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Title: CALCULATION OF AXIAL MODE SEPARATION OF A SEMICONDUCTOR LASER FROM REFLECTANCE SPECTRUM

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It is reported that the axial mode separation of a semiconductor laser can be computed from the reflectance spectrum of a narrow spectral range near the lasing frequency. The Kramers-Kronig dispersion relation is used in this computation.

GaAs semiconductor laser is taken as an example. The computed values of the normalized frequency separation for GaAs at lasing photon energy of 1.38 eV range from 0.107 to 0.111 for various widths of the reflectance spectrum. These results are in good agreement with the measured ones.

Calculation of Axial Mode Separation of a Semiconductor Laser From Reflectance Spectrum

by

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I. INTRODUCTION

A simple laser cavity consists of two parallel and highly reflecting mirrors, in which there exists a great number of transverse electromagnetic (TEM_{mnq}) modes. However for a practical laser, higher order modes are suppressed. As a result, only one or a few fundamental normal modes are sustained.

The allowed modes in a laser that actually oscillate will depend on the gain characteristics of the laser medium, which will depend on the spectral linewidth, i. e., the spontaneous emission linewidth of the laser transition. Any mode falling outside of the linewidth will not oscillate because of an insufficient gain.

Since the mode separation is small relative to the linewidth, many modes will in fact oscillate. For selecting a single-mode operation sometimes mode selectors (19) will be required in the cavity. Recently Popov and Shuikin (15) used a compound resonator to obtain single-mode emission from a semiconductor.

To design a laser with single mode operation such as the work cited above requires the knowledge of the mode separation. Furthermore it is useful to know the mode separation in determining the gain of a desired mode (8).. It follows that the prediction of the mode

separation of a semiconductor laser is very desirable.

In a semiconductor laser, modes are determined by the length and the refractive index n of the medium. It is known that the refractive index of a semiconducting material is very frequency-sensitive. For predicting mode separation the value of n versus frequency is usually obtained experimentally. For instance, the mode separation of a GaAs junction laser was measured by Burns, Dill, and Nathan (3). Later Marple (9) measured the refractive index n versus wavelength λ and computed the mode separation for GaAs laser.

As a matter of fact, those direct measurements of n and mode separation are not easy. Robinson (16) suggested that the calculation of the optical constants such as the refractive index n, and the extinction coefficient k of a material can be made from its reflectance spectrum by using the Kramers-Kronig dispersion relation. The application of this relation required the knowledge of a whole spectral range. Later Roessler (17) suggested a modified approach, which required only a limited range of spectrum.

Since the reflectance spectrum of a semiconductor is easy to obtain experimentally and readily available, attempt has been made to calculate its axial mode separation from the reflectance data. Furthermore, justification of using a narrow reflectance spectrum to obtain the mode separation with reasonable accuracy has also been

made. To the author's knowledge, such an attempt has not been explored.

Due to the frequency-sensitivity of the refractive index n in a dispersive medium, the calculation of the mode separation requires the knowledge of $dn/d\nu$, i.e., the slope of n versus frequency. The purpose of this work is to show how the quantity $dn/d\nu$ and hence the mode separation of a semiconductor laser are obtained from a narrow spectral reflectance range around the lasing frequency. Also in this work the change of the calculated results for mode separation as a function of spectral width was also examined. The GaAs junction laser was taken as an example. The value of the mode separation obtained in such a computation was compared to that calculated from the conventional method, i.e., the method using a whole spectral range, and to the measured data as well. As a result, the calculated values of the axial mode separation for GaAs laser were in good agreement with the measured ones.

II. REFLECTANCE AND OPTICAL CONSTANTS

Relations Among Optical Constants

When radiation is incident upon the surface of a material, one part is reflected, another is absorbed, and the remainder is transmitted through the material. Approximately the expressions for the reflectance R, transmittance T, and absorptance A at normal incidence are given by (23)

$$R = r^2\left[\frac{1+(1-2r^2)\exp(-2\alpha d)}{1-r^4\exp(-2\alpha d)}\right] \tag{2.1}$$

$$T = \frac{(1-r^2)\exp(-\alpha d)}{1-r^4\exp(-2\alpha d)} \tag{2.2}$$

$$A = \frac{(1-r^2)[1-\exp(-\alpha d)]}{1-r^2\exp(-\alpha d)} \tag{2.3}$$

where $r = \frac{N-1}{N+1}$ is the Fresnel reflection coefficient at normal incidence with $N = n-ik$, the complex refractive index of the crystal, $\alpha = 4\pi k/\lambda$ the absorption coefficient at normal incidence, and d the sample thickness. It is easily seen that $A + R + T = 1$.

Expressions (2.1) and (2.2) have been widely used for determining the optical properties of solids in many experiments.

Actually, the expression for reflectance was used in the case of $\alpha d \gg 1$. For this reason, only the information of the front-surface

reflectance was needed. Thus Equation (2.1) becomes

$$R = r^2 .$$

The expression for r can be written as

$$r = \frac{n-ik-1}{n-ik+1} = |r|e^{i\theta} \tag{2.4}$$

Then the magnitude of the measured reflectance is

$$R = |r|^2 = \frac{(n-1)^2+k^2}{(n+1)^2+k^2} \tag{2.5}$$

and the phase is

$$\theta = \tan^{-1} \frac{-2k}{n^2+k^2-1} \tag{2.6}$$

Solving for n and k in Equation (2.4), one obtains

$$n = \frac{1-R}{1+R-2\sqrt{R}\cos\theta} \tag{2.7}$$

and

$$k = \frac{-2\sqrt{R}\sin\theta}{1+R-2\sqrt{R}\cos\theta} \tag{2.8}$$

The expressions (2.7) and (2.8) show that the quantities n and k are functions of the magnitude R and phase θ of reflectance. The variables R and θ are related to each other as will be seen in the next chapter. The study of the behavior of R for a semiconductor, particularly for GaAs, is as follows.

Reflectance of GaAs

As stated in the previous chapter, GaAs laser was taken as an example. The reflectance of GaAs at room temperature is shown in Figures 1A, 1B, and 1C. The data tabulated in Appendix I were gathered from the references as quoted in (4, 12, 14, 23).

Three spectral regions are distinguished (13). The first region (Figure 1B) covering up to about 8 or 10 eV is characterized by the sharp structures associated with the band-to-band transitions. The second region (Figure 1C) extending to about 20 eV shows a rapid decrease in the reflectance which is reminiscent of the behavior of certain metals in the ultraviolet region. This is because the valence electrons become unbound and able to perform collective oscillations.

In the third region (Figure 1C) the reflectance again rises indicating the onset of additional optical absorption. This situation can be thought of as the presence of the transitions between filled d bands, lying below the valence band, and empty conduction band states. It should be noted that in Figure 1A the sharp structure covering from 0.03 eV to 0.05 eV is due to the transition in reststrahlen band.

These curves are used as measured data for the mode separation computation.

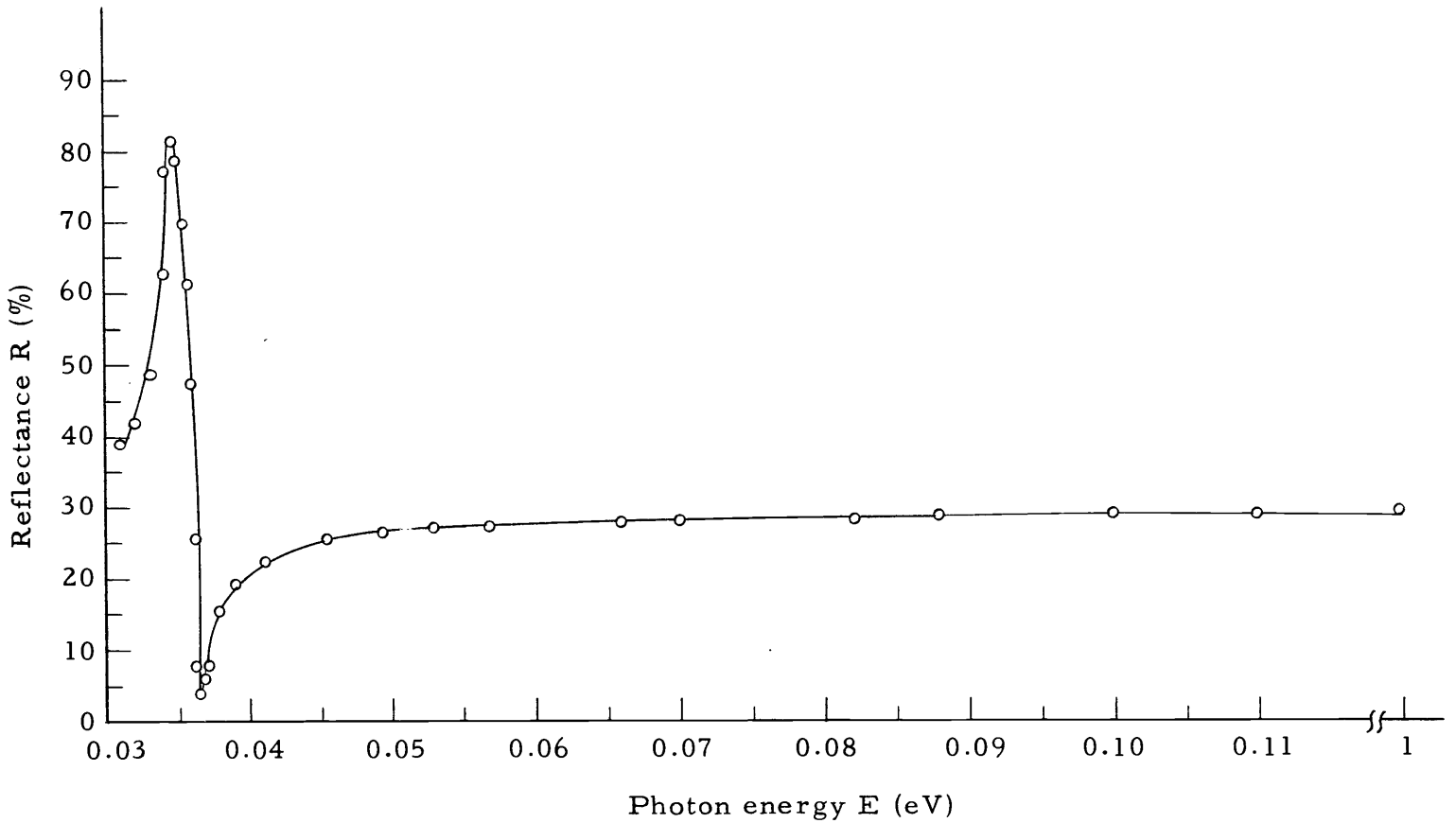

Figure 1A. Reflectance data versus photon energy of GaAs at room temperature.

