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Effect of Band Tails on Stimulated Emission of Light in Semiconductors*

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The dependence of the stimulated emission of radiation in semiconductors on temperature and on impurity concentration has been calculated using a Kane model with a Gaussian band tail for the density of states, and an optical model with a constant matrix element and no selection rule for the radiative transitions. The screening length and the characteristic energies for the widths of the conduction- and valence-band tails are calculated by a self-consistent procedure, and the calculation has no adjustable parameters. Numerical results are obtained using parameters appropriate for GaAs injection lasers. The presence of band tails leads to a more nearly linear dependence of gain on excitation level, in better agreement with experiment, than did the calculation without band tails by Lasher and Stern. Increasing impurity concentration leads to a weaker temperature dependence of the excitation rate required to reach a given gain.

1. INTRODUCTION

THE qualitative features of stimulated emission of radiation in semiconductors are by now well understood. We consider here only one aspect of this subject, namely the effect of band tails on stimulated emission, particularly on its temperature dependence.

There is considerable experimental evidence for the presence of band tails associated with random impurity distributions in semiconductors. Most relevant to this paper are experiments on optical absorption,[1–3] on radiative recombination and electroluminescence,[4–6] and on electrical properties.[7,8] Our detailed considerations are limited to gallium arsenide, and even for this material the papers just cited represent only a small part of the published literature.

Theory has lagged considerably behind experiment in giving quantitative information about band tails in solids. While many papers treat the energy spectrum of disordered systems,[9,10] the results are usually not in a form that can be readily used for further calculations. Only a few models have been treated exactly. One of these is the density of states associated with deep impurity levels, which acquire a range of energies because of fluctuating Coulomb potentials.[11] Another is the structure of the band edge in a one-dimensional crystal with random impurities.[12] We shall use in this calculation the approximate band-tailing model of Kane,[13] which is described in the following section.

The present work is a simple extension of the calculation by Lasher and Stern.[14,15] The need for an extended calculation is apparent from two kinds of experiments. The first is the finding that the gain in injection lasers is a linear function of current, as shown for example by Pilkuhn, Rupprecht, and Blum.[16] This contradicts the calculated results of LS, who found the gain to vary superlinearly with current for temperatures of the order of 80°K and above. The second is the experimentally observed relation between the temperature dependence of threshold current density and the method of preparing semiconductor lasers.[17–19]

In Sec. 2 we describe the model used in the calculation. It is relatively straightforward, and contains no arbitrary parameters. We call attention in particular to the calculation of the screening length, which is carried through self-consistently. In this calculation we introduce the concept of diffusion energy, which appears in the expression for the screening length and in the relation between diffusion constant and mobility. An outline of the details of the calculation is given in

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[1] J. I. Pankove, Phys. Rev. **140**, A2059 (1965). I am indebted to Dr. Pankove for a copy before publication.

[2] G. Lucovsky, Appl. Phys. Letters **5**, 37 (1964).

[3] I. Kudman and T. Seidel, J. Appl. Phys. **33**, 771 (1962).

[4] G. Lucovsky, A. J. Varga, and R. F. Schwarz, Solid State Commun. 3, 9 (1965).

[5] G. Lucovsky, in *Physics of Quantum Electronics*, edited by P. L. Kelley, B. Lax, and P. E. Tannenwald (McGraw-Hill Book Company, New York, 1966), p. 467. I am indebted to Dr. Lucovsky for a copy before publication.

[6] N. N. Winogradoff and H. Kessler, Solid State Commun. **2**, 119 (1964).

[7] O. V. Emelianenko. T. S. Lagunova, D. N. Nasledov, and G. N. Talalakin, Fiz. Tverd. Tela **7**, 1315 (1965) [English transl.: Soviet Phys.—Solid State **7**, 1063 (1965)].

[8] O. Ohtsaki, T. Kotani, Y. Iwai, and I. Tsurumi, Japan. J. Appl. Phys. **4**, 314 (1965.)

[9] I. M. Lifshitz, Advan. Phys. **13**, 483 (1964).

[10] V. L. Bonch-Bruevich and R. Roman, Fiz. Tverd. Tela **5**, 2117 (1964) [English transl.: Soviet Phys.—Solid State **5**, 2890 (1963)].

[11] T. N. Morgan, Phys. Rev. **139**, A343 (1965).

[12] See, for example, B. I. Halperin, Phys. Rev. **139**, A104 (1965), and references cited therein.

[13] E. O. Kane, Phys. Rev. **131**, 79 (1963).

[14] G. Lasher and F. Stern, Phys. Rev. **133**, A553 (1964), to be referred to as LS.

[15] The expression in brackets in Eq. (5c) of LS should have a superscript −1. Also, the expression in braces in Eq. (5d) of LS should be replaced by 2, which brings that equation into agreement with the corresponding result of Dumke (see Ref. 20). I am indebted to B. H. Sacks and to T. N. Morgan, respectively, for pointing out these errors.

[16] M. Pilkuhn, H. Rupprecht, and S. Blum, Solid-State Electron. **7**, 905 (1964).

[17] G. C. Dousmanis, H. Nelson, and D. L. Staebler, Appl. Phys. Letters **5**, 174 (1964).

[18] M. Pilkuhn, H. Rupprecht, and J. Woodall, IEEE J. Quant. Electron. **QE-1**, 184 (1965).

[19] M. Pilkuhn and H. Rupprecht, J. Appl. Phys. (to be published).

Sec. 3. We use parameters appropriate for GaAs throughout.

Our results are given in Sec. 4. Most important is the temperature dependence of the excitation rate required to maintain a given gain for various donor and acceptor concentrations. We also give values for the photon energy at which the stimulated emission rate has its peak, for the screening length, and for the characteristic energies of the conduction- and valence-band tails. The application of these results to GaAs-injection lasers is given in Sec. 5.

In the last section the results are discussed and some directions in which the theory must be improved are indicated.

