

Evaluation of semiconductor optical parameters for laser diodes

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Abstract: The small-signal modulation and noise properties (electrical voltage, optical power and phase) of laser diodes depend on ten real parameters relating to the semiconductor material employed. Among these, the phase-amplitude coupling factor α is of particular importance. These parameters are evaluated for GaAs at $0.87 \mu\text{m}$, GaInAsP at $1.55 \mu\text{m}$ and InAsSb at $3.87 \mu\text{m}$ at room temperature. Revised expressions for the optical gain are used. The light-hole contribution, the plasma effect and band-gap shrinkage are taken into account. The latter leads to a significant reduction of α , particularly below the peak-gain frequency. The α -factors for the three materials listed above are found to be, respectively, 2.9, 3.85 and 8.3 for conventional diodes.

1 Introduction

Stringent requirements concerning modulation characteristics and fluctuations are imposed upon laser diodes used in sensor and optical communication systems. The noise properties of laser diodes can be obtained in full generality from Nyquist's expression of fluctuations associated with resistors and the energy-conservation law [1]. This Nyquist theory gives expressions for the spectral density of fluctuating quantities that are in exact agreement with the results of quantum optics [2], even in the case of electrical feedback and nonclassical states of light [3]. For frequency-independent losses, one may equivalently postulate independent shot-noise fluctuations of the light fluxes. They are in approximate agreement with standard rate equations [4-6] for simple laser models but significant discrepancies may occur when spatial inhomogeneities are accounted for [7].

Besides geometrical parameters (thickness, width and length of the active volume) and the injected current and its fluctuations, the modulation and noise properties of laser diodes depend on ten parameters relating to the properties of the semiconductor employed in the active region. They are defined below.

Let U denote the voltage across the diode, the voltage drop across the confining layers and contacts being considered separately. U is equal to the energy spacing between the conduction and valence band quasi-Fermi levels divided by e (the absolute value of the electron charge), and is a function of the carrier density n .

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We define the dimensionless differential parameter $u \equiv (n/U) dU/dn$. The parameter u , which expresses the change of the electrical voltage U for some small change of carrier density n , is important for the optoelectrical characterisation of the diode particularly when electrical feedback from an optical detector is employed to reduce power or phase fluctuations.

Let $S(n)$ denote the total spontaneous recombination rate. The parameter $s \equiv (n/S) dS/dn$ expresses the dependence of S on the carrier density n . At $T = 0\text{K}$ the radiative spontaneous recombination rate is proportional to n and thus $s = 1$. At elevated temperatures, the electron-hole collision theory is an acceptable approximation and $s = 2$. The s -factor may reach the value of 3 when Auger effects are dominant.

Let us further define, as in Reference 8, the complex conductivity $\sigma(\nu, n) \equiv \sigma'(\nu, n) + i\sigma''(\nu, n)$. Note that time-variations are denoted with an $\exp(-i2\pi\nu t)$ notation at optical frequencies and an $\exp(j2\pi ft)$ notation at base-band frequencies [1]. The gain (or loss) is simply related to σ' , whereas the refractive index n_r is simply related to σ'' . The refractive index n_r determines, in conjunction with the refractive index of the confining layers, the confinement factor Γ (and thus the modal gain), the facet reflectivity for TE or TM polarisations, and the far-field radiation pattern. The differential gain $\partial\sigma'/\partial n$ importantly influences the laser diode relaxation frequency, and we define $g \equiv (n/\sigma') \partial\sigma'/\partial n$. The dependence of σ' on the optical frequency ν is very small for semiconductors and is unimportant when only one oscillating mode is considered. We therefore do not evaluate the parameter $\partial\sigma'/\partial\nu$. However, it is important to evaluate the group velocity v_g which is related to $\partial\sigma''/\partial\nu$. The group index $n_g \equiv c/v_g$ determines in conjunction with the confining-layer group index the intermode frequency spacing (precisely, one must average the product $n_r n_g$, with Γ as a weighting factor). Strictly speaking, these indices are complex numbers, but we find it sufficiently accurate to consider only the real parts. The most important factor is probably the phase-amplitude coupling factor $\alpha \equiv -(\partial\sigma''/\partial n)/(\partial\sigma'/\partial n)$. This factor, introduced in laserlinewidth theory by Lax [9] and Haug [10] is of major practical importance for laser diodes, as Henry first showed [11]. Finally, one must split σ' into $\sigma'_a - \sigma'_e$, where σ'_a expresses stimulated absorption and σ'_e stimulated emission. The factor $n_s \equiv -\sigma'_e/\sigma'$ (sometimes called 'spontaneous emission factor' and denoted n_{sp}) is unity for full inversion of the carrier population.

To summarise, we shall evaluate five steady-state parameters: $U(n_0)$, $S(n_0)$, $\sigma'(\nu_0, n_0)$, $n_r(\nu_0, n_0)$ and $n_s(\nu_0, n_0)$, and five differential parameters, namely $u(n_0)$, $s(n_0)$, $g(\nu_0, n_0)$, $\alpha(\nu_0, n_0)$, $n_g(\nu_0, n_0)$ at the steady-state frequency ν_0 and carrier density n_0 .