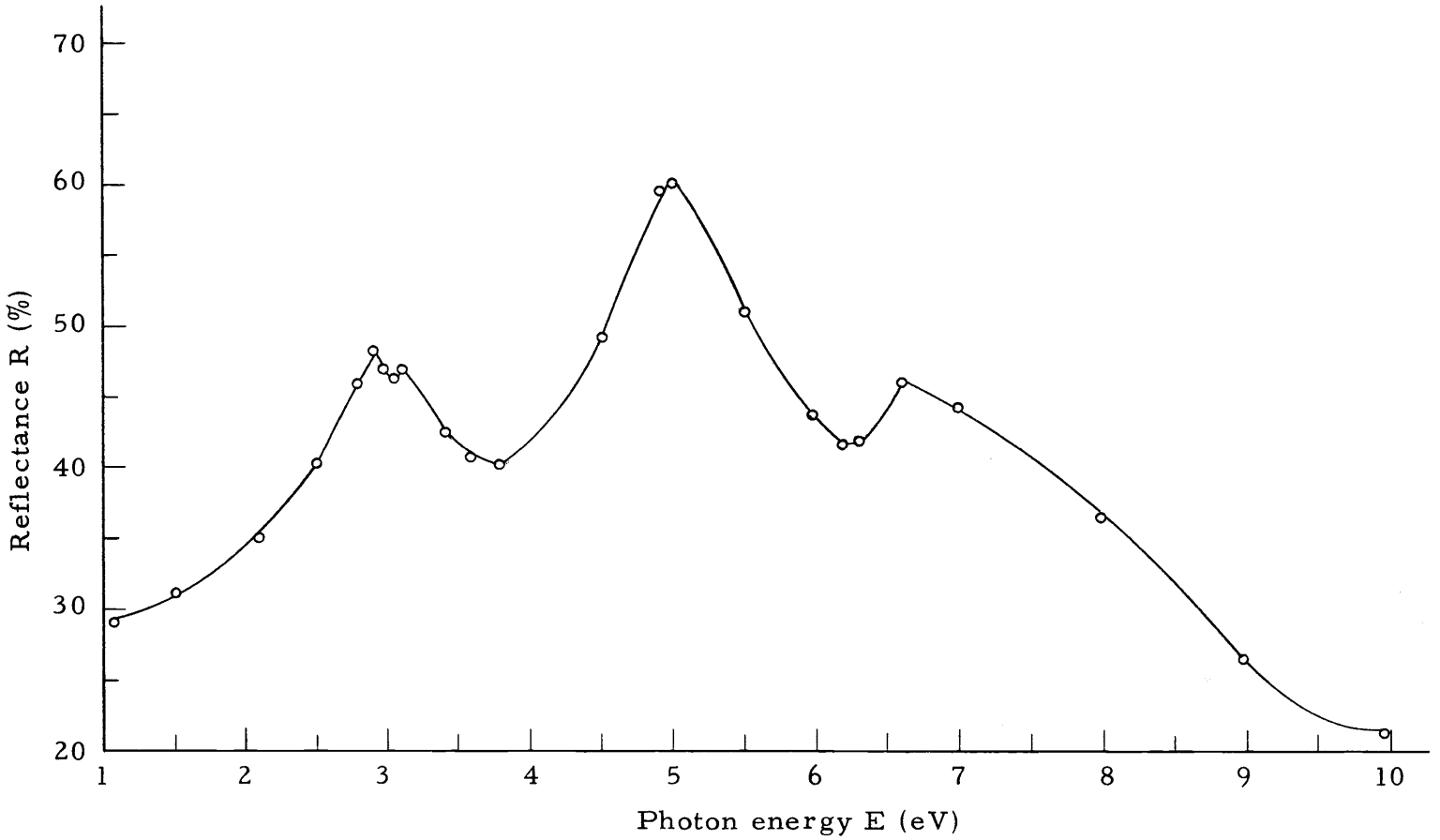

Figure 1B. Reflectance data of GaAs (continued).

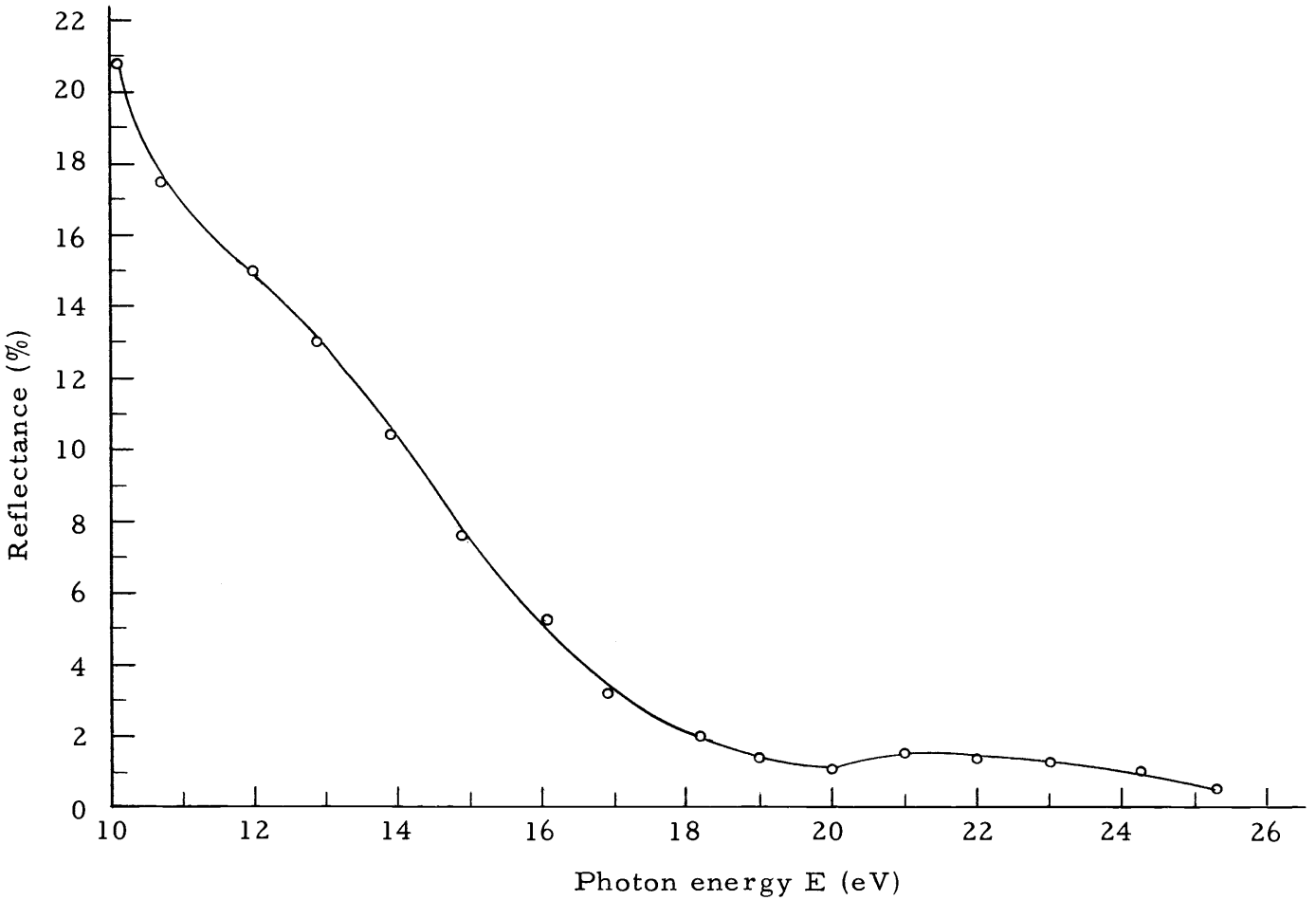

Figure 1C. Reflectance data of GaAs (continued).

III. KRAMERS-KRONIG ANALYSIS

Kramers-Kronig Dispersion Relation

In general the dispersion relation is the relation between the real and imaginary parts of a complex quantity (2). Consequently, the relation between the magnitude and phase of the reflectance is called the dispersion relation or Kramers-Kronig dispersion relation. The application of this relation to reflectance data of normal incidence permits the determination of the refractive index n, the extinction coefficient k, and other optical quantities.

Taking the logarithm of both members of Equation (2.4) gives

$$\ln r = \ln|r| + i\theta$$

or

$$\ln r = 1/2 \ln R + i\theta$$

where the relation between R and θ can be written in terms of frequency as (11, 21)

$$\theta(\nu_o) = \frac{\nu_o}{\pi} P \int_0^\infty \frac{\ln R(\nu)}{\nu^2 - \nu_o^2} d\nu \tag{3.1}$$

or in terms of photon energy E as

$$\theta(E_o) = \frac{E_o}{\pi} P \int_0^\infty \frac{\ln R(E)}{E^2 - E_o^2} dE \tag{3.2}$$

where P stands for the Cauchy principal value of the integral. Equations (3.1) or (3.2) is called Kramers-Kronig dispersion relation.