2. DESCRIPTION OF THE MODEL

A. The Optical Model

We consider a homogeneous semiconductor in which radiative transitions between states in the perturbed conduction band and states in the perturbed valence band take place with a matrix element independent of the initial and final states. Thus the shape of the emitted spectrum depends only on the densities of states in the two bands, and on the occupations of the levels.

The light emitted per unit volume and per unit energy is then given by [LS, Eq. (6a)]

$$r_{\text{spon}}(E)=B\int\rho_c(E')\rho_v(E'-E)f_c(E')\times[1-f_v(E'-E)]dE',\quad(1)$$

where E is the photon energy, ρ_c and ρ_v are the densities of states per unit volume and unit energy in the conduction and valence bands, and f_c and f_v are the probabilities that these states are occupied by electrons. The relation between B and the matrix element is given by LS, Eqs. (6c) and (12), and by Dumke.[20]

We suppose that the electrons scatter one another in times short compared to their recombination lifetime, so that they are in equilibrium with one another, and can be characterized by a quasi-Fermi level F_n and a temperature T, which we suppose to be the same as the lattice temperature. We make the same assumptions for holes, characterized by quasi-Fermi level F_p, and thus find

$$f_v(E'')=[1+\exp([E''-F_p]/KT)]^{-1},\quad(2)$$

where K is Boltzmann's constant.

The absorption coefficient $\alpha(E)$ can easily be obtained from the spontaneous emission rate $r_{\text{spon}}(E)$ and from the difference

$$\Delta F=F_n-F_p\quad(3)$$

between the electron and hole quasi-Fermi levels from the relation [LS, Eqs. (8) and (9)]

$$\alpha(E)=\pi^2c^2\hbar^3n^{-2}E^{-2}r_{\text{spon}}(E)\times\{\exp[(E-\Delta F)/KT]-1\},\quad(4)$$

where n is the index of refraction at photon energy E. We see that α is negative, corresponding to amplification of light, when $E<\Delta F$.

We assume that stimulated emission occurs in p-type material,[21] and use Gaussian units throughout.

B. The Band Model

The density of states to be inserted in Eq. (1) is taken from the results of Kane[13] to be, for the conduction band

$$\rho_c(E')=\pi^{-2}\hbar^{-3}m_c^{3/2}(2\eta_c)^{1/2}y[(E'-E_c)/\eta_c],\quad(5)$$

where m_c is the conduction-band effective mass, E_c is the energy of the nominal conduction band edge,

$$y(x)=\pi^{-1/2}\int_{-\infty}^{x}(x-z)^{1/2}\exp(-z^2)dz,\quad(6)$$

and η_c is a band-tail spreading energy given by

$$\eta_c=(e^2/\kappa_s)(4\pi N_DL_{\text{scr}})^{1/2},\quad(7)$$

where κ_s is the static dielectric constant, N_D is the donor concentration, and L_{scr} is the screening length to be discussed below.

When the characteristic energy η_c goes to zero, Eq. (5) reduces to the standard expression for the density of states in a band of effectke mass m_c, since $y(x)\rightarrow x^{1/2}$ as $x\rightarrow\infty$. Then the calculation of r_{spon} and α reduces to the one given by LS.

A measure of the importance of the band tail is given by the total number of states per unit volume whose energy is below that of the nominal conduction band edge. We find

$$\int_{-\infty}^{E_c}\rho_c(E')dE'=6^{-1}\pi^{-5/2}\hbar^{-3}(2m_c\eta_c)^{3/2}\Gamma(5/4),\quad(8)$$

where $\Gamma(5/4)=0.9064$. This is the same as the number of carriers at absolute zero in a conventional parabolic band with effective mass m_c if the Fermi level relative to the band edge is 0.403 η_c. In an uncompensated sample with N_D ionized donors per unit volume, the screening length at absolute zero calculated without band tails is given by Eq. (12) below, and the ratio of the number of states below the band edge to the total electron concentration is approximately

$$N_D^{-1}\int_{-\infty}^{E_c}\rho_c(E')dE'=3^{-9/8}\pi^{-13/8}2^{5/4}\Gamma(5/4)(N_Da^{*3})^{-3/8},$$
$$\approx2.5\times10^8(\kappa_sm/m_c)^{-9/8}N_D^{-3/8},\quad(9)$$

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[20] W. P. Dumke, Phys. Rev. **132**, 1998 (1963).

[21] See, for example, G. Burns and M. I. Nathan, Proc. IEEE **52**, 770 (1964).

where $a^*=\kappa_s\hbar^2/m_ce^2$ is the effective Bohr radius. If we put $\kappa_s=12.5$, and $m_c=0.072$ m, as appropriate for GaAs, and take $N_D=10^8$ cm^{-3}, we find that 14% of the electrons are in states in the conduction band tail.[22] As N_D increases, the absolute number of states in the tail increases, but their importance relative to the total number of carriers decreases.

So far, our discussion has been for an uncompensated n-type semiconductor. The results of Eqs. (5) to (9) can easily be extended to p-type semiconductors if we replace $E'-E_c$ in (5) by E_v-E', where E_v is the energy of the nominal valence band edge, and replace m_c, η_c, and N_D by m_v, η_v, and N_A, respectively. If we take $m_v=0.5m$, we find that in uncompensated p-type material with 10^{18} acceptor ions per cm^3, there are about as many states in the tail as there are carriers.

When both donors and acceptors are present, we make the further approximation that the conduction-band edge is affected only by the donor ions, and the valence-band edge is affected only by the acceptor ions. This is certainly not rigorously true, but Morgan's[11] results suggest that our approximation is valid qualitatively.

In addition to the band tailing, there is also a shift in the position of the nominal band edges, which has been estimated by Wolff[23] for uncompensated semiconductors. For very large carrier concentrations, conduction and valence bands will experience equal shifts. In transitions between conduction and valence bands in homogeneous material, it is only the difference in the positions of the nominal conduction- and valence-band edges which is of significance. We shall suppose that this difference is the same as in pure material.