In the present paper we concentrate on the theoretical evaluation of bulk semiconductor parameters. To our knowledge, this has not been done before in a unified manner. The evaluation is based on measured values of a number of primary parameters such as the effective mass of electrons in the conduction band and on Kane's $\kappa - p$ method [12] using a strict electron-wavenumber (κ) conservation law. The distribution in energy of the electrons and holes is given by Fermi-Dirac's law and the imaginary part σ'' of the complex conductivity is obtained from the real part σ' through Kramers-Kronig's (or Hilbert's) relations. The high-frequency behaviour of σ' is modelled by Dirac's δ -function, whose position and weight are fitted to measured values of refractive indices below the band-gap. Finally, the spontaneous radiative recombination rate is obtained from the radiation of the Nyquist current sources into an homogeneous space [13]. First-principle derivations are not given, but the essential formulas are listed in Appendix 8 with concise explanations.

For GaAs (0.87 μm), nonradiative recombinations remain small and are neglected. For InAsSb (3.87 μm) the spin-orbit splitting energy Δ is comparable to the band-gap energy E_{g0} , and this causes strong nonradiative (nr) recombinations due to the Auger effect. We have used the expression $S_{nr}(n, T) = C(T)n^3$, where $C(T)$ is crudely estimated. In the Figures, the three materials considered; GaAs, GaInAsP and InAsSb are labelled by 1, 2 and 3, respectively.

Let us now clarify the approximations made. The theory of optical gain is the simplest when there is only one kind of hole with a mass equal to the effective mass of the electron in the conduction band as is the case for lead salts such as PbSe. (The bands are anisotropic in these materials, however, and their properties are not discussed in detail here). In that case, the quasi-Fermi levels are symmetrically positioned with respect to the middle of the band gap. At $T = 0\text{K}$, transparency occurs in principle for arbitrarily small carrier densities and injected currents. The α -factor at maximum-gain is then as low as 1.7 according to our calculations, plasma and band-gap shrinkage effects being neglected here.

At $T = 0\text{K}$, Kane's four-band theory [12] predicts that the minimum value of the conductivity (maximum gain) is $\sigma' = -4 \cdot 10^{-5} n^{1/3}$ in S.I. units when $\Delta \ll E_g$ and $m_h \approx m \gg m_c \approx m_l$, where m is the free-space electron mass, and m_c, m_h, m_l are, respectively, the conduction band, heavy and light-hole masses [14, 7]. This expression is applicable to any direct band-gap III-V compound and is independent of the refractive index. It has been pointed out recently [15] that alternative expressions given in the literature for σ' (or for the gain) are too low by a factor of two, notwithstanding other correction factors discussed below. Note that an upward revision of the expression for the optical gain implies not only reduced threshold currents but also reduced α -factors. Indeed, the enhancement of the α -factor by the plasma effect is reduced when the optical gain is increased.

The light-hole contribution to the gain cannot be neglected even in the limit in which the heavy-hole mass goes to infinity [16]. At low temperatures ($T = 2\text{K}$) the $\sigma'(v)$ curve shown in Fig. 1 (shifted to the right for the sake of comparison with room-temperature curves) distinctly exhibits the light-hole and heavy-hole contributions to the gain. At room temperature, the ratio of light-hole to heavy-hole contributions is almost independent of frequency and is equal to one-half when the approximation $m_h \gg m_c \approx m_l$ holds.

Kane's theory, when restricted to only four bands, is

not sufficiently accurate for wide band-gap materials such as GaAs. The conduction-band electron mass that determines the transition matrix differs somewhat from the measured mass because of higher-lying conduction bands [15, 17]. This forces us to multiply the expression for the

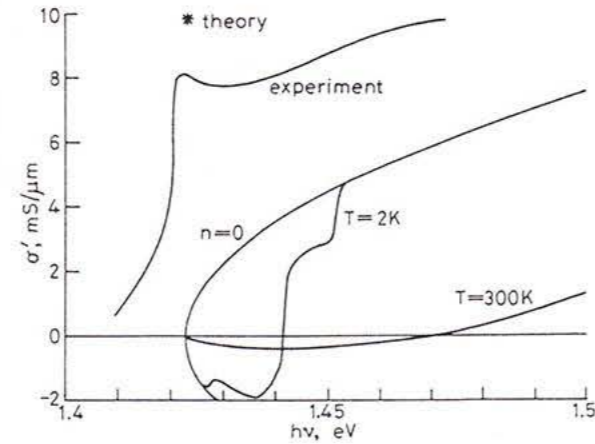


Fig. 1 Variation of the real part σ' of the conductivity as a function of frequency ν .

The upper part of the parabola with horizontal axis follows from Kane's theory for the unpumped material. The curve for $T = 2\text{K}$ is calculated for a carrier density $n = 1.5 \times 10^{17} \text{ cm}^{-3}$, and shifted to the right for the sake of comparison. This curve exhibits light-hole and heavy-hole contributions. The curve labelled $T = 300\text{K}$ includes all the contributions except those originating from excitons and is calculated for $n = 2 \times 10^{18} \text{ cm}^{-3}$. The star is calculated with the excitonic contribution taken into account. The upper curve is experimental for very pure GaAs at 300K.

gain by a factor which is estimated at 1.2 for GaAs [15] but can be omitted for the narrower band-gap materials 2 and 3.