Accordingly with the knowledge of the reflectance spectrum, the phase angle θ can be calculated with a computer. The integral in Equation (3.2) can be represented by a usual one as

$$\theta(E_o) = \frac{E_o}{\pi} P \int_0^\infty \frac{\ln R(E)}{E^2 - E_o^2} dE$$

$$= \frac{E_o}{\pi} P \int_0^\infty \frac{\ln R(E) - \ln R(E_o)}{E^2 - E_o^2} dE$$

$$= \frac{E_o}{\pi} \int_0^\infty \frac{\ln R(E) - \ln R(E_o)}{E^2 - E_o^2} dE \qquad (3.3)$$

because

$$P \int_0^\infty \frac{dE}{E^2 - E_o^2} = 0 \qquad (3.4)$$

The proof of Equation (3.4) is shown in Appendix II.

The integrand in Equation (3.3) is finite for $E = E_o$ provided the reflectance spectrum does not have an infinite slope at E_o. Such infinite slopes are never encountered experimentally.

It is clear that from Equations (3.3) and (3.4) one can see that a constant reflectance gives $\theta = 0$.

Calculation of the Phase Angle Using an Entire Spectral Range

For the evaluation of the phase angle θ, in principle, the reflectance data should cover the entire spectral region from zero to infinity. Since the spectral region of the reflectance measurements is always bounded, it is necessary to extrapolate the measured reflectance curve $R(E)$ to infinite energy in order to compute the integral in Equation (3.3) and hence the refractive index n in Equation (2.7).

The most reasonable extrapolation procedure assumes that above the valence electron plasma frequency ω_p the following expressions are usually used.

$$n^2 - k^2 = 1 - \frac{\omega_p^2}{\omega^2}$$

and

$$2nk = \frac{\omega_p^2 \tau}{\omega^2 \tau^2} \approx 0 .$$

These expressions (11) are valid only for $\omega^2 \tau^2 >> 1$ and $\omega > \omega_p$, where τ is the relaxation time of free carriers in the conduction band of a semiconductor.

Thus at high frequencies

$$n \approx 1 - \frac{1}{2}\frac{\omega_p^2}{\omega^2}$$

and

$$R = \frac{(n-1)^2}{(n+1)^2} \approx \frac{1}{16}\frac{\omega_p^4}{\omega^4} \tag{3.5}$$

Therefore if the upper frequency limit of the measurement ω_1 is larger than ω_p, it is logical to extrapolate $R(\omega)$ beyond ω_1 by

$$R = R_1\left(\frac{\omega_1}{\omega}\right)^4$$

or

$$R = (R_1\omega_1^4)\omega^{-4} \tag{3.6}$$

where R_1 is the measured reflectance at ω_1.

On the other hand, for low frequencies the reflectance is approximately constant and hence there is no contribution to θ as mentioned in the previous section. Thus no extrapolation for R to zero frequency is needed.

Calculation of the Phase Angle Using a Limited Spectral Range

In the case of a limited spectrum, the method described above should be modified to calculate the phase angle θ. The modified approach was treated by Roessler (17) as mentioned in the introduction.

In fact, the integral in Equation (3.3) can be broken into three parts as

$$\theta(E_o) = \theta_{0a}(E_o) + \theta_{ab}(E_o) + \theta_{b\infty}(E_o) \tag{3.7}$$

where

$$\theta_{0a}(E_o) = \frac{1}{2\pi}\int_0^a f(R, E_o)dE \tag{3.8}$$

$$\theta_{ab}(E_o) = \frac{E_o}{\pi}\int_a^b \frac{\ln R(E) - \ln R(E_o)}{E^2 - E_o^2}\, dE \tag{3.9}$$

and

$$\theta_{b\infty}(E_o) = \frac{1}{2\pi}\int_b^\infty f(R, E_o)dE \tag{3.10}$$

where

$$f(R, E_o) = \ln\frac{R(E)}{R(E_o)}\ \frac{d}{dE}\left(\ln\left|\frac{E+E_o}{E-E_o}\right|\right)$$

Here $\theta_{ab}(E_o)$ is the contribution from the region of the experimental data, $\theta_{0a}(E_o)$ and $\theta_{b\infty}(E_o)$ are not known because of the lack of data. But the integrals θ_{0a} and $\theta_{b\infty}$ can be found as follows.

According to Equation (3.8), in the interval $(0, a)$, E is everywhere less than E_o since E_o lies in (a, b). Hence the continuous function $\frac{d}{dE}\ln\left|\frac{E+E_o}{E-E_o}\right|$ is monotonic with E.

Thus applying the generalized mean value theorem for integrals to the integral in Equation (3.8) gives

$$\theta_{0a}(E_o) = \frac{\ln[R(\zeta)/R(E_o)]}{2\pi} \int_0^a \frac{d}{dE} \ln\left|\frac{E+E_o}{E-E_o}\right| dE$$

$$= [A - \frac{\ln R(E_o)}{2\pi}] \ln\left|\frac{a+E_o}{a-E_o}\right| \qquad (3.11)$$

where $A = \ln R(\zeta)/2\pi$ and varies only slowly with E_o, ζ being some value of E in the interval $(0, a)$.

Similarly, the integral in Equation (3.10) can be written as

$$\theta_{b\infty}(E_o) = \frac{\ln[R(\eta)/R(E_o)]}{2\pi} \int_b^\infty \frac{d}{dE} \ln\left|\frac{E+E_o}{E-E_o}\right| dE$$

$$= [B - \frac{\ln R(E_o)}{2\pi}] \ln\left|\frac{b+E_o}{b-E_o}\right| \qquad (3.12)$$

where $B = \ln R(\eta)/2\pi$, η belonging to the interval (b, ∞).

Thus Equation (3.7) has the form

$$\theta(E_o) = [A - \frac{\ln R(E_o)}{2\pi}] \ln\left|\frac{a+E_o}{a-E_o}\right| + \theta_{ab}(E_o)$$

$$+ [B - \frac{\ln R(E_o)}{2\pi}] \ln\left|\frac{b+E_o}{b-E_o}\right| \qquad (3.13)$$

where the unknown quantities A and B may be determined by the fact that the phase angle $\theta(E_o)$ is zero at energies below the onset of absorption. As a matter of fact theoretically the phase angle θ

should be zero in regions of no absorption, i.e., for energies less than the energy gap or $E = h\nu < E_g$.

Therefore it is easy to choose two frequencies ν_1 and ν_2 such that $h\nu_{1,2} < E_g$ within the range (a, b) to obtain two zero θ's.

Consequently, the quantities A and B in Equation (3.13) can be solved for the following simultaneous equations

$$[A - \frac{\ln R(E_1)}{2\pi}] \ln\left|\frac{a+E_1}{a-E_1}\right| + \theta_{ab}(E_1) + [B - \frac{\ln R(E_1)}{2\pi}] \ln\left|\frac{b+E_1}{b-E_1}\right| = 0 \tag{3.14}$$

$$[A - \frac{\ln R(E_2)}{2\pi}] \ln\left|\frac{a+E_2}{a-E_2}\right| + \theta_{ab}(E_2) + [B - \frac{\ln R(E_2)}{2\pi}] \ln\left|\frac{b+E_2}{b-E_2}\right| = 0 \tag{3.15}$$

where $E_1 = h\nu_1$ and $E_2 = h\nu_2$.

Thus the computation of $\theta(E_o)$ is essentially as follows: $R(E)$ is determined experimentally in (a, b) and, using (3.14) and (3.15), the constants A and B are found by computing $\theta_{ab}(E_1)$ and $\theta_{ab}(E_2)$. Then $\theta(E_o)$ is calculated from Equation (3.13).

IV. CAVITY AND MODES IN A SEMICONDUCTOR LASER

Cavity and Resonant Modes

A semiconductor laser is usually fabricated with two parallel cleaved surfaces and the other two sawed or roughened. The cavity in a semiconductor laser so obtained is essentially a Fabry-Perot structure. As commonly known, a Fabry-Perot interferometer consists of two optically flat, partially reflecting plates of glass or quartz with their reflecting surfaces held accurately parallel.

Radiation propagating perpendicularly to these reflecting surfaces forms standing waves in the cavity. Standing waves occur whenever the cavity contains an integral number of half-wavelength. For a cavity length L, this resonance condition is

$$m\frac{\lambda}{2} = L \tag{4.1}$$

where m is the axial mode number, λ wavelength in air.

Expression (4.1) above is valid for a passive cavity. In a semiconductor laser of refractive index n, the radiation propagates with wavelength λ/n. Thus, the resonance condition given by Equation (4.1) becomes

$$m\frac{\lambda}{2n} = L$$

or

$$m\lambda = 2nL \tag{4.2}$$

In an actual laser not all the frequencies satisfying Equation (4. 2) are permitted to oscillate because of losses due to diffraction, reflection, and absorption. The medium between the mirrors has a net gain that will compensate for these losses. Lower order modes will usually have greater gain than the higher order ones. As a consequence only a few fundamental modes will exist. Furthermore, it is possible to design a laser of single mode operation, i. e., highly monochromatic light output (15, 19). Such a design requires the knowledge of the mode separation.

Axial Mode Separation of a Semiconductor Laser

The refractive index n of a semiconductor is very frequency-sensitive, i. e., a function of wavelength. Thus differentiating Equation (4. 2) with respect to λ gives

$$\lambda \frac{dm}{d\lambda} + m = 2L \frac{dn}{d\lambda} \tag{4. 3}$$

For the separation of two adjacent modes and for large m, substituting

$$d\lambda \sim \Delta\lambda$$

$$dm = -1$$

$$m = 2nL/\lambda$$

into Equation (4. 3), one obtains

$$1 - \frac{\lambda}{n}\frac{dn}{d\lambda} = \frac{1}{2nL}\frac{\lambda^2}{\Delta\lambda}$$

or

$$\Delta\lambda = \frac{\lambda^2}{2L(n-\lambda\frac{dn}{d\lambda})}$$

or in terms of frequency as

$$\Delta\nu = \frac{c}{2L(n+\nu\frac{dn}{d\nu})} \tag{4.4}$$

(by noting that $\lambda = c/\nu$, $\Delta\lambda = -c\Delta\nu/\nu^2$, $d\nu/d\lambda = -c/\lambda^2$, and $dn/d\lambda = (dn/d\nu)(d\nu/d\lambda)$), where c is the velocity of light.