C. The Screening Length

Since we are dealing with nonparabolic energy bands, the simple formula for the classical screening length L_{scr} which enters in Eq. (7) cannot be used. It must be modified in our case also because we are dealing with a nonequilibrium system characterized by more than one quasi-Fermi level. Under these more general circumstances the conventional derivation[24] of the screening length leads to the result

$$L_{\mathrm{scr}}^{-2}=(4\pi e^2/\kappa_s)\sum_i(dN_i/dF'_i)\,, \tag{10}$$

where N_i is the concentration of carriers in band i, and F'_i is the quasi-Fermi level for these carriers relative to the band edge, measured positively into the band. In particular, since we deal only with one kind of conduction band and one kind of valence band, we have $F'_n=F_n-E_c$ and $F'_p=E_v-F_p$.

It is convenient to introduce an energy $E_{d,i}$, which we call the diffusion energy, defined by

$$E_{d,i}=N_i/(dN_i/dF'_i)\,. \tag{11}$$

For parabolic bands at absolute zero, $E_{d,i}=2F'_i/3$, for which

$$L_{\mathrm{scr}}=2^{-1}(\pi/3)^{1/6}N_i^{-1/6}a^{*1/2}\,, \tag{12}$$

where a^* has the same meaning as in (9). Numerically this gives

$$L_{\mathrm{scr}}[\mathrm{cm}]=3.67\times10^{-5}(N_i[\mathrm{cm}^{-3}])^{-1/6}\times(\kappa_s m/m_c)^{1/2}\,. \tag{13}$$

For any band to which Boltzmann statistics apply, $E_d=KT$. We call E_d the diffusion energy because it is the energy which appears in the generalized Einstein relation[25,26]

$$D_i=E_{d,i}\mu_i/e \tag{14}$$

between the diffusion constant D_i and the mobility μ_i of the carriers in band i.

The screening length depends on the density of states of the carriers, on the degree of excitation F' in each band, and on the temperature. But the density of states depends on the screening length through Eqs. (5) and (7). Thus the problem of determining η_c, η_v and L_{scr} must be solved self-consistently. This has been done, as described more fully below.[27]

Although the screening length given by Eq. (10) does not accurately describe the screening of ionic potentials in a semiconductor under all conditions, its use is warranted in our calculation for two reasons: first, because it qualitatively describes the changes in the screening with temperature and with excitation of the system, and second, because we avoid the lower range of carrier concentrations, for which its validity is most questionable.

D. Discussion of the Model

The model used in our calculations has a number of advantages. It is relatively simple, since the Kane band model has only a single parameter to characterize the band tailing. It is free of arbitrariness, since we use the standard screening-length expression, and find the band structure and the screening length by a self-consistent procedure.

The model does have many limitations, of course, most of which appear to be unavoidable at the present stage of development of the theory of impure semiconductors. The Kane model is not exact for uncom-

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[22] A self-consistent calculation for the screening length and η_c that includes the effect of the band tail increases the numerical coefficient in Eq. (9) by about 2% for this example.

[23] P. A. Wolff, Phys. Rev. **126**, 405 (1962).

[24] See, for example, R. B. Dingle, Phil. Mag. **46**, 831 (1955).

[25] E. Spenke, *Elektronische Halbleiter* (Springer-Verlag, Berlin, 1965), 2nd ed., p. 424. References to the original papers by Nernst, Townsend, and Einstein are cited there. See also R. Kubo, J. Phys. Soc. Japan **12**, 570 (1957).

[26] The connection between the screening length and the Einstein relation has been pointed out, for a case with a single type of carrier present, by W. Bernard, H. Roth, A. P. Schmid, and P. Zeldes, Phys. Rev. **131**, 627 (1963).

[27] A self-consistent solution at absolute zero, using a somewhat different model, was carried out by Morgan, Ref. **11**.

pensated materials; its use for compensated materials is even less clearly justified. In particular, independent treatment of the conduction- and valence-band densities of states neglects the correlations which arise because each transition takes place in a small part of the crystal, where a potential fluctuation is likely to affect both bands. These correlations will appear in the matrix elements in a more exact treatment.

The use of a constant matrix element is also unjustified, since states far in the tail are likely to have more tightly localized wave functions than do states at higher energy. These differences will certainly affect the matrix element, but there appear to be no quantitative results for heavily doped semiconductors on which to base a better approximation than the constant-matrix-element approximation which we use.

An alternative approach to the question of absorption-edge tails to the one given here is that of Redfield,[28] who considers the effect of fluctuating electric fields on the absorption edge. This approach does take the correlations between the bands into account and may provide an independent way to deal quantitatively with the effects of random impurities on stimulated emission.

There are certain limitations we must impose on the impurity concentrations if our calculation is to be reasonable. The Kane model applies only for impurity concentrations high enough that the impurity levels have actually merged with the adjacent band edge. An approximate condition for this to happen is that the characteristic energy η_c or η_v exceeds the ionization energy of the donor or acceptor impurity. This condition is fulfilled when $N_D \gtrsim 10^{17}$ cm^{-3} and when $N_A \gtrsim 3\times10^{18}$ cm^{-3}, with some variation depending on the carrier concentration, which enters η_c and η_v through L_{scr}. These limits are approximately the same as those at which impurity activation energies found from electrical measurements[7,8] approach zero. There cannot be a precise determination of a cutoff impurity concentration in any case, since the minimum in the density of states between the impurity level and the adjacent band fills up gradually as the carrier concentration is increased.

All the numerical calculations reported here meet the conditions for applicability of the Kane model mentioned above. We also made some calculations with acceptor concentrations down to 10^{18} cm^{-3}. The density of states for that carrier concentration is not well described by a Kane model, and may be somewhat better approximated by a model with a discrete level with Gaussian broadening.[5,29]

The optical model which we use is valid provided the carrier concentration does not exceed approximately 4×10^{18} cm^{-3}. This is because the constant matrix element of our no-selection-rule model is obtained by dividing the matrix element for a direct transition among all the states perturbed by the impurities. We essentially use up the available phase space at the indicated carrier concentration, as was pointed out by Dumke.[20] Our carrier concentrations are near the upper limit of the allowable range.