The optical loss of a very pure GaAs sample measured as a function of frequency at room temperature [18, 19] is compared in Fig. 1 with the prediction of Kane's theory discussed above, which corresponds to the parabola with horizontal axis. In pure materials excitonic absorption is significant even when kT (26 meV) is larger than the excitonic binding energy (4.6 meV for heavy-hole excitons in GaAs). The band-gap-edge optical loss is nonzero when excitons are taken into account [18] and is simply related to the parabolic loss-law discussed previously. The theoretical result shown by a star in Fig. 1 at the band edge is in acceptable agreement with the measured value. This gives us confidence that Kane's theory, when properly interpreted, is accurate. For most semiconductor samples, excitons are in fact screened by residual impurities even if the samples are nominally undoped as we assume here, or by injected carriers if n exceeds approximately 10^{16} cm^{-3} . For that reason excitons are not considered further in this paper. When the plasma effect is omitted calculated values of α at a peak gain of 200 cm^{-1} are 2.45 instead of 2.93 for GaAs, 2.7 instead of 3.85 for GaInAsP and 4.0 instead of 8.33 for InAsSb.

Band-gap shrinkage (renormalisation of the band-gap energy) is accounted for. This effect is mainly due to Coulomb interaction and is inversely proportional to the average electron spacing. The $\sigma'(v)$ curve is assumed to shift rigidly frequency-wise by the amount $\delta\nu = -\Delta E_g/h$. We have $\Delta E_g = \beta n^{1/3}$, with β a constant. This third-power law established at $T = 0\text{K}$ is valid at room temperature for the rather high carrier densities that we are considering [20]. The coefficient β is equal to $3.2 \cdot 10^{-8}$, if ΔE_g is expressed in eV and n in cm^{-3} [See eqn. 20]. Band-gap shrinkage explains why most laser diodes oscil-

late below the band-gap frequency. An alternative explanation rests on band-tail states. Band-gap shrinkage reduces the α -values, particularly at frequencies below the peak-gain frequency.

In summary, the calculations presented in this paper take into consideration accurate expressions for the gain, light-hole contributions, plasma effects and band-gap shrinkage. These effects are treated consistently and not simply added. We do not take into account excitons, non κ -conservation, band-tail states, intraband relaxation or spectral hole burning [21, 22]. The conduction-band nonparabolicity is not explicitly taken into account, but we indicate (interrupted lines in the Figures) when the parabolic approximation may be inaccurate. X and L conduction band valleys need not be considered for the materials that we study. Free-carrier and intravalence band (IVB) absorptions are not taken into account. The role of IVB absorption on the refractive index is usually considered negligible [16].

2 Primary semiconductor parameters

Since it is impractical to deduce all semiconductor parameters from the chemical composition, some of them have to be measured. The primary parameters that we shall need are listed in Table 1.

Table 1: (Primary) unpumped semiconductor parameters at $T = 300\text{K}$

Material	1	2	3
E_{g0} (eV)	1.423	0.801	0.319
Δ (eV)	0.341	0.316	0.347
m_c/m	0.0632	0.0450	0.023
m_h/m	0.5	0.438	0.410
m_l/m	0.088	0.0575	0.025
m_c^*/m	0.05	0.0450	0.023
$n_r, 0.9$	3.53	3.51	3.50
$n_r, 0.8$	3.46	3.47	3.48
ϵ_r	12.85		
C (cm^6/s)	negligible	10^{-27}	10^{-27}
Derived masses			
m_h/m , eqn. 17	0.524	0.452	0.414
μ_n/m , eqn. 23	0.0561	0.0408	0.0218
μ_l/m , eqn. 23	0.0368	0.0252	0.012
m_l/m , eqn. 26	0.0541	0.0397	0.0215

1 \equiv GaAs, 2 \equiv $\text{In}_{0.582}\text{Ga}_{0.418}\text{As}_{0.898}\text{P}_{0.102}$, 3 \equiv $\text{InAs}_{0.95}\text{Sb}_{0.05}$. E_{g0} is the band-gap energy, m is the vacuum electron mass and m_c the band-edge (direct Γ -valley) conduction-band electron mass. m_c^* is the effective electron mass in the conduction band that should be used (instead of m_c) in a four-band approximation, h \equiv heavy hole, l \equiv light hole and $n_r, 0.9$ and $n_r, 0.8$ are refractive indices measured at $\nu = 0.9$ and $0.8\nu_{g0}$, respectively, ($h\nu_{g0} \equiv E_{g0}$). ϵ_r is the static relative permittivity and C the estimated Auger coefficient. The data for materials 1, 2, 3 are, respectively, from References 18 and 19, 5, and 27.

The band-gap energies E_{g0} and Δ are most conveniently measured from electroreflection techniques. Effective masses have been determined, for example, from Faraday rotation, and the refractive indices below the band-gap frequency from sample optical reflectivities. The electron and hole mobilities and electronic affinities are not needed here.