Equation (4.4) can be written as

$$\frac{L\Delta\nu}{c} = \frac{1}{2(n+\nu\frac{dn}{d\nu})} \tag{4.5}$$

or

$$\frac{L\Delta\nu}{c} = \frac{1}{2(n+E\frac{dn}{dE})} \tag{4.6}$$

where E is the photon energy. The quantity $L\Delta\nu/c$ can be called the normalized frequency separation of a semiconductor laser.

V. PROCEDURE OF CALCULATING AXIAL MODE SEPARATION

As mentioned in Chapter I, the GaAs semiconductor laser was taken as an example. The reflectance data of GaAs used here were referred to Chapter II. The Kramers-Kronig dispersion relation was applied to calculate the phase angle θ and hence the refractive index n and the quantity dn/dE in Equation (4.6). In other words the normalized frequency separation $L\Delta\nu/c$ of a semiconductor laser was predicted by using the reflectance data through the dispersion relation.

To achieve the calculation of the quantity $L\Delta\nu/c$, the conventional method using Equation (3.3) was first used, then followed by the narrow spectrum method, which was derived in Equation (3.13).

Computation of $L\Delta\nu/c$ Versus Photon Energy Using Conventional Method

As shown in Equation (3.3), this method of calculation requires the whole spectral range from zero to infinity to compute the phase angle θ. Practically to calculate the integral in Equation (3.3) with a computer, the upper integration limit of this integral should be finite. In the present work, 50 eV was chosen as this upper limit.

Since the reflectance data of GaAs was not available beyond 25 eV, an extrapolation for $R(E)$ to 50 eV should be needed. Yet the upper energy limit of 25 eV is larger than the plasma energy

($h\omega_p \sim 16$ eV) for GaAs (4, 13). Thus the behavior of $R(E)$ beyond 25 eV has the form of Equation (3.6):

$$R = R_1 \omega_1^4 \omega^{-4}$$

or in terms of energy as

$$R = R_1 E_1^4 E^{-4} \tag{5.1}$$

where $E_1 = 25$ eV and $R_1 = 0.006$.

On the other hand, the lower integration limit was chosen as 0.03 eV instead of 0 eV. This is because below 0.03 eV the reflectance is constant and hence there is no contribution to θ as stated in Chapter III.

The Simpson's numerical method (10) was used to handle the integral $\theta(E_o)$ in Equation (3.3) with the aid of a computer. Since this numerical method requires equal intervals, an interpolation of the reflectance data was needed to obtain a set of equally spaced data points.

The spectrum was divided into 0.001 eV intervals within the reststrahlen region, i.e., from 0.03 eV to 0.05 eV due to the sharp variation of reflectance. The rest of the spectrum extending up to 50 eV was divided into 0.015 eV intervals. Then the Lagrangian formula (10) was used to interpolate the reflectance data points. Since the integrand in Equation (3.3) becomes indeterminate when

$E = E_o$, it has another form as described in Appendix III.

Then the refractive index n given by Equation (2.7) was computed. The quantity dn/dE was hence obtained numerically as

$$\frac{dn_j}{dE} \approx \frac{n_{j+1} - n_{j-1}}{2\Delta E} \tag{5.2}$$

where ΔE is the equal energy interval of the spectrum.

Finally the normalized frequency separation $L\Delta\nu/c$ versus photon energy as expressed in Equation (4.6) was found. All these computations were included in a Fortran program named MODSEP1 (see Appendices IV and V).

Computation of $L\Delta\nu/c$ Versus Photon Energy Using Narrow Spectrum Method

The narrow spectrum method was described in detail in the third part of Chapter III. The lower limit a and upper limit b of the integral θ_{ab} in Equation (3.9) were chosen near the lasing energy $E = 1.38$eV. Consequently in this computation b was used as a parameter and a fixed at 0.1 eV. In this case b was chosen as 2 eV and 3 eV.

The reflectance data points were interpolated to obtain equally spaced points with equal interval of 0.015 eV by using 3-point Lagrangian interpolation as stated before.

The integral θ_{ab} in Equation (3.9) was then calculated using

Simpson's rule as mentioned in the previous section. To compute the integral $\theta(E_o)$ in Equation (3.13), the unknown quantities A and B were determined first from the Equations (3.14) and (3.15). The quantities E_1 and E_2 in these two equations were chosen to be 0.3 eV and 0.5 eV respectively. These values were actually chosen more or less arbitrarily from any value near and less than the energy gap. As a matter of fact, the values E_1 and E_2 were not sensitive to the resultant A and B.

The knowledge of $\theta(E_o)$ in Equation (3.13) permitted the calculation of the refractive index n, of dn/dE and hence of the quantity $L\Delta\nu/c$ versus photon energy as expressed in Equation (4.6). A program named MODSEP2A (see Appendices VII and VIII) was written to complete those calculations.

Computation of $L\Delta\nu/c$ Versus Upper Integration Limit b

In this computation the narrow spectrum method was also used to calculate the mode separation at lasing photon energy of 1.38 eV (corresponding to the wavelength of 9000 angstroms) as the upper integration limit b varied. The reflectance data points were interpolated using the same interval of 0.015 eV.

In computing the integral $\theta(E_o)$ in Equation (3.13), the lower integration limit a was chosen as 0.1 eV and the upper integration limit b varied from 2 eV to 24 eV. Two vanishing θ's

corresponding to $E_1 = 0.3$ eV and $E_2 = 0.5$ eV were adopted. The quantities A and B in Equations (3.14) and (3.15) vary with b. The integral $\theta_{ab}(E_o)$, where $E_o = 1.38$ eV, was calculated similarly by using the Simpson's rule.

As usual, with the knowledge of the phase angle θ, n and hence the normalized frequency separation $L\Delta\nu/c$ were calculated as a function of the upper integration limit b. A program named MODSEP2B (see Appendices VII and X) was written for the calculation.

VI. RESULTS AND DISCUSSION

Figure 2 shows the calculated normalized frequency separation $L\Delta\nu/c$ of GaAs laser versus photon energy. This curve is the result obtained from the conventional method of computation. The computer output for Figure 2 is included in Appendix VI. As one can see, the normalized mode separation $L\Delta\nu/c$ at lasing energy of 1.38 eV is 0.1086.

The calculated values of $L\Delta\nu/c$ from the narrow spectrum method are shown in Figure 3 which is plotted from the computer output tabulated in Appendix IX. The two curves in this figure correspond to b of 2 eV and 3 eV. At the lasing energy of 1.38 eV the mode separation $L\Delta\nu/c$ is 0.107 for b = 2 eV and 0.108 for b = 3 eV. As shown in Figure 3 these two curves are very close to each other and to the curve in Figure 2.

The mode separation $L\Delta\nu/c$ as a function of b at lasing photon energy is shown in Figure 4. Appendix XI shows the data of the computer output for this figure. Here the values of $L\Delta\nu/c$ swing only between 0.107 and 0.111. Consequently the quantity $L\Delta\nu/c$ does not vary much as the spectral width changes.

For the sake of comparison, the measured values for $L\Delta\nu/c$ at lasing frequency are searched in the literature. The value $L\Delta\nu/c$ was reported by Burns, Dill and Nathan (3) to be 0.114 ± 0.01 percent

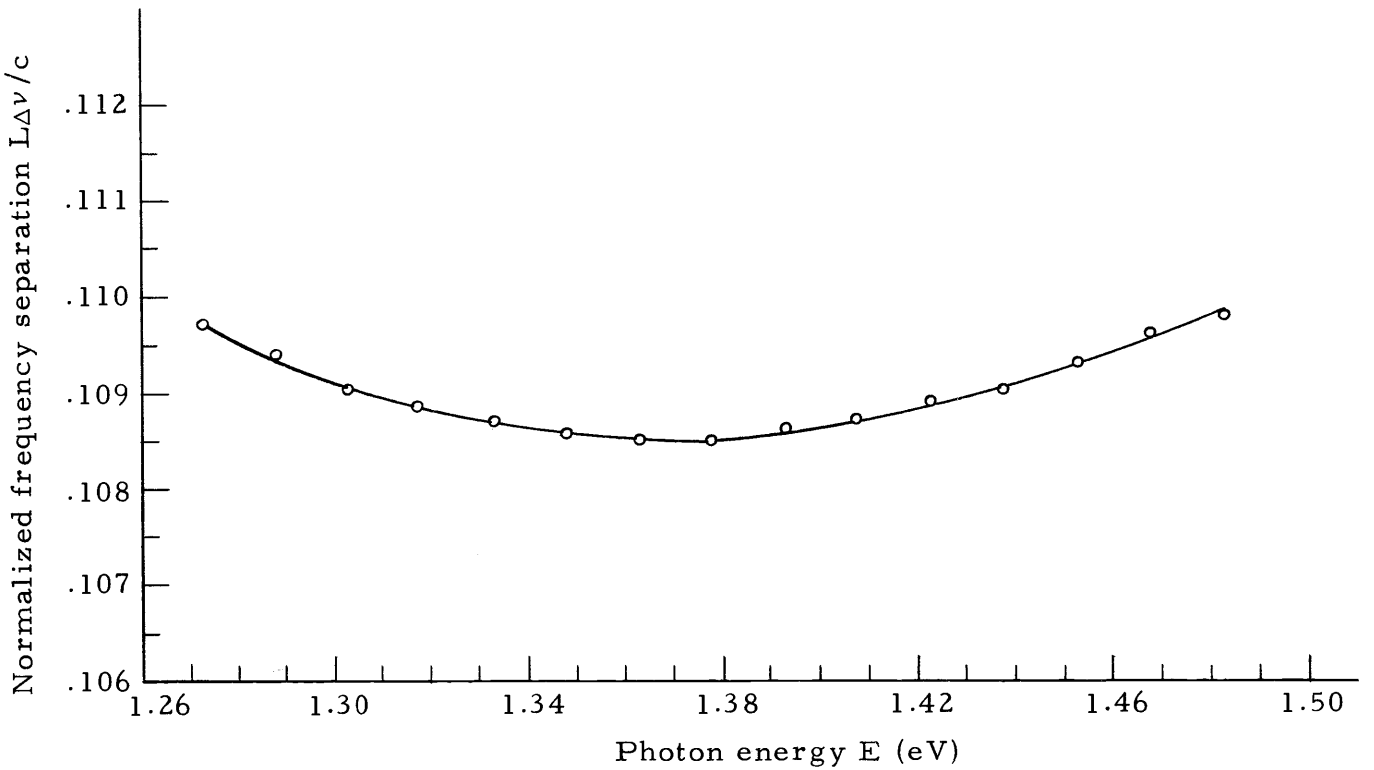

Figure 2. Calculated normalized frequency separation L$\Delta\nu$/c of GaAs laser versus photon energy from the conventional method.

