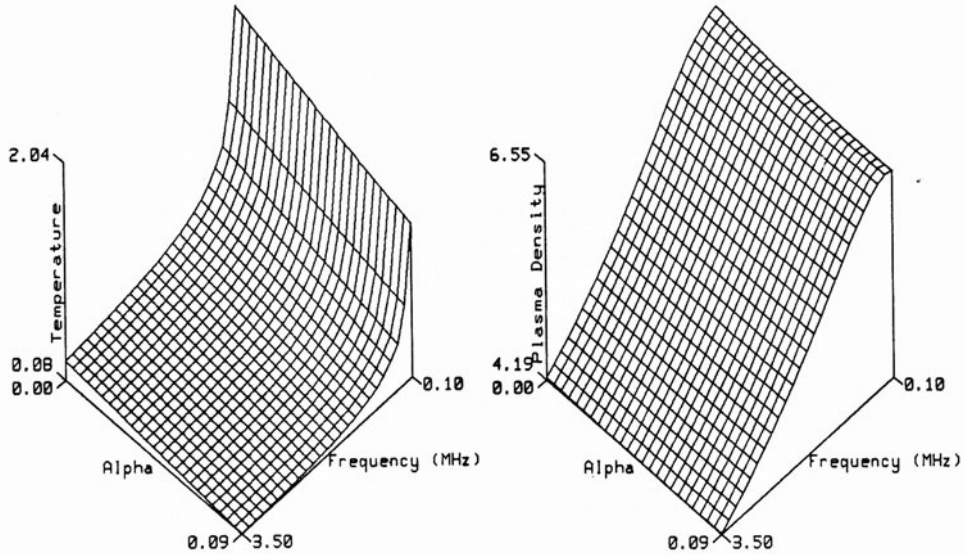

Fig. 3 Surface temperature T(0) ($^\circ$C) and plasma density N(0) ($10^{17}/cm^3$) as functions of α and modulation frequency with $\beta/\alpha = 10$, $\tau = 0.1$ μsec, and Q = 3.2 kW/cm^2.

To understand the effect of this coupling, we consider Eq.(22) in a manner analogous to what we did earlier in obtaining Eq. (30). Specifically, we assume $k_1 = p$, $k_2 = q$, $C_2 = 0$, and $\epsilon = 0$. For the surface temperature we then obtain

$$T(0) = \frac{iQ}{q\kappa}o \left[1 - \beta \left[\frac{q}{p + q} \right] \right] \tag{31}$$

Equation (31) predicts a dependence of T(0) on β similar in form to that for N(0) on α in Eq. (30) but with a different dependence on the wavevectors p and q. At 0.1 MHz we therefore expect the dependence for T(0) to be $\sim [1 - .5\beta]$ but at higher frequencies becoming stronger and approaching the limit $[1 - .8\beta]$ as recombination becomes insignificant. These predictions are consistent with the calculations shown in Fig. 3. The surface temperature at 0.1 MHz decreases from 2.04 $^\circ$C to 1.45 $^\circ$C and at 3.5 MHz decreases from 0.25 $^\circ$C to 0.08 $^\circ$C as β increases from 0 to 0.9.

Although our examples so far have been limited to effects in 1-dimension, the generalization of the solutions, Eqs. (21) and (22) to 3-dimensions is easily accomplished as described in [3]. We should note, however, that the theory portion of this talk, Eqs. (1) through (14), is general and valid in 3-dimensions. Thus, the expressions for C_1 and C_2,

Eqs. (26) and (27), are also valid in 3-dimensions. The only changes that need to be made are to the wave vectors k_1 and k_2 wherever they explicitly appear in Eqs. (21), (22) and (23). As discussed in [3] these are replaced by there respective z-components, k_{1z} and k_{2z}, where

$$k_{1z} = [\ k_1^2 - q_r^2\ ]^{\frac{1}{2}} \tag{32}$$

$$k_{2z} = [\ k_2^2 - q_r^2\ ]^{\frac{1}{2}} \tag{33}$$

The new N(0) and T(0) obtained with these replacements are multiplied by their respective spatially transformed sources, P_0 and Q_0, then multiplied by exp(iq_r·r) and the resulting products integrated over the q_r plane. In Fig. (4) we show the surface temperature and plasma density at the center (r = 0) of a source with a 2-dimensional gaussian profile along the surface, exp(-r²/a²). In this particular example, recombination plays no role whatsoever since Dτ >> a². However, the arguments are analogous to those employed earlier for the 1-dimensional case; the plasma wave essentially saturates at significantly higher frequencies than does the thermal wave since D >> κ/ρC with the result that the effect of coupling on N and T will be frequency dependent.
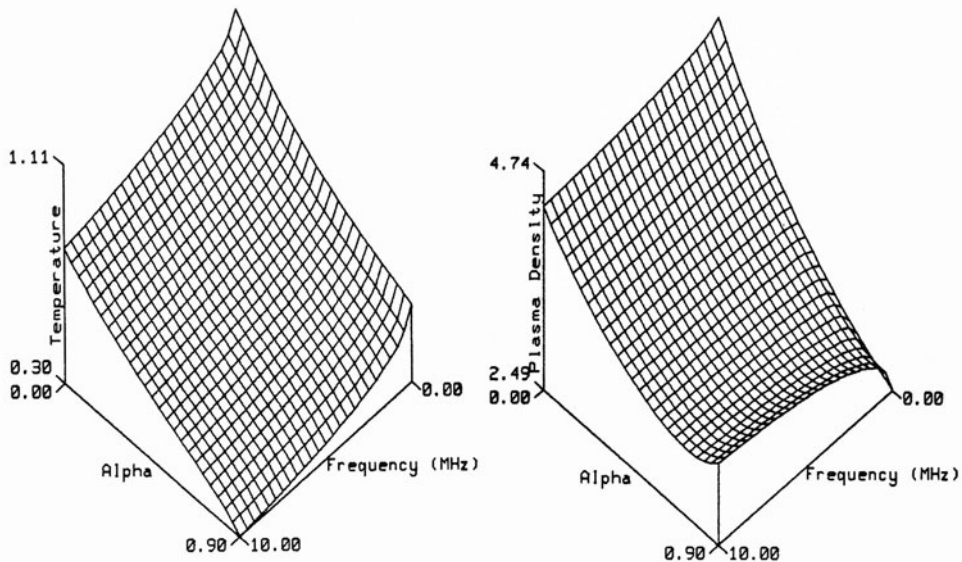

Fig. 4 Surface temperature T(0) (°C) and plasma density N(0) (10^{17}/cm³) as functions of α and modulation frequency at the center of a gaussian source of radius a = 1 μm assuming β/α = 1, τ = 1 msec and 1 mW of total absorbed power.

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