3. DESCRIPTION OF THE CALCULATION

The numerical evaluation of the expressions for the spontaneous spectrum, for the total spontaneous emission rate, and for the carrier concentrations and quasi-Fermi levels in the conduction and valence bands is straightforward, and is described briefly here.

Our calculation is carried out for GaAs, for which we take the following values of constants:

$$\begin{aligned}
\text{electron effective mass}^{30}\ m_c &= 0.072m\,,\\
\text{hole effective mass}^{31}\ m_v &= 0.5m\,,\\
\text{static dielectric constant}^{32}\ \kappa_s &= 12.5\,, \qquad (15)\\
\text{index of refraction}^{33}\ n &= 3.6\,,\\
\text{recombination constant}^{34}\ B &= 7.5\times10^{-10}\ \text{cm}^3/\text{sec}.
\end{aligned}$$

Primary input parameters are the donor and acceptor concentrations N_D and N_A. The net hole concentration is then $P-N=N_A-N_D$.

For a given difference ΔF of the quasi-Fermi levels and a given temperature T, a trial value of the screening length L_{scr} is assumed, and the band-spread parameters η_c and η_v are calculated from Eq. (7). With these values, the electron and hole quasi-Fermi levels are found by an iterative procedure, and the values of N, P, $E_{d,n}$ and $E_{d,p}$ are found. From these values a new screening length is calculated from Eqs. (10) and (11), and the process is repeated until input and output values of L_{scr} agree within 0.1%. Convergence is quite rapid, since the screening length depends mainly on the carrier concentrations and temperature, and only weakly on the band shape.

Once the quasi-Fermi levels are known, we calculate r_{spon} from Eq. (1) and $\alpha(E)$ from Eq. (4). The maximum value of $-\alpha$ is the gain g, which increases with increasing ΔF. In presenting our results, we usually give g not as a function of ΔF, but of the related quantity $\mathcal{R}=BNP$. It is convenient to express $\mathcal{R}$ as a nominal current

$$J_{\mathrm{nom}}=1.602\times10^{-23}\mathcal{R}\,, \qquad (16)$$

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[28] D. Redfield, Phys. Rev. **130**, 916 (1963); Solid State Commun. **1**, 151 (1963).

[29] G. Lucovsky, Solid State Commun. **3**, 105 (1965). This paper calculates the characteristic energies η_c and η_v using Eqs. (7) and (12), but using impurity concentrations rather than carrier concentrations to determine the screening length. The good agreement found between the calculated and measured values may therefore be fortuitous.

[30] H. Ehrenreich, J. Appl. Phys. **32**, 2155 (1961).

[31] C. Hilsum, in *Physics of Semiconductors* (Dunod Cie, Paris, 1964), p. 1127.

[32] K. G. Hambleton, C. Hilsum, and B. R. Holeman, Proc. Phys. Soc. (London) **77**, 1147 (1961).

[33] D. T. F. Marple, J. Appl. Phys. **35**, 1241 (1964).

[34] This value was calculated by LS, using the same constants given here and assuming an acceptor ionization energy of 34 MeV.

the current which must flow to maintain the recombination rate $\mathcal{R}$ per cm^3 sec in a layer 1μ thick if the internal quantum efficiency is 100%.

For one value of ΔF, the calculation required about 12 sec on an IBM 360/40 system. At each temperature, a number of values of ΔF were used to find the dependence of maximum gain on J_{nom}. The temperature dependence is determined by finding the values of J_{nom} required to maintain a given value of g at each temperature.

As input to the calculation we also used the energy gap of GaAs as found by Sturge.[35] Because of the uncertainty in the positions of the nominal band edges, mentioned in Sec. 2B, the values of photon energy found for the spectrum are rather uncertain and should not be compared with experiment without further consideration. Relative values, such as line widths and shifts with current at a fixed temperature are, however, valid results of the model.

A rather coarse grid was used in the various integrations, and numerical interpolation was used to find the values shown in the figures and tables for specified values of g. We expect the error in J_{nom} to be $\lesssim 2\%$, and the error in photon energies, quasi-Fermi levels, and line widths to be less than 2 meV. The values of L_{scr}, E_d, and η_c and η_v should be correct within 1%. These numerical uncertainties are small compared to the physical approximations involved in the calculation.

4. RESULTS

We first show, in Fig. 1, the dependence of gain g on nominal current density J_{nom} for donor and acceptor concentrations of 1×10^{18} and 4×10^{18} cm^{-3}, respectively, for five temperatures between absolute zero and room temperature. Shown for comparison are the results without band tails, as in LS, for 80°K and 300°K. We see that the presence of band tails makes the gain up to about 160°K vary nearly linearly with current, while the dependence of gain on current at 300°K is much less superlinear than that found by LS. Since experiment indicates that the gain is a linear function of current,[16,18] these results are in much better agreement with experiment than those found without band tails.

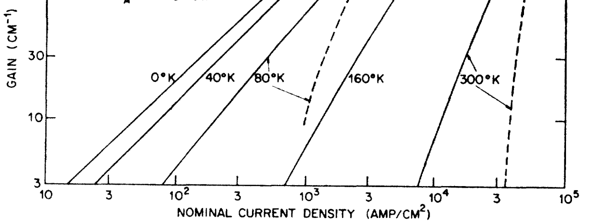

FIG. 1. Variation of gain with nominal current density [defined in Eq. (16)] for recombination in a region with 1×10^{18} donor atoms and 4×10^{18} acceptor atoms per cm^3. The dashed curves show results calculated without band tails, as in Ref. 14.