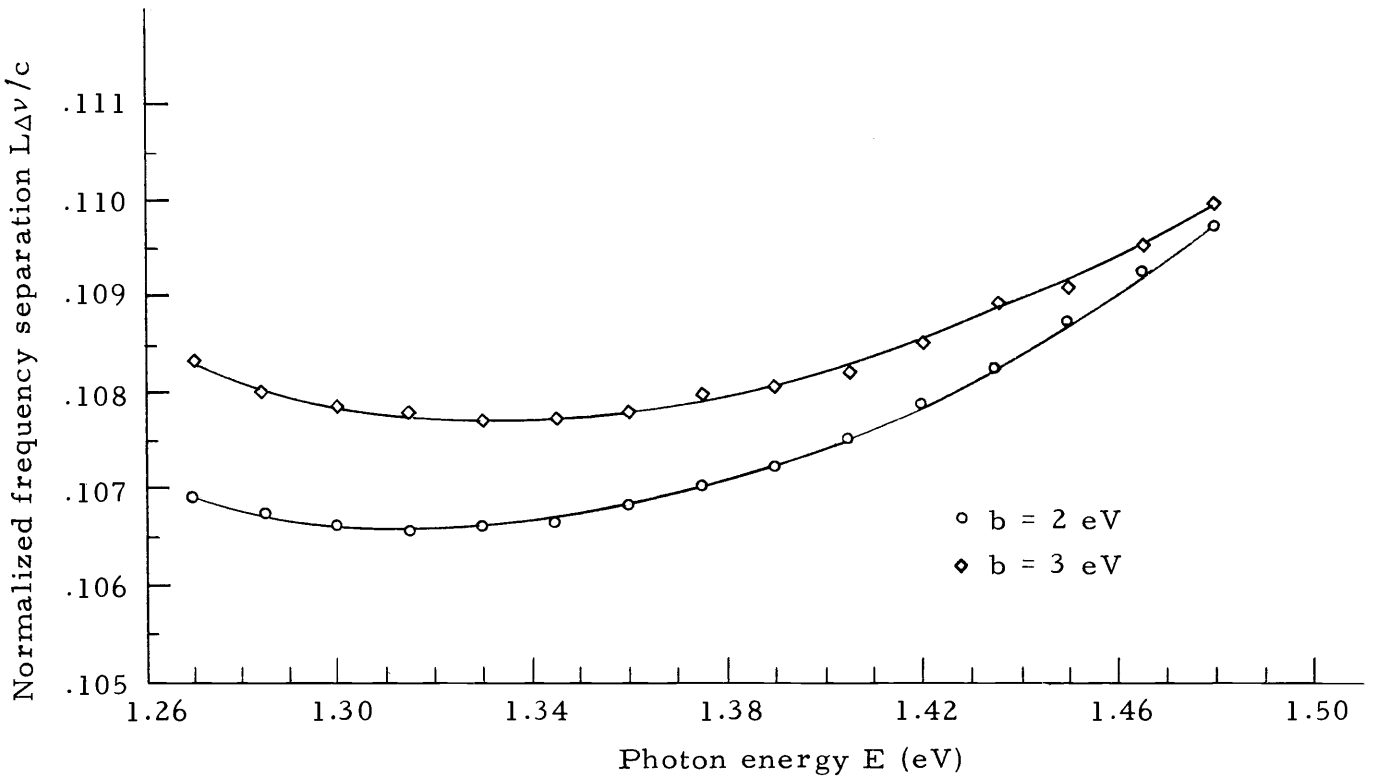

Figure 3. Calculated normalized frequency separation $L\Delta\nu/c$ of GaAs laser versus photon energy from the narrow spectrum method.

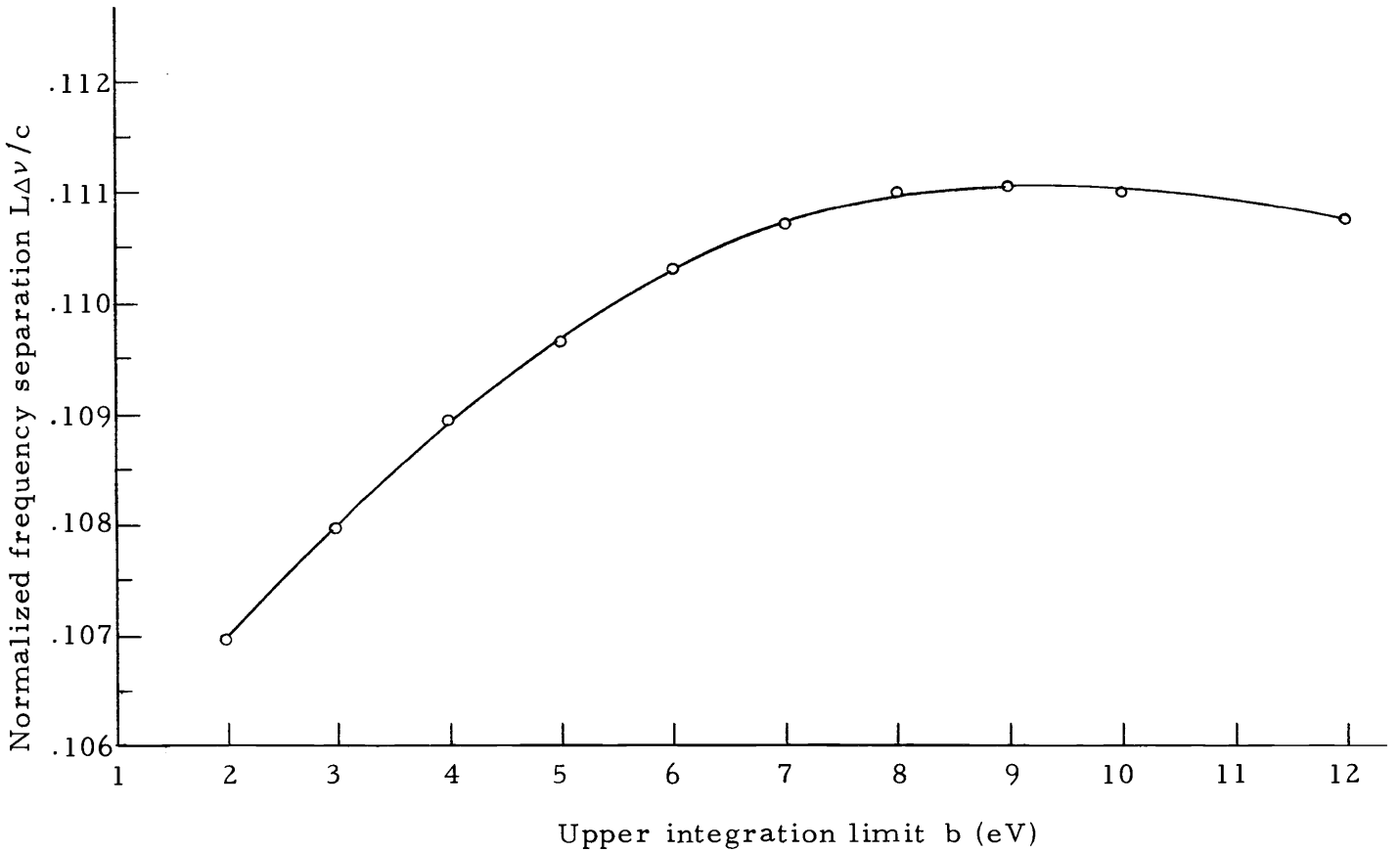

Figure 4. Calculated normalized frequency separation $L\Delta\nu/c$ of GaAs laser at 1.38 eV versus upper integration limit b.

and 0.105. Therefore it is reasonable to say that the computed results in this work are in good agreement with the measured ones. The table below shows the comparison between those values.

$L\Delta\nu/c$ at lasing energy of 1.38 eV for GaAs laser

Measured	Computed		
	Conventional Method	Narrow Spectrum Method	
		b = 2 eV	b = 3 eV
0.114 and 0.105	0.1086	0.107	0.108

It is also included that the results for the refractive index n of GaAs obtained from both methods of computation are shown in Figure 5. These curves are very close to each other, and the computed values for n agree satisfactorily with the measured ones (9).

In conclusion, in calculating the axial mode separation of a semiconductor laser from reflectance spectrum, the narrow spectrum method has many important advantages. Firstly, this method requires only a narrow spectral range near the energy gap of a semiconductor. Secondly, the set up for measuring such a narrow reflectance spectrum will be much simpler and cost less. In addition, the computing time is tremendously reduced as compared to the conventional method. This work has shown that the narrow spectrum method can be used to compute the mode separation of a semiconductor laser with a reasonable accuracy.