3 Definition of secondary parameters

The electrical voltage U applied to the intrinsic diode (that is, not considering the voltage drop in the confinement layers and contacts) is equal to the energy spacing between quasi-Fermi levels in the conduction and valence bands divided by the absolute value e of the electron charge. Bernard and Durrafourg have shown that optical

transparency is achieved at frequency ν if $E_g < h\nu < eU$. We assume that the semiconductor is undoped and neutral: $p = n$. U is a monotonically increasing function of n , see eqn. 19. We define the dimensionless differential parameter

$$u \equiv \frac{n}{U} \frac{dU}{dn} \quad (1)$$

The complex conductivity $\sigma(\nu, n) \equiv \sigma' + i\sigma''$ is the ratio of total current density to impressed electrical field. It depends on the optical frequency ν and carrier density n . The power loss α_p and power gain g_p are related to σ' by

$$\alpha_p \equiv -g_p \approx \sqrt{\left(\frac{\mu}{\epsilon}\right)} \sigma' \quad (2)$$

if the loss or gain are small. Here, $\mu = \mu_0$ is the free-space permeability and $\epsilon = \epsilon_0 n_r^2$, where ϵ_0 denotes the free-space permittivity and n_r the refractive index. For example, a gain value $g_p = 200 \text{ cm}^{-1}$ corresponds to $\sigma' = -190 \text{ S/m}$ if $n_r = 3.6$ (AsGa). An exact form for g_p is given in eqn. 7 below. The expression of σ' follows from Kane's theory and the measurement of primary parameters (see eqn. 21). The dimensionless differential gain g is defined as

$$g \equiv \frac{n}{\sigma'} \frac{\partial \sigma'}{\partial n} \quad (3)$$

g is equal to 0 at $T = 0\text{K}$ but usually exceeds unity and may reach large values at small carrier densities.

The real part σ' of the conductivity σ may be split into a term σ'_e expressing stimulated emission minus a term σ'_a expressing stimulated absorption. The population inversion factor

$$n_s \equiv -\frac{\sigma'_e}{\sigma'} \quad \sigma' \equiv \sigma'_a - \sigma'_e \quad (4)$$

is readily evaluated once the quasi-Fermi levels have been located.

The spontaneous emission rate $S(n)$ is the sum of the radiative spontaneous emission rate $S_r(n)$ that can be evaluated from the radiation of Nyquist sources, and the nonradiative spontaneous emission rate $S_{nr}(n)$. The differential parameter s is defined as

$$s \equiv \frac{n}{S} \frac{dS}{dn} \quad (5)$$

and is a value between 1 and 3.

The imaginary part σ'' of σ is obtained from the real part σ' through a Kramers-Kronig's transformation, for some n -value (see eqn. 26). The refractive index $n_r(\nu, n)$ is then obtained from

$$n_r^2 = \frac{\sqrt{(\sigma'^2 + \sigma''^2) - \sigma''}}{4\pi\nu\epsilon_0} \approx \left| \frac{\sigma''}{2\pi\nu\epsilon_0} \right| \quad (6)$$

The power gain $g_p(\nu, n)$ is given exactly by

$$g_p^2 = 4\pi\nu\mu_0 [\sqrt{(\sigma'^2 + \sigma''^2) + \sigma''}] \quad (7)$$

The group refractive index is defined from the group velocity v_g as

$$n_g \equiv \frac{c}{v_g} = \frac{\partial[\nu n_r(\nu)]}{\partial \nu} \quad (8)$$

Finally, the phase-amplitude coupling factor α defined at some frequency ν by

$$\alpha \equiv -\frac{\partial \sigma''/\partial n}{\partial \sigma'/\partial n} \quad (9)$$

is usually positive and valued between 1 and 10. α is sometimes referred to as the 'antiguating parameter'.

4 Pumped semiconductor parameters

The optical gain is expressed by the real part σ' of the conductivity represented in Fig. 2 as a function of the

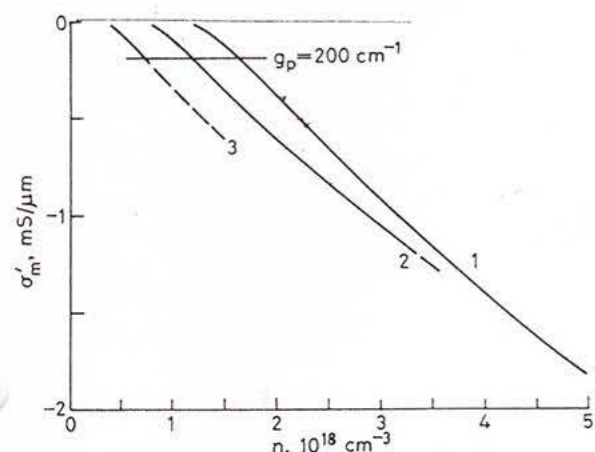


Fig. 2 Variation of the real part σ' of the conductivity at peak gain as a function of carrier density

The labels 1, 2, 3 correspond to the three materials at 0.87, 1.55 and 3.87 μm , respectively. Negative σ' -values correspond to positive gains.

carrier density n . The subscript 'm' indicates that this conductivity is evaluated at the peak-gain frequency. The value corresponding to an optical power gain $g_p = 200 \text{ cm}^{-1}$ is shown by a horizontal line (the three materials considered have almost the same refractive index). The corresponding n -values are 1.65, 1.24, and $0.75 \cdot 10^{18} \text{ cm}^{-3}$ for materials 1, 2, 3, respectively. The curves are interrupted when the parabolic-band approximation is questionable.