If the impurity concentration is increased, we find that the room temperature gain becomes still more linear with current. These results are summarized in Table I, in which the exponent b in the relation $g=\beta J_{\text{nom}}{}^b$ is a measure of the linearity. We determine b from the values of J_{nom} required to reach a gain of 30 cm^{-1} and 300 cm^{-1}, i.e.,

$$b=1/\log_{10}[J_{\text{nom}}(g=300)/J_{\text{nom}}(g=30)]. \tag{17}$$

The temperature dependence of the excitation rate required to reach a gain of 100 cm^{-1} is shown in Fig. 2. Because of the nonlinearity at the higher temperatures, the temperature dependence will be somewhat different at other gains. The necessary corrections over a limited range of gain values can be made by using the exponent b as given in Table I.

The striking variation of the temperature dependence with donor content is quite clear from Fig. 2. We also find that changing the net hole concentration from 3×10^{18} cm^{-3} to 1×10^{18} cm^{-3} gives a similar set of curves. Since the principal effect of the change in impurity content is to vary the width of the band tails, we conclude that these have a pronounced effect on the temperature dependence of threshold. Other defects which introduce band tails would have a similar effect.

A number of other results are given in Table I. We note in particular the diffusion energy E_d and the screening length L_{scr}, which are required to find the characteristic energies η_c and η_v of the band structure. These quantities will depend on the degree of excitation of the system, because the carrier concentrations and carrier quasi-Fermi levels increase as the degree of excitation increases. An example of this dependence is given in Table II.

Although our main concern is with stimulated emission, we show the spontaneous spectrum for a number of temperatures in Fig. 3, since this is of interest in comparing the model used in the present calculation with other models. Some of the features of the spontaneous emission are given in Table II.

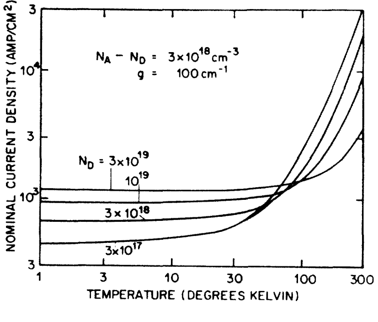

FIG. 2. Temperature dependence of nominal current density required to reach a gain of 100 cm^{-1} for four compositions with $N_A-N_D=3\times10^{18}$ cm^{-3}.

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[35] We interpolated between the values given by M. D. Sturge, Phys. Rev. 127, 768 (1962), to find the values given in the caption of Table I.

TABLE I. Calculated results for gain $g = 100$ cm^{-1} for a series of compositions with $N_A - N_D = 3\times10^{18}$ cm^{-3}, where N_A and N_D are the acceptor and donor concentrations, respectively. J_{nom} is the nominal current density defined in Eq. (16); b is the exponent defined in Eq. (17); $E_{m,g}$ is the photon energy at which $-\alpha(E)$ of Eq. (4) has its peak; ΔF is the difference between the electron and hole quasi-Fermi levels; F'_n and F'_p are the quasi-Fermi levels of electrons and holes with respect to the corresponding nominal band edges, with positive values into the band and negative values into the gap; $E_{d,c}$ and $E_{d,v}$ are the diffusion energies for electrons and holes, respectively, defined in Eq. (11); L_{scr} is the screening length defined in Eq. (10); η_c and η_v are the characteristic band-tail energies for the conduction and valence bands, respectively, defined in Eq. (7); and N is the electron concentration in the active layer. The nominal energy gap is taken to be 1.521, 1.519, 1.513, 1.487, and 1.433 eV, respectively, at 0°, 40°, 80°, 160°, and 300°K.

N_D (cm^{-3})	N_A (cm^{-3})	T (°K)	J_{nom} (A/cm^2)	b	$E_{m,g}$ (eV)	ΔF (eV)	F'_n (meV)	F'_p (meV)	$E_{d,c}$ (meV)	$E_{d,v}$ (meV)	L_{scr} (Å)	η_c (meV)	η_v (meV)	N (cm^{-3})
3×10^{17}	3.3×10^{18}	0	450	0.96	1.514	1.522	−3	3	4.3	17.2	19.7	9.9	32.9	1.2×10^{16}
		40	700	1.06	1.509	1.518	−4	3	5.8	17.6	19.9	10.0	33.1	1.9×10^{16}
		80	1540	1.28	1.499	1.509	−4	0	9.2	18.7	20.4	10.1	33.4	4.2×10^{16}
		160	6100	1.78	1.468	1.480	1	−8	18.5	22.4	21.5	10.4	34.4	1.6×10^{17}
		300	31000	2.7	1.414	1.427	22	−28	39.2	31.9	22.7	10.6	35.3	7.0×10^{17}
1×10^{18}	4×10^{18}	0	540	0.95	1.500	1.511	−10	1	6.8	18.4	20.4	18.4	36.9	1.5×10^{16}
		40	710	1.00	1.496	1.509	−11	0	7.7	18.7	20.6	18.5	37.0	2.0×10^{16}
		80	1360	1.09	1.488	1.500	−10	−3	10.4	19.7	21.0	18.7	37.4	3.7×10^{16}
		160	5100	1.57	1.458	1.471	−5	−11	18.8	23.2	22.0	19.2	38.3	1.4×10^{17}
		300	27000	2.4	1.404	1.419	16	−30	38.5	32.3	23.2	19.7	39.3	6.2×10^{17}
3×10^{18}	6×10^{18}	0	680	0.94	1.472	1.488	−26	−7	10.9	21.3	22.0	33.1	46.8	1.9×10^{16}
		40	800	0.96	1.469	1.485	−26	−8	11.5	21.6	22.1	33.2	47.0	2.2×10^{16}
		80	1210	1.04	1.461	1.478	−25	−10	13.4	22.4	22.4	33.4	47.3	3.3×10^{16}
		160	3600	1.30	1.432	1.449	−20	−18	20.0	25.3	23.3	34.1	48.3	9.8×10^{16}
		300	19200	1.86	1.378	1.396	1	−38	37.3	33.4	24.5	35.0	49.4	4.6×10^{17}
1×10^{19}	1.3×10^{19}	0	950	0.93	1.397	1.423	−65	−33	19.5	29.1	25.6	65.3	74.5	2.6×10^{16}
		40	1010	0.94	1.395	1.420	−65	−34	19.8	29.2	25.7	65.4	74.6	2.8×10^{16}
		80	1220	0.96	1.388	1.413	−64	−35	20.9	29.7	25.8	65.6	74.8	3.4×10^{16}
		160	2300	1.06	1.359	1.385	−60	−42	25.0	31.7	26.4	66.4	75.7	6.2×10^{16}
		300	8900	1.34	1.302	1.329	−43	−61	37.6	37.8	27.5	67.7	77.2	2.3×10^{17}
3×10^{19}	3.3×10^{19}	0	1200	0.91	1.228	1.271	−152	−98	34.1	44.1	31.4	125	131	3.3×10^{16}
		40	1230	0.91	1.226	1.269	−151	−99	34.3	44.2	31.4	125	131	3.4×10^{16}
		80	1320	0.91	1.219	1.262	−151	−100	34.8	44.4	31.5	125	131	3.6×10^{16}
		160	1690	0.94	1.189	1.233	−149	−105	36.9	45.5	31.8	126	132	4.6×10^{16}
		300	3500	1.04	1.129	1.173	−140	−121	44.2	49.2	32.6	127	134	9.5×10^{16}