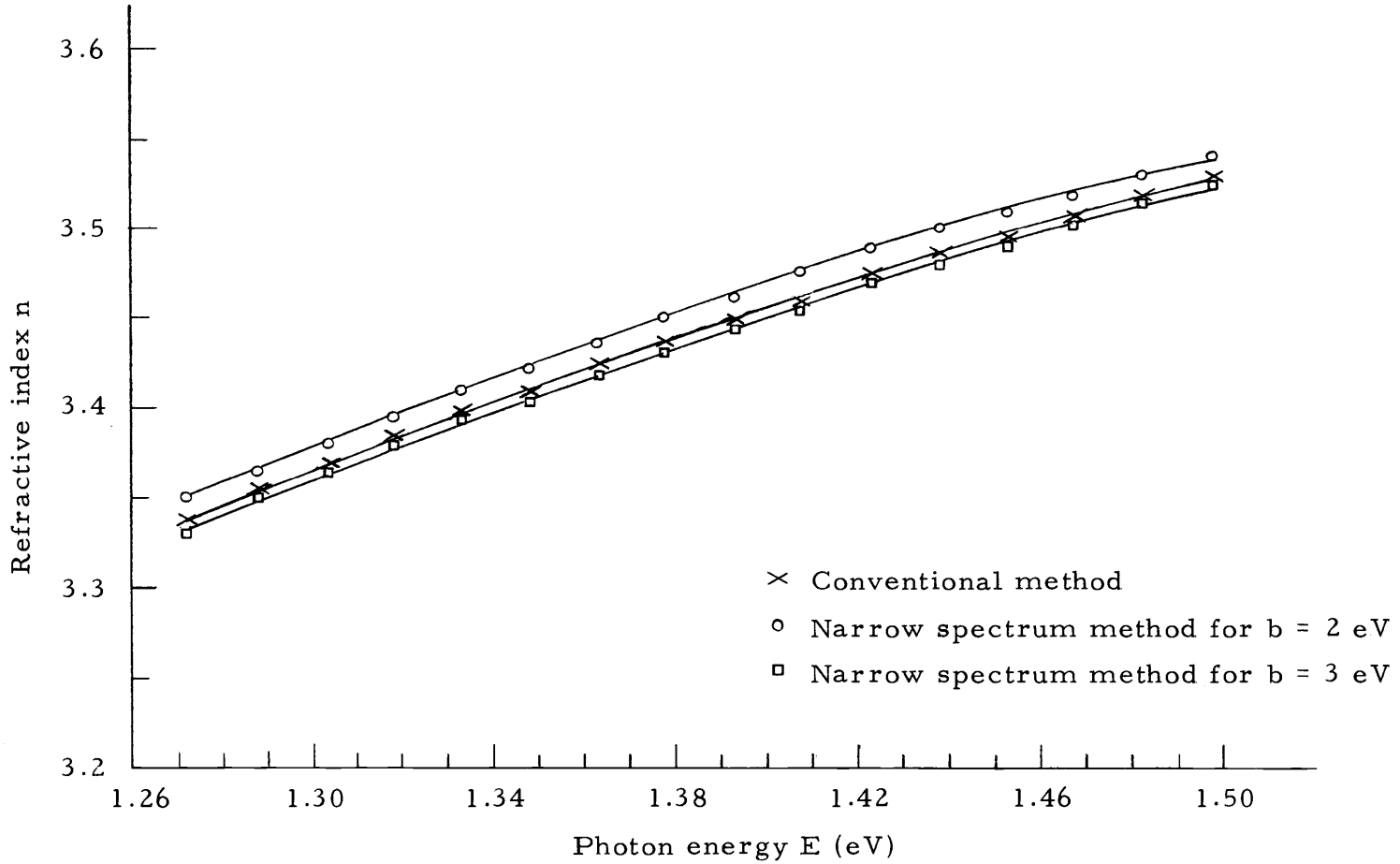

Figure 5. Calculated refractive index n of GaAs versus photon energy at room temperature.

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APPENDICES

APPENDIX I

Reflectance Data of GaAs at Room Temperature (from Reference 23).

Wavelength λ (μ)	Frequency γ (cps)	Photon Energy E (eV)	Reflectance R
4.0000E 01	7.5000E 12	3.1000E-02	3.9000E-01
3.9730E 01	7.5510E 12	3.1211E-02	3.9500E-01
3.9470E 01	7.6007E 12	3.1416E-02	4.0100E-01
3.9210E 01	7.6511E 12	3.1625E-02	4.0700E-01
3.8960E 01	7.7002E 12	3.1828E-02	4.1400E-01
3.8710E 01	7.7499E 12	3.2033E-02	4.2200E-01
3.8460E 01	7.8003E 12	3.2241E-02	4.3100E-01
3.8210E 01	7.8513E 12	3.2452E-02	4.4200E-01
3.7970E 01	7.9010E 12	3.2657E-02	4.5400E-01
3.7730E 01	7.9512E 12	3.2865E-02	4.6900E-01
3.7500E 01	8.0000E 12	3.3067E-02	4.8700E-01
3.7260E 01	8.0515E 12	3.3280E-02	5.1600E-01
3.7030E 01	8.1015E 12	3.3486E-02	5.3900E-01
3.6810E 01	8.1500E 12	3.3686E-02	5.7600E-01
3.6580E 01	8.2012E 12	3.3898E-02	6.2800E-01
3.6360E 01	8.2508E 12	3.4103E-02	6.9900E-01
3.6140E 01	8.3011E 12	3.4311E-02	7.6900E-01
3.5920E 01	8.3519E 12	3.4521E-02	8.0400E-01
3.5710E 01	8.4010E 12	3.4724E-02	8.1200E-01
3.5500E 01	8.4507E 12	3.4930E-02	8.0600E-01
3.5290E 01	8.5010E 12	3.5137E-02	7.8800E-01
3.5080E 01	8.5519E 12	3.5348E-02	7.5600E-01
3.4880E 01	8.6009E 12	3.5550E-02	7.0400E-01
3.4680E 01	8.6505E 12	3.5755E-02	6.1700E-01
3.4480E 01	8.7007E 12	3.5963E-02	4.7300E-01
3.4280E 01	8.7515E 12	3.6173E-02	2.5500E-01
3.4090E 01	8.8002E 12	3.6374E-02	8.0000E-02
3.3890E 01	8.8522E 12	3.6589E-02	4.6000E-02
3.3700E 01	8.9021E 12	3.6795E-02	5.9000E-02
3.3520E 01	8.9499E 12	3.6993E-02	8.0000E-02
3.3330E 01	9.0009E 12	3.7204E-02	1.0000E-01
3.3140E 01	9.0525E 12	3.7417E-02	1.1700E-01
3.2960E 01	9.1019E 12	3.7621E-02	1.3200E-01
3.2780E 01	9.1519E 12	3.7828E-02	1.4400E-01
3.2600E 01	9.2025E 12	3.8037E-02	1.5500E-01
3.2430E 01	9.2507E 12	3.8236E-02	1.6400E-01
3.2250E 01	9.3023E 12	3.8450E-02	1.7300E-01
3.2080E 01	9.3516E 12	3.8653E-02	1.8000E-01
3.1910E 01	9.4014E 12	3.8859E-02	1.8600E-01
3.1740E 01	9.4518E 12	3.9067E-02	1.9200E-01
3.1570E 01	9.5027E 12	3.9278E-02	1.9700E-01
3.1410E 01	9.5511E 12	3.9478E-02	2.0200E-01
3.1250E 01	9.6000E 12	3.9680E-02	2.0600E-01
3.1080E 01	9.6525E 12	3.9897E-02	2.1000E-01
3.0920E 01	9.7025E 12	4.0103E-02	2.1400E-01
3.0760E 01	9.7529E 12	4.0312E-02	2.1700E-01
3.0610E 01	9.8007E 12	4.0510E-02	2.2000E-01
3.0450E 01	9.8522E 12	4.0722E-02	2.2300E-01
3.0300E 01	9.9010E 12	4.0924E-02	2.2500E-01
3.0150E 01	9.9502E 12	4.1128E-02	2.2800E-01
3.0000E 01	1.0000E 13	4.1333E-02	2.3000E-01
2.7270E 01	1.1001E 13	4.5471E-02	2.5600E-01
2.5000E 01	1.2000E 13	4.9600E-02	2.6600E-01
2.3070E 01	1.3004E 13	5.3749E-02	2.7200E-01
2.1420E 01	1.4006E 13	5.7890E-02	2.7600E-01
2.0000E 01	1.5000E 13	6.2000E-02	2.7800E-01
1.8750E 01	1.6000E 13	6.6133E-02	2.8000E-01
1.7640E 01	1.7007E 13	7.0295E-02	2.8200E-01
1.6660E 01	1.8007E 13	7.4430E-02	2.8300E-01
1.5780E 01	1.9011E 13	7.8580E-02	2.8300E-01
1.5000E 01	2.0000E 13	8.2667E-02	2.8400E-01
1.4600E 01	2.1429E 13	8.8571E-02	2.8500E-01
1.3000E 01	2.3077E 13	9.5385E-02	2.6600E-01
1.2000E 01	2.5000E 13	1.0333E-01	2.8600E-01
1.1000E 01	2.7273E 13	1.1273E-01	2.8700E-01
1.0000E 01	3.0000E 13	1.2400E-01	2.8700E-01
9.0000E 00	3.3333E 13	1.3778E-01	2.8800E-01
8.0000E 00	3.7500E 13	1.5500E-01	2.8700E-01
7.0000E 00	4.2857E 13	1.7714E-01	2.8800E-01
6.0000E 00	5.0000E 13	2.0667E-01	2.8800E-01
5.0000E 00	6.0000E 13	2.4800E-01	2.8900E-01
4.0000E 00	7.5000E 13	3.1000E-01	2.8900E-01
3.0000E 00	1.0000E 14	4.1333E-01	2.8900E-01
2.0000E 00	1.5000E 14	6.2000E-01	2.8900E-01
1.0000E 00	3.0000E 14	1.2400E 00	2.8900E-01
8.2700E-01	3.6276E 14	1.4994E 00	3.1400E-01
7.2900E-01	4.1152E 14	1.7010E 00	3.2300E-01
6.5300E-01	4.5942E 14	1.8989E 00	3.3500E-01
5.9000E-01	5.0847E 14	2.1017E 00	3.5000E-01
5.3900E-01	5.5659E 14	2.3006E 00	3.7300E-01
4.9600E-01	6.0484E 14	2.5000E 00	4.0200E-01
4.5900E-01	6.5359E 14	2.7015E 00	4.3600E-01
4.4300E-01	6.7720E 14	2.7991E 00	4.6100E-01
4.2500E-01	7.0588E 14	2.9176E 00	4.8400E-01
4.1900E-01	7.1599E 14	2.9594E 00	4.6800E-01
4.0900E-01	7.3350E 14	3.0318E 00	4.6500E-01
4.0000E-01	7.5000E 14	3.1000E 00	4.6600E-01
3.6500E-01	8.2192E 14	3.3973E 00	4.2500E-01
3.4400E-01	8.7209E 14	3.6047E 00	4.0800E-01
3.2600E-01	9.2025E 14	3.8037E 00	4.0200E-01
3.1800E-01	9.4340E 14	3.8994E 00	4.0400E-01
2.7600E-01	1.0870E 15	4.4928E 00	4.9400E-01
2.5300E-01	1.1858E 15	4.9012E 00	5.9800E-01
2.4800E-01	1.2097E 15	5.0000E 00	6.0500E-01
2.2500E-01	1.3333E 15	5.5111E 00	5.1000E-01
2.0700E-01	1.4493E 15	5.9903E 00	4.3800E-01
2.0000E-01	1.5000E 15	6.2000E 00	4.1800E-01
1.9700E-01	1.5228E 15	6.2944E 00	4.1900E-01
1.8800E-01	1.5957E 15	6.5957E 00	4.6000E-01
1.7700E-01	1.6949E 15	7.0056E 00	4.4300E-01
1.5500E-01	1.9355E 15	8.0000E 00	3.6500E-01
1.3800E-01	2.1739E 15	8.9855E 00	2.6500E-01
1.2400E-01	2.4194E 15	1.0000E 01	2.0800E-01
1.1500E-01	2.6087E 15	1.0783E 01	1.7500E-01
1.0300E-01	2.9126E 15	1.2039E 01	1.5100E-01
9.6000E-02	3.1250E 15	1.2917E 01	1.3100E-01
8.9000E-02	3.3708E 15	1.3933E 01	1.0400E-01
8.3000E-02	3.6145E 15	1.4940E 01	7.7000E-02
7.7000E-02	3.8961E 15	1.6104E 01	5.3000E-02
7.3000E-02	4.1096E 15	1.6986E 01	3.2000E-02
6.8000E-02	4.4118E 15	1.8235E 01	2.0000E-02
6.5000E-02	4.6154E 15	1.9077E 01	1.4000E-02
6.2000E-02	4.8387E 15	2.0000E 01	1.1000E-02
5.9000E-02	5.0847E 15	2.1017E 01	1.5000E-02
5.8000E-02	5.1724E 15	2.1379E 01	1.5000E-02
5.6000E-02	5.3571E 15	2.2143E 01	1.4000E-02
5.4000E-02	5.5556E 15	2.2963E 01	1.3000E-02
5.1000E-02	5.8824E 15	2.4314E 01	1.0000E-02
4.9000E-02	6.1224E 15	2.5306E 01	6.0000E-03