Fig. 3a gives the electrical voltage across the intrinsic diode as a function of the carrier density n . The semiconductor transparency occurs when $U - U_g > 0$, where $U_g \equiv E_g/e$. Fig. 3b gives the peak-gain frequency $\nu_m \equiv E_m/h$ as a function of the carrier density n . For the three materials $\nu_m < \nu_{g0}$ in the usual range of n -values, and therefore Fabry-Perot laser diodes would oscillate below the band-gap frequency (about 30 meV below E_{g0} for GaAs).

The refractive index n_r is shown in Fig. 4 as a function of frequency for unpumped GaAs (label '0') and various carrier densities expressed in units of 10^{18} cm^{-3} . These curves show that the refractive index n_{rm} at the peak-gain frequency increases slightly with n (note that the frequency varies) and is of the order of 3.63. The group index n_g at peak-gain frequency is about 4.85.

From a practical stand-point, the most important parameter in laser-diode theory is the spontaneous recombination rate $S(n)$, which determines the threshold current $I_{th} = eV S$, where V denotes the active volume. The radiative part of S is essentially the integral over frequency of the stimulated emission conductivity $\sigma'_s \equiv -n_s \sigma'$, as shown in eqn. 25, and is represented by dotted lines in Fig. 5. The nonradiative part is due essentially to

the Auger effect and is of the form Cn^3 . Estimated values of the C coefficients have been given in Table 1. Because of the high value of C for InAsSb, room-temperature operation of laser diodes using this material would require careful optimisation [28]. Operation at $T = 160\text{K}$, and low threshold currents at 70K have been reported [29].

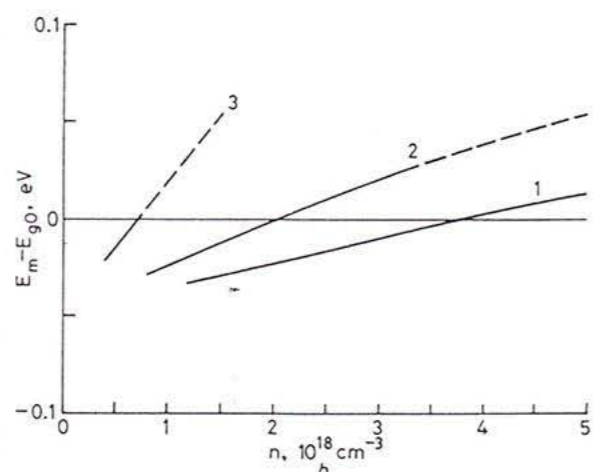
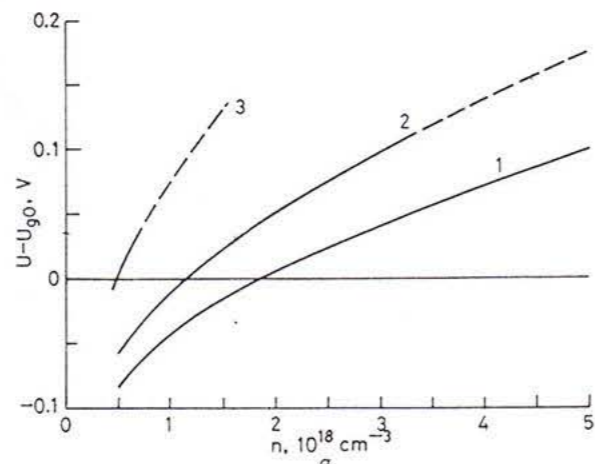


Fig. 3 Variation of the voltage and peak-gain frequency as a function of carrier density for the three materials

a Variation of voltage U across the intrinsic diode (energy spacing between quasi-Fermi's levels divided by e)
b Variation of the peak-gain frequency $\nu_m \equiv E_m/h$

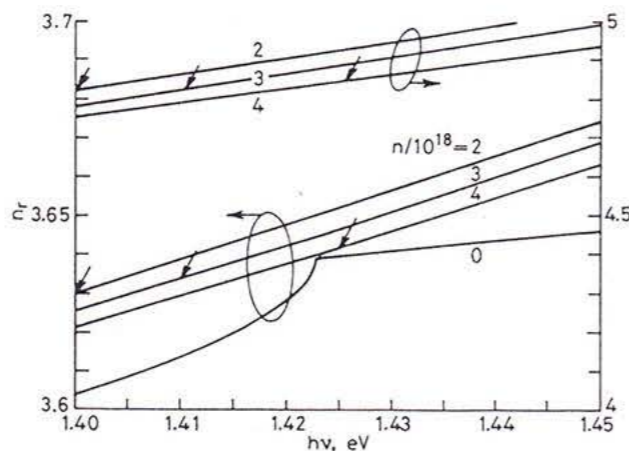


Fig. 4 Variation of the refractive index (left) and group index (right) of GaAs as a function of frequency ν for different carrier densities n expressed in units of 10^{18} cm^{-3} . Arrows correspond to peak-gain frequencies. The label '0' corresponds to the unpumped material

The dimensionless differential gain g_m at peak-gain frequency is shown in Fig. 6 as a function of carrier density.