5. APPLICATION TO GaAs LASERS

To apply our results to GaAs lasers, we must convert from the nominal current density J_{nom}, which is the current density required to maintain the gain g in a layer one micron thick if there are no losses, to the actual current density J that is required to maintain the same gain in the active layer of a semiconductor laser.

The conversion factor depends on three quantities. One is the thickness d of the active layer, and the second is the quantum efficiency η, which is the fraction of exciting particles[36] that produces radiative recombination in the spectral range of interest. The third factor Γ takes into account the incomplete confinement of the mode propagating along the active layer to the layer itself,[37] and is approximately equal to the fraction of the energy of the propagating mode which is within the active layer. With these three quantities we can write

$$J = J_{\text{nom}} d / \eta \Gamma, \tag{18}$$

where d is measured in microns.

There is experimental evidence that the internal

TABLE II. Variation of several calculated quantities with the degree of excitation for $N_D = 3\times10^{18}$ and $N_A = 6\times10^{18}$ cm^{-3} at 0, 80, and 300°K. $E_{m,\text{sp}}$ and ΔE_{sp} are the peak photon energy and the half-intensity width, respectively, of the spontaneous emission. All other quantities are as in Table I.

	J_{nom}(A/cm^2)			$E_{m,\text{sp}}$(eV)			ΔE_{sp}(meV)			$E_{d,c}$(meV)			L_{scr}(Å)		
g(cm^{-1})	0°K	80°K	300°K	0°K	80°K	300°K	0°K	80°K	300°K	0°K	80°K	300°K	0°K	80°K	300°K
1	5.6	16.7	2 200	1.435	1.438	1.441	30	56	130	6.7	8.7	28.2	22.2	22.7	27.1
3	17.5	45	3 400	1.442	1.444	1.444	31	55	129	7.3	9.3	29.2	22.2	22.7	26.8
10	61	137	6 000	1.451	1.451	1.447	32	54	128	8.2	10.2	30.9	22.2	22.7	26.3
30	191	380	10 200	1.460	1.459	1.452	33	53	127	9.2	11.4	33.3	22.1	22.6	25.6
100	680	1210	19 200	1.472	1.470	1.461	35	53	127	10.9	13.4	37.3	22.0	22.4	24.5

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[36] The calculation is carried out for an injection laser structure, but can be easily modified if the exciting particles are photons or energetic electrons incident on the surface.

[37] F. Stern, in *Radiative Recombination in Semiconductors* (Dunod Cie., Paris, 1965), p. 165.

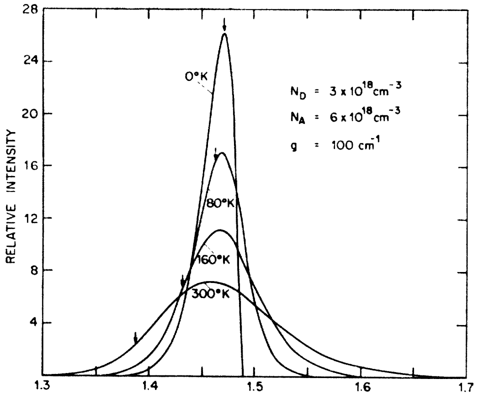

FIG. 3. Calculated spontaneous emission line shape for $N_D = 3\times10^{18}$ and $N_A = 6\times10^{18}$ cm^{-3}. The curves have been normalized to unit area. The arrows mark the energies at which $-\alpha(E)$ has its peak.

quantum efficiency of GaAs diodes and lasers is close to 1 at low temperatures, and is of the order of 0.5 at room temperature.[17,19,38] There is indirect evidence that in diffused diode lasers the active layer thickness d is about 1.5μ, and that the coefficient Γ is about 0.9, both at 77°K.[37] There is some reason to suppose that the dispersion of the index of refraction is less steep near the absorption edge at room temperature than at low temperatures, and that the radiation confinement effects associated with index changes will be less pronounced at high temperatures. This would lead to a smaller value of Γ. No estimates based on room-temperature experiments are yet available, however.

We can make some qualitative predictions about the temperature dependence of the active layer thickness for injection lasers in diodes with linearly graded junctions from the relation[39]

$$d = s(D/AB)^{1/3}, \tag{19}$$

where D is the diffusion coefficient of the electrons, A is the gradient of the net impurity concentration $N_A - N_D$ in the active layer, B is the rate constant introduced in Eq. (1), and s is a numerical constant of the order of unity. The quantities A and B are here considered to be independent of temperature,[40] so it is only the temperature dependence of D which affects the temperature dependence of d. Since D is given by Eq. (14), it depends both on the mobility μ and on the diffusion energy E_d. For the high impurity concentrations in the active layer which we consider, the mobility varies by about a factor 2 over the temperature range from 0°K to 300°K.[41,42] The diffusion energy increases monotonically with increasing temperature, as shown in Table I, with a change between 80°K and 300°K that varies between a factor 4 at the lowest impurity concentrations and a factor 1.3 at the highest. The changes in μ and in E_d tend to oppose each other for the lower impurity concentrations.