APPENDIX II

Proof of Equation (3.4)

This integral can be written as

$$P\int_0^{\infty}\frac{dE}{E^2-E_o^2} = \lim_{\epsilon\to 0}\left[\int_0^{E_o-\epsilon}\frac{dE}{E^2-E_o^2}+\int_{E_o+\epsilon}^{\infty}\frac{dE}{E^2-E_o^2}\right] \qquad (1)$$

Since $E^2 > E_o^2$ in the second integral in brackets one has from the integral table

$$\int_{E_o+\epsilon}^{\infty}\frac{dE}{E^2-E_o^2} = \frac{1}{2E_o}\ln\left(\frac{E-E_o}{E+E_o}\right)\Bigg|_{E_o+\epsilon}^{\infty}$$

$$= -\frac{1}{2E_o}\ln\left(\frac{\epsilon}{2E_o}\right)$$

On the other hand the first integral in brackets can not be calculated directly from the table because the condition $E^2 > E_o^2$ is not satisfied. Thus one should proceed as follows.

The integrand in Equation (1) can be written as

$$\frac{1}{E^2-E_o^2} = -\frac{1}{E_o^2}\,\frac{1}{(1-p^2)}$$

where $E = pE_o$, $p < 1$.

Then, $\dfrac{1}{1-p^2}$ has series form as

$$\frac{1}{1-p^2} = 1 + p^2 + p^4 + p^6 + \ldots$$

With corresponding change in integration variable and integration limits one obtains

$$\int_0^{E_o-\epsilon} \frac{dE}{E^2-E_o^2} = -\frac{1}{E_o^2}\int_0^{1-\frac{\epsilon}{E_o}} (1+p^2+p^4+\ldots)E_o dp$$

$$= -\frac{1}{E_o}\left[p+\frac{p^3}{3}+\frac{p^5}{5}+\ldots\right]_0^{1-\frac{\epsilon}{E_o}}$$

The quantity in brackets is the series expansion of $\frac{1}{2}\ln(\frac{1+p}{1-p})$, thus

$$\int_0^{E_o-\epsilon} \frac{dE}{E^2-E_o^2} = -\frac{1}{E_o}\left[\frac{1}{2}\ln(\frac{1+p}{1-p})\right]_0^{1-\frac{\epsilon}{E_o}}$$

$$= -\frac{1}{2E_o}\ln\frac{2E_o}{\epsilon}$$

$$= \frac{1}{2E_o}\ln\frac{\epsilon}{2E_o}$$

Therefore two integrals in brackets in Equation (1) cancel out and the proof is completed.

APPENDIX III

Calculation of the Integrand in Equation (3.3) in the Case $E = E_o$

This integrand is written as

$$Y = \frac{\ln R(E) - \ln R(E_o)}{E^2 - E_o^2}$$

When $E = E_o$, Y becomes indeterminate. Using L'Hospital's rule gives

$$\lim_{E \to E_o} Y = \frac{\frac{d}{dE} \ln R}{2E} = \frac{\frac{1}{R}\frac{dR}{dE}}{2E}$$

Numerically

$$\left.\frac{dR}{dE}\right|_{E=E_j} = \frac{R_{j+1} - R_{j-1}}{2\Delta E}$$

Then

$$Y\big|_{E=E_j} = \frac{R_{j+1} - R_{j-1}}{4E_j R \Delta E}$$

where ΔE is equal interval of the spectrum.

APPENDIX IV

Symbols and Procedures of Calculation for Program MODSEP1

1) Dimension

XWL: wavelength available in data

XR: reflectance data values

XE: photon energy corresponding to XWL

CXE: interpolated photon energy

CXR: interpolated reflectance data

Y: integrand in Equation (3.3)

THETA: $\theta(E_o)$ in Equation (3.3)

RN: refractive index n

DRN: dn/dE in Equation (4.6)

2) Read reflectance data given in Appendix I

3) Converting wavelength XWL into energy XE

4) Some constants--

DE1: interval size within the reststrahlen range

DE2: interval size outside the reststrahlen range

C: the value of $R_1E_1^4$ in Equation (5.1)

NF1: number of equally spaced data points in the restrahlen range

NF: total number of interpolated data points covering up to 25 eV

5) CALL Subroutine LAGINT in the reststrahlen range

6) CALL Subroutine LAGINT outside the reststrahlen range

7) Extrapolation of R(E) curve for $E \geq 25$ eV

$CXR(I) = C/CXE(I)^4$

CXE(3499) = 50 eV

8) Calculating integrand Y in the case $E \neq E_o$

9) Calculating integrand Y in the case $E = E_o$ (see Appendix III)

10) Calculating $\theta(E_o)$ using Simpson's rule

THETA1: values of θ in the reststrahlen range

THETA2: values of θ outside the restrahlen range

11) Calculating refractive index n in Equation (2.7)

DENOM: denominator of the expression in Equation (2.7)

12) Calculating dn/dE using Equation (5.2)

13) Calculating the normalized frequency separation $L\Delta\nu/c$ in Equation (4.6)