The reciprocal of the u -factor defined in eqn. 1 is shown in Fig. 7 as a function of the carrier density n . It agrees well with Reference 30.

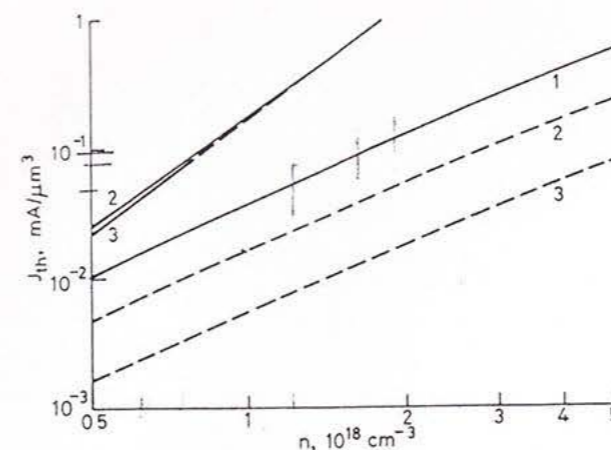


Fig. 5 Variation of the recombination rates S or threshold current densities ($J_{th} \equiv eS$) as a function of carrier density for the three materials. Dotted lines correspond to radiative recombination rates

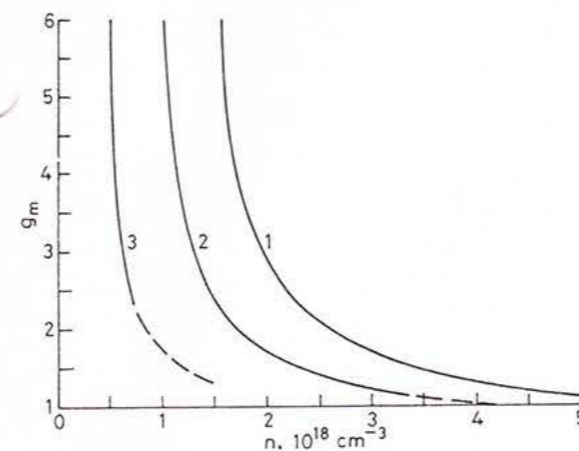


Fig. 6 Variation of the dimensionless differential gain g_m at peak gain as a function of carrier density for the three materials

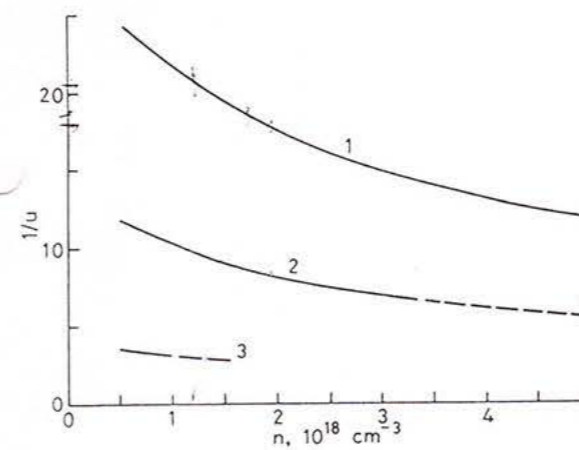


Fig. 7 Variation of the dimensionless differential voltage u as a function of carrier density for the three materials

The differential spontaneous emission parameter s follows from Fig. 5 and is shown in Fig. 8 as a function of the carrier density n .

Self-focusing in the layer plane and phase fluctuations depend mostly on the phase-amplitude α -factor defined in eqn. 9. This factor is shown in Fig. 9 for GaAs as a function of the carrier density by plain lines, at the peak-gain

frequency $\nu_m(\alpha_m)$, at 90% of peak gain and $\nu > \nu_m(\alpha_+)$, and at 90% of peak gain and $\nu < \nu_m(\alpha_-)$. The latter two results are of interest for distributed Bragg reflector

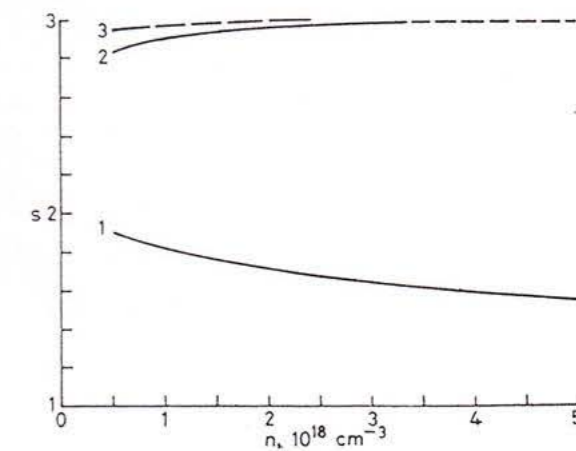


Fig. 8 Variation of the dimensionless differential recombination rate s as a function of carrier density for the three materials