TABLE III. Estimated current density required to reach a gain of 100 cm^{-1}, and the corresponding gain parameter β of Eq. (20), in comparison with the experimental results of Ref. 16 for a sample made by diffusing Zn into n-type GaAs with 5×10^{18} donors/cm^3. The calculated values of J_{nom} are for $N_D = 3\times10^{18}$ cm^{-3} and $N_A = 6\times10^{18}$ cm^{-3}. The active layer thickness d, the internal quantum efficiency η, and the radiation confinement parameter Γ are estimated, as discussed in the text.

	80°K	300°K
J_{nom}(A/cm^2)	1210	19200
d (microns)	1.5	2.0
η	0.7	0.5
Γ	0.9	0.8
J(A/cm^2)	2900	96000
β_{calc} (cm/A)	3.5×10^{-2}	1.04×10^{-3}
β_{exp} (cm/A)[a]	2.5×10^{-2}	0.49×10^{-3}

[a] Data of Ref. 16, for 77°K and 296°K, respectively.

We conclude that for all the cases we consider the temperature dependence of d is rather weak, with an increase between 77°K and 300°K of perhaps 30%.

A summary of the parameters that enter the threshold current density of GaAs lasers at liquid-nitrogen temperature and room temperature, estimated using the considerations outlined above and the data of Table I, is given in Table III. We have used $N_D = 3\times10^{18}$ cm^{-3} and $N_A = 6\times10^{18}$ cm^{-3}, and compare with the data of Pilkuhn, Rupprecht and Blum[16] for a laser diode made by diffusion into a substrate with $N_D \sim 5\times10^{18}$ cm^{-3}. The constant β is given by

$$\beta = g/J, \tag{20}$$

where J is the current density required to reach gain g. In Table III we used the calculated results for $g = 100$ cm^{-1}.

The value $g = 100$ cm^{-1} which we use as a typical gain throughout this calculation is the gain required to reach threshold for a laser about 150 microns long. This length leads to an end loss $L^{-1}\log R^{-1}$ equal to 75 cm^{-1}, and we allow for internal losses, due to free carrier absorption and penetration of the beam into absorbing material, of about 25 cm^{-1}. The experimentally observed internal losses[16,18] are somewhat smaller at low temperatures and somewhat higher at room temperature, but the calculated temperature dependence of β is not very sensitive to small changes in the value of g that is used.

The observed temperature dependence is somewhat

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[38] S. V. Galginaitis, J. Appl. Phys. **35**, 295 (1964).

[39] F. Stern, in *Semiconductors and Semimetals Physics of III-V Compounds*, edited by R. K. Willardson and A. C. Beer (Academic Press Inc., New York, 1966), Vol. 2.

[40] Dumke, Ref. 20, found that the average value of B decreases by about a factor 2 between low temperature and room temperature. The decrease arises because the matrix element is not a constant, but decreases for electron states with higher crystal momentum, which are more populated at higher temperatures. This is one of the effects which must be taken into account in a more accurate theory.

[41] C. Hilsum, Progr. Semicond. **9**, 135 (1965).

[42] J. F. Woods (private communication).

stronger than the calculated one, but the agreement between the calculated and observed values in Table III is quite satisfactory, both for the absolute values and for the temperature dependence. The theory is certainly not reliable enough for precise comparisons, and the experimental data still fluctuate somewhat from one sample to another in a set of nominally equivalent samples.

The pronounced effect of heavy doping on the temperature dependence of J_{nom} shown in Fig. 2 remains to be compared with experiment. This would require a series of experiments like those of references 16 and 18, using samples with varying impurity content, together with determinations of the quantities d, η, and Γ of Eq. (18). One could also study homogeneous samples excited by light or by electron beams.

The comparison between diodes prepared by diffusion and those prepared by solution growth does not at present give a complete test of the theory, since the chemical structure near the active layer, and therefore also the quantities d and Γ of Eq. (18), may be quite different for these two kinds of structures. One indication that this is so is given by Pilkuhn and Rupprecht,[19] who find that the linewidth of the radiation from the solution-grown diodes is substantially larger than that of the diffused diodes even though both were made using the same n-type starting material. The greater linewidth in solution-grown diodes suggests that band-tailing effects are more pronounced in these, and thus their weaker temperature dependence is consistent with our calculation. This is not the only possible explanation, of course, and quantitative comparisons must be deferred until more is known about the chemical structure of solution-grown diodes.

6. DISCUSSION

The temperature dependence of the excitation rate required to reach a gain g can be rather easily understood, if we rewrite Eq. (4) [following LS, Eq. (25)] in the form

$$\mathcal{R}=(n^2E_{m,g}{}^2/\pi^2c^2\hbar^2)\gamma g\Delta E\,, \tag{21}$$

where $E_{m,g}$ is the photon energy of the lasing peak,[43] and ΔE is the half-intensity width of the spontaneous emission spectrum. The value of $E_{m,g}$ decreases, and the linewidth increases, with increasing temperature, but these effects are easily measured and require no further discussion. The main part of the temperature dependence of the excitation rate lies in the factor γ of Eq. (21), which we can write as a product of three factors:

$$\gamma=\frac{\int r_{\mathrm{spon}}(E)dE}{r_{\mathrm{spon}}(E_{m,sp})\Delta E}\times\frac{r_{\mathrm{spon}}(E_{m,sp})}{r_{\mathrm{spon}}(E_{m,g})}\times\frac{1}{1-\exp[(E_{m,g}-\Delta F)/KT]}\,, \tag{22}$$

where $E_{m,sp}$ is the photon energy of the spontaneous emission peak.

The first factor in Eq. (22) is a line shape factor, and will be close to 1 at all temperatures. The second factor is essentially equal to 1 at low temperature, since then the spontaneous emission and $-\alpha(E)$ have their maximum values at almost[43] the same photon energy. At higher temperatures, however, the spontaneous emission peak lies at higher photon energy than the stimulated emission peak, and the middle factor can reach values substantially greater than 1. The last factor in Eq. (22) is also equal to 1 at low temperature, and will be somewhat greater than 1 at higher temperatures.

We give a numerical example for 300°K for $N_D=3\times10^{18}$ and $N_A=6\times10^{18}$ cm^{-3}, and $g=100$ cm^{-1}. For that case $\gamma=9.7$, and the three factors in Eq. (22) equal 1.1, 4.6, and 1.9, respectively. Because the lasing peak lies at lower energy than the spontaneous emission peak, much of the excitation is "wasted."

The relatively weaker temperature dependence of the excitation rate required for a given gain in heavily doped units is mainly caused by a variation in the second factor in Eq. (22). This variation is rather simply understood, since in lightly doped semiconductors the density of states is increasing rather steeply with increasing energy near the electron and hole quasi-Fermi levels. Thus an increase in temperature leads to a large increase in the height of the spontaneous emission peak, as the mean energy of the excited carriers rises above the quasi-Fermi levels. In heavily doped materials, where the density of states is varying less rapidly with photon energy, this increase in the spontaneous spectrum is weaker, and the middle factor in Eq. (22) rises only gradually with increasing temperature.

Alternatively, we may say that the increase in carrier concentration necessary to maintain a given gain with increasing temperature is greater, the steeper the variation of the density of states with energy. This is essentially the explanation given by Dousmanis *et at.*[17] although their numerical examples are hard to justify quantitatively. The usefulness of heavy doping or compensation[6] in obtaining good laser performance at higher temperatures can be readily understood from these simple arguments.

Our calculation points out the great need for more work on the theory of energy levels and interband matrix

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[43] $E_{m,g}$ is the energy at which $-\alpha(E)$ reaches its maximum, and is essentially the same as the energy at which the stimulated function r_{stim} of LS has its maximum. When the ratio $\Delta E/E_{m,g}$ is no longer very small compared to 1, it may be necessary to distinguish between these two energies.

elements in impure and compensated semiconductors. For example, a calculation of these quantities even for a one-dimensional model would be very helpful. It would also be useful to have a quantitative description of the density of states near the band edge for the difficult range of impurity concentrations in which the minimum in the density of states between the impurity level and the adjacent band disappears.

In spite of the many shortcomings of the model used in our calculations, we conclude that it gives a reasonable account of the stimulated emission of radiation in impure GaAs for the range of impurity and carrier concentrations for which the model can be expected to apply. For small-gap semiconductors, such as InAs and InSb, the model may not be applicable directly, since small errors in the calculated position of the lasing peak lead to large errors in the factor E^{-2} of Eq. (4), an effect which is of minor importance in a semiconductor with a larger energy gap.

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Paramagnetic-Resonance Absorption in the Optically Populated State $^2F_{5/2}$, $E_{5/2}$ of Tm^{2+} in CaF_2

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Paramagnetic-resonance absorption was observed in the metastable state $^2F_{5/2}$, $E_{5/2}$ of CaF_2:Tm^{2+} which was populated by an optical source. The measured g value of 1.453 ± 0.002 can be compared with the calculated value of (−) 1.478. The g discrepancy of 0.025 is the same as found for the ground state. From the hyperfine constant for two values of J, a core-polarization correction of (+) 14±3 Mc/sec is derived for the ground state.

INTRODUCTION

PARAMAGNETIC-resonance absorption has been extensively used to analyze the structure of the ground state of paramagnetic ions and the interaction of these ions with their diamagnetic neighbors. Currently, this method is being exploited to examine the properties of excited states which can be populated by an optical source. Paramagnetic resonance absorption in a metastable state populated by optical pumping has already been reported for Dy^{2+} in CaF_2.[1] We wish to report on the paramagnetic-resonance spectrum of an excited state of Tm^{2+} in CaF_2, the emitting state of the laser, populated by incoherent unpolarized light. The optical spectrum of CaF_2:Tm^{2+} has been observed by Kiss[2] and it was also demonstrated that this system could be operated as a laser[3] at a wave number of about 9000 cm^{-1}. The ground-state paramagnetic-resonance spectrum and the ground-state nuclear-double-resonance spectrum have been investigated by Hayes and Twidell,[4] and Bessent and Hayes,[5] respectively. It has also been shown[6] that the broad $4f^{n-1}5d$ absorption bands show circular dichroism and that the ground-state Zeeman levels can be selectively pumped using polarized radiation. The ground configuration of Tm^{2+} consists of only a single term, ^2F, and therefore any breakdown of L-S coupling due to the crystalline field can be readily taken into account. Because of the simplicity of the Tm^{2+} system, the combination of paramagnetic-resonance data for both excited and ground states yields information about covalent bonding and core polarization. It is felt that investigations of the divalent thulium ion hold the most promise for reaching some conclusions about covalent bonding and core polarization in rare-earth ions since it is theoretically the most straightforward system and a considerable amount of data can be obtained on both of the J states in the ground configuration.

OPTICAL SPECTRUM OF Tm^{2+}:CaF_2

The divalent thulium ion (isoelectronic with Yb^{3+}) has 13 electrons in the incomplete $4f$ shell. The spin-orbit coupling $\zeta \mathbf{L}\cdot\mathbf{S}$ splits the energy levels into two spin-orbit states $^2F_{5/2}$ and $^2F_{7/2}$, spaced by $\frac{7}{2}\zeta$ with the latter lower. An ideal cubic field further splits these two

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