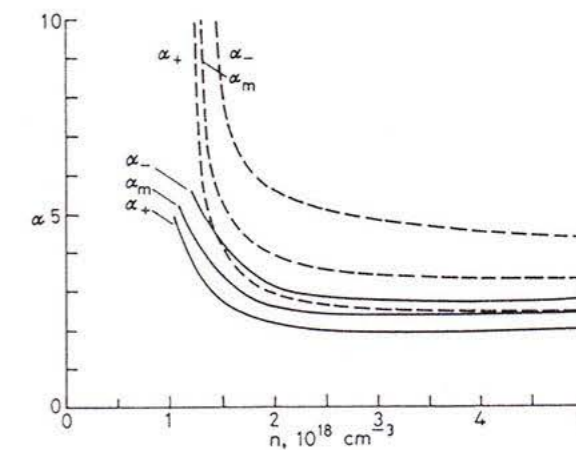


Fig. 9 Variation as a function of carrier density of the α -factor for GaAs at peak gain (α_m), at 90% of peak gain and $\nu < \nu_m(\alpha_-)$, and at 90% of peak gain and $\nu > \nu_m(\alpha_+)$ (plain lines)

Dotted curves are similar except that band-gap shrinkage is not accounted for

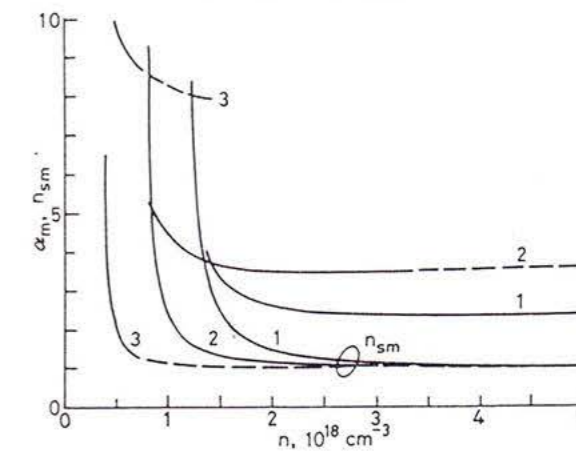


Fig. 10 Variation as a function of carrier density of the α -factors at peak-gain for the three materials

The lower curves give the population inversion factor n_{sm} at peak gain

(DBR) lasers since this type of laser may not oscillate at the peak-gain frequency. It is advantageous to operate at $\nu > \nu_m$ if one wishes to reduce the laser linewidth, as is well known. The carrier density should be moderately large if α is to be minimised. The dotted lines in Fig. 9 give the result of the calculation made without taking band-gap shrinkage into account. Band-gap shrinkage

The voltage $U(n)$ across the intrinsic diode is given by

$$U = \frac{kT}{e} [x_F + x_g(n)] \quad x_g(n) = \frac{E_{g0} - \beta n^{1/3}}{kT} \quad (19)$$

$$\beta = 0.73 \left(\frac{3}{\pi}\right)^{1/3} \frac{e^2}{2\pi\epsilon} \quad \epsilon = \epsilon_0 \epsilon_r \quad (20)$$

ϵ_r is the static relative permittivity given in Table 1, and ϵ_0 is the free-space permittivity. The coefficient β expresses the band-gap renormalisation due to Coulomb effects, the exchange integral being neglected. The factor 0.73 in front of eqn. 20 follows from Reference 32. Thus $\beta \approx 3.2 \cdot 10^{-8}$ if the energy is expressed in eV and n in cm^{-3} .

The real part $\sigma'(v, n)$ of the conductivity is given from Kane's theory by

$$\sigma' = -\frac{2\pi e^2}{3 h^2} \frac{1 + \Delta/E_{g0}}{1 + \frac{2}{3} \Delta/E_{g0}} \sqrt{(2m_c kT) \left(\frac{m_c}{m_c^*} - \frac{m_c}{m}\right)} \\ \times \left[\left(\frac{\mu_h}{m_c}\right)^{3/2} (f_{ch} - f_{vh}) + \left(\frac{\mu_l}{m_c}\right)^{3/2} (f_{cl} - f_{vl}) \right] \\ \times \sqrt{(x)(1 + x/x_g)^{-1}} \quad (21)$$

for $v > 0$ and $\sigma'(-v) = \sigma'(v)$. The quantities introduced in eqn. 21 are defined below. This parabolic law holds only for x -values not exceeding a few units. We have defined f_{ch} and f_{vh}

$$f_{ch}^{-1} \equiv 1 + \exp\left(-\eta_c + \frac{\mu_h}{m_c} x\right) \\ f_{vh}^{-1} \equiv 1 + \exp\left(\eta_v - \frac{\mu_h}{m_h} x\right) \quad (22)$$

where

$$\frac{1}{\mu_h} = \frac{1}{m_c} + \frac{1}{m_h} \quad \frac{1}{\mu_l} = \frac{1}{m_c} + \frac{1}{m_l} \quad (23a)$$

Two other functions f_{cl} , f_{vl} are similarly defined with 'h' changed to 'l'. For unpumped materials, $f_{ch} = f_{cl} = 0$, $f_{vh} = f_{vl} = 1$, and $\sigma' \approx B\sqrt{(x)}$, with B a constant. The first term in parenthesis in eqn. 21, which corrects for the fact that m_c is not quite negligible compared with m and for upper-lying conduction bands, is equal to 1.2 for GaAs. The last term in eqn. 21 can be neglected when the gain is evaluated, but it is important in the Kramers-Kronig transformation, eqn. 26, since the integration extends in principle to infinity. We have also defined

$$x \equiv \frac{h\nu - E_g}{kT} \quad x_g \equiv \frac{E_g}{kT} \quad (23b)$$

where E_g is the reduced band-gap energy in eqn. 19.

After lengthy but straightforward calculations, one finds that the population inversion factor $n_s(v, n)$ defined in eqn. 4 from the above expression of σ' is given exactly by the simple expression

$$n_s = \frac{1}{1 - \exp(x - x_F)} \quad (24)$$

The radiative spontaneous emission rate per unit volume $S_r(n)$ into a homogeneous medium of refractive index equal to n_r can be evaluated from the classical radiation of the Nyquist-current noise sources provided both the active material and absorbers at spatial infinity are considered [13]. The expression is

$$S_r = 8\pi\mu_0 n_r \int_0^\infty -n_s(v)\sigma'(v)v^2 dv \quad (25)$$

Alternatively, Einstein's relation between stimulated and spontaneous emission coefficients can be used.

Once the real part $\sigma'(v, n)$ of the conductivity has been obtained, the imaginary part σ'' follows from Kramers-Kronig's (KK) relation, at some value of n and $v > 0$

$$\sigma''(v, n) = -2\pi v \epsilon_0 + \frac{e^2}{2\pi v} \left[\frac{n}{m_c} + \frac{p_h}{m_h} + \frac{p_l}{m_l} \right] \\ - \frac{1}{\pi} \wp \int_{-\infty}^{+\infty} \frac{\sigma'(z, n)}{z - v} dz \\ p_h/p_l = (m_h/m_l)^{3/2} \quad p_h + p_l = p = n \quad (26)$$

The term in brackets in eqn. 26 can be written simply as n/m_r if we define a reduced mass m_r ,

$$m_r^{-1} \equiv m_c^{-1} + (m_h^{1/2} + m_l^{1/2})/(m_h^{3/2} + m_l^{3/2}) \quad (27)$$

The first term in the expression of σ'' is the vacuum contribution and the second term is the plasma effect, whose corresponding loss is not included in σ' . \wp denotes a 'principal value', that is, the interval $z = v - \epsilon$ to $z = v + \epsilon$ is omitted in the integration. The numerical accuracy was checked against analytically known solutions, such as eqn. 28 below. A value $h\epsilon/kT = 0.02$ is found to be appropriate. When the expression for $\sigma'(v)$ in eqn. 21 is introduced in eqn. 26 we find that the integral converge at large z -values because of the last term in this expression. In the absence of pumping, the analytical result, first obtained by Cardona [33] from an integration in the complex plane, can alternatively be obtained by integration along the real z -axis if an appropriate limiting procedure is used. We have

$$\wp \int_0^\infty \frac{\sqrt{(u)} du}{(u+1)(u-\alpha)} = \begin{cases} \pi/(1+\alpha) & \alpha > 0 \\ \pi/(1+\sqrt{(-\alpha)}) & \alpha < 0 \end{cases} \quad (28)$$

The expression in eqn. 21 for $\sigma'(v)$ describes the optical conductivity near the band-gap frequency only. Thus, in the KK's transformation this expression must be supplemented by a Dirac's δ -function of such position and weight that measured values of the refractive index of the unpumped material at two frequencies below ν_g are fitted ($n_{r,0.9}$ and $n_{r,0.8}$ values in Table 1). This procedure has been performed analytically using eqn. 28.

To introduce easily the band-gap shrinkage effect, the integral in eqn. 26 is split into a positive- z part and a negative- z part of lesser importance. These two functions are calculated in matrix form with discretised x and n values, to calculate their partial derivatives. The δ -function fitting procedure can be improved by requiring that the sum-rule be obeyed; the integral of $\sigma'(v)$ from minus to plus infinity must be proportional to the total number of electrons in the semiconductor. Since this number remains unchanged when electrons are promoted from the valence band to the conduction band, the following sum-rule must be obeyed at any temperature

$$-\frac{4m}{e^2 n} \int_0^\infty [\sigma'(v, n) - \sigma'(v, 0)] dv \\ = \frac{m}{m_c} + \frac{m}{m_h} \frac{p_h}{n} + \frac{m}{m_l} \frac{p_l}{n} \quad (29)$$

The numerical value of the right-hand side of this expression is 18.5 for GaAs. The left-hand side, evaluated on the basis of Kane's four-band approximation, is found to be equal to 20.1, indicating a fair agreement.