SEPMOD = $L\Delta\nu/c$

14) Subroutine LAGINT

Using 3-point Lagrangian interpolation

APPENDIX V

Computer Program
Program MODSEP1

```
      PROGRAM MODSEP1
      DIMENSION XWL(130),XR(130),XE(130),CXE(3500),CXR(3500),Y(3500),
     1THETA(140),RN(140),DRN(140)
C READ TABULATED DATA WAVELENGTH XWL AND REFLECTANCE XR
      READ(60,10) (XWL(I),XR(I),I=2,120)
   10 FORMAT(12F6.3)
C CONVERTING WAVELENGTH INTO ENERGY
      DO300I=2,120
  300 XE(I)=1.24/XWL(I)
      WRITE(61,77)
   77 FORMAT(#1#,25X,#OUTPUT#////)
C SOME CONSTANTS
      DE1=0.001
      DE2=0.015
      CXE(1)=XE(2)
      CXR(1)=XR(2)
      C=XR(120)*XE(120)**4
      NF1=1.0+(XE(56)-XE(2))/DE1
      NF2=NF1+1
      NF=NF1+(XE(120)-XE(56))/DE2
      NF3=NF+1
C CALL SUBPROGRAM LAGINT FOR OBTAINING EQUALLY SPACED POINTS
      DO111I=1,NF1
      CALL LAGINT(XE,XR,CXE(I),CXR(I),2,56)
      CXE(I+1)=CXE(I)+DE1
  111 CONTINUE
      DO112I=NF2,NF
      CALL LAGINT(XE,XR,CXE(I),CXR(I),56,120)
      CXE(I+1)=CXE(I)+DE2
  112 CONTINUE
C THIS DO LOOP USED TO EXTRAPOLATE R(E) CURVE
      DO220I=NF3,3499
      CXE(I)=CXE(I-1)+DE2
  220 CXR(I)=C/CXE(I)**4
      DO110I=106,129
      E0=CXE(I)
      R1=CXR(I)
      DO100J=1,3499
      EJ=CXE(J)
      R2=CXR(J)
      IF(J.EQ.I)GOTO15
      Y(J)=(ALOG(R2/R1))/(EJ*EJ-E0*E0)
      GOTO100
   15 Y(J)=(CXR(J+1)-CXR(J-1))/4./DE2/CXE(J)/CXR(J)
  100 CONTINUE
      ESUM=0.0
      OSUM=0.0
      DO50M=2,3498,2
   50 ESUM=ESUM+Y(M)
      DO40M=3,3497,2
   40 OSUM=OSUM+Y(M)
C CALCULATING INTEGRAL USING SIMPSON RULE
      IF(NF1/2*2.EQ.NF1)GOTO2
      NFF=NF1
      GOTO3
    2 NFF=NF1+1
    3 THETA1=(E0/3.14159)*(DE1/3.)*(Y(1)+4.*ESUM+2.*OSUM+Y(NFF))
      NFG=NFF+1
      THETA2=(E0/3.14159)*(DE2/3.)*(Y(NFG)+4.*ESUM+2.*OSUM+Y(3499))
      THETA(I)=THETA1+THETA2
      DENOM=1.+CXR(I)-2.*SQRT(CXR(I))*COS(THETA(I))
      RN(I)=(1.-CXR(I))/DENOM
  110 CONTINUE
C CALCULATING NUMERICAL DIFFERENTIATION AND NORMALIZED FREQUENCY SPACING
      DO330I=107,128
      DRN(I)=(RN(I+1)-RN(I-1))/(2.*DE2)
      SEPMOD=0.5/(RN(I)+CXE(I)*DRN(I))
      WRITE(61,70) CXE(I),RN(I),SEPMOD
   70 FORMAT(3E17.4)
  330 CONTINUE
      STOP
      END

      SUBROUTINE LAGINT(X,Y,XA,YA,K,L)
      DIMENSION X(130),Y(130)
      DO8I=K,L
      IF(XA-X(I))9,8,8
    8 CONTINUE
    9 TERM1=(XA-X(I))*(XA-X(I+1))*Y(I-1)/((X(I-1)-X(I))*(X(I-1)-X(I+1)))
      TERM2=(XA-X(I-1))*(XA-X(I+1))*Y(I)/((X(I)-X(I-1))*(X(I)-X(I+1)))
      TERM3=(XA-X(I-1))*(XA-X(I))*Y(I+1)/((X(I+1)-X(I-1))*(X(I+1)-X(I)))
      YA=TERM1+TERM2+TERM3
      RETURN
      END
```

APPENDIX VI

Output of Program MODSEP1

E (eV)	n	$L\Delta\nu/c$
1.2430E 00	3.3145E 00	1.1761E-01
1.2580E 00	3.3287E 00	1.1046E-01
1.2730E 00	3.3431E 00	1.0975E-01
1.2880E 00	3.3573E 00	1.0936E-01
1.3030E 00	3.3714E 00	1.0907E-01
1.3180E 00	3.3852E 00	1.0886E-01
1.3330E 00	3.3989E 00	1.0871E-01
1.3480E 00	3.4122E 00	1.0861E-01
1.3630E 00	3.4254E 00	1.0856E-01
1.3780E 00	3.4382E 00	1.0856E-01
1.3930E 00	3.4508E 00	1.0862E-01
1.4080E 00	3.4630E 00	1.0872E-01
1.4230E 00	3.4750E 00	1.0888E-01
1.4380E 00	3.4866E 00	1.0907E-01
1.4530E 00	3.4979E 00	1.0931E-01
1.4680E 00	3.5088E 00	1.0957E-01
1.4830E 00	3.5194E 00	1.0963E-01
1.4980E 00	3.5299E 00	1.1422E-01
1.5130E 00	3.5364E 00	1.2009E-01
1.5280E 00	3.5423E 00	1.2061E-01
1.5430E 00	3.5483E 00	1.2015E-01
1.5580E 00	3.5542E 00	1.1955E-01

APPENDIX VII

Symbols and Procedures of Calculation for Programs MODSEP2A and MODSEP2B

1) Dimension. (same as in MODSEP1).

2) Read reflectance data. (same as in MODSEP1).

3) Converting wavelength into energy.

4) Some constants--

   DE: interval size

   A: the lower integration limit a = 0.1 eV

   C: the value of energy $h\nu_1$ = 0.3 eV

   D: the value of energy $h\nu_2$ = 0.5 eV

5) CALL Subroutine LAGINT.

6) Read upper integration limit data (NJ) given in Appendix XII.

7) Determining the quantities A and B in Equations (3.14) and (3.15).

   DET: determinant of coefficients of unknowns A and B

8) Calculating integrand Y in the case $E \neq E_o$.

9) Calculating integrand Y in the case $E = E_o$ (see Appendix III).

10) Calculating $\theta(E_o)$ using Simpson's rule.

    THETA = θ_{ab}

    THETA(18) = $\theta_{ab}(h\nu_1)$

    THETA(31) = $\theta_{ab}(h\nu_2)$

    THETA1 = θ_{0a}

THETA3 $= \theta_{b\infty}$

THETAT $= \theta(E_o)$

The rest of this program is similar to that of MODSEP1.

Computer Program
Program MODSEP2A

```
      PROGRAM MODSEP2A
      DIMENSION XWL(130),XR(130),XE(130),CXE(1700),CXR(1700),Y(1700),

     1THETA(120),RN(120),DRN(120)
C READ TABULATED DATA, WAVELENGTH XWL AND REFLECTANCE XR
      READ (60,10) (XWL(I),XR(I),I=2,120)
   10 FORMAT(12F6.3)
C CONVERTING WAVELENGTH INTO ENERGY
      DO300I=2,120
      XE(I)=1.24/XWL(I)
  300 CONTINUE
C SOME CONSTANTS
      DE=0.015
      CXE(1)=XE(46)
      CXR(1)=XR(46)
      NF=1.0+(XE(120)-XE(46))/DE
C CALL SUBROUTINE LAGINT FOR INTERPOLATION
      DO111I=1,NF
      CALL LAGINT(XE,XR,CXE(I),CXR(I),120)
      CXE(I+1)=CXE(I)+DE
  111 CONTINUE
      A=CXE(5)
      C=CXE(18)
      D=CXE(31)
      CA=(C+A)/(C-A)
      DA=(D+A)/(D-A)
      A1=ALOG(CA)
      A2=ALOG(DA)
C READ UPPER LIMITS OF INTEGRATION
  555 READ(60,11) NJ
   11 FORMAT(I4)
      WRITE(61,77)
   77 FORMAT(#1#,25X,#OUTPUT#////)
      IF(EOF(60)) GOTO55
      B=CXE(NJ)
      BC=(B+C)/(B-C)
      BD=(B+D)/(B-D)
      B1=ALOG(BC)
      B2=ALOG(BD)
      DET=A1*B2-A2*B1
      DO110I=80,100
      E0=CXE(I)
      R1=CXR(I)
      DO100J=5,NJ
      EJ=CXE(J)
      R2=CXR(J)
      IF(J.EQ.I) GOTO15
      Y(J)=(ALOG(R2/R1))/(EJ*EJ-E0*E0)
      GOTO100
   15 Y(J)=(CXR(J+1)-CXR(J-1))/4./DE/CXE(J)/CXR(J)
  100 CONTINUE
      ESUM=0.0
      OSUM=0.0
      NF2=NJ-1
      DO50M=2,NF2,2
   50 ESUM=ESUM+Y(M)
C CALCULATING INTEGRAL USING SIMPSON RULE
      THETA(I)=(E0/3.14159)*(DE/3.)*(Y(5)+4.*ESUM+2.*OSUM+Y(NJ))
  110 CONTINUE
      TC=THETA(18)-(0.5/3.1416*ALOG(CXR(18)))*(A1+B1)
      TD=THETA(31)-(0.5/3.1416*ALOG(CXR(31)))*(A2+B2)
      IF(DET.EQ.0.0)STOP
      AA=(TD*B1-TC*B2)/DET
      BB=(TC*A2-TD*A1)/DET
C NUMERICAL DIFFERENTIATION AND NORMALIZED FREQUENCY SPACING
      DO330I=80,100
      E0=CXE(I)
      AR1=(E0+A)/(E0-A)
      AR2=(B+E0)/(B-E0)
      F=0.5/3.1416*ALOG(CXR(I))
      THETA1=(AA-F)*ALOG(AR1)
      THETA3=(BB-F)*ALOG(AR2)
      THETAT=THETA1+THETA(I)+THETA3
      DENOM=1.+CXR(I)-2.*SQRT(CXR(I))*COS(THETAT)
      RN(I)=(1.-CXR(I))/DENOM
  330 CONTINUE
      DO333I=81,99
      DRN(I)=(RN(I+1)-RN(I-1))/(2.*DE)
      SEPMOD=0.5/(RN(I)+CXE(I)*DRN(I))
      WRITE(61,70) CXE(I),RN(I),SEPMOD
   70 FORMAT(3E17.4)
  333 CONTINUE
      GOTO555
   55 STOP
      END
      SUBROUTINE LAGINT(X,Y,XA,YA,N)
      DIMENSION X(130),Y(130)

      DO8I=46,N
      IF(XA-X(I))9,9,8
    8 CONTINUE
    9 TERM1=(XA-X(I))*(XA-X(I+1))*Y(I-1)/((X(I-1)-X(I))*(X(I-1)-X(I+1)))
      TERM2=(XA-X(I-1))*(XA-X(I+1))*Y(I)/((X(I)-X(I-1))*(X(I)-X(I+1)))
      TERM3=(XA-X(I-1))*(XA-X(I))*Y(I+1)/((X(I+1)-X(I-1))*(X(I+1)-X(I)))
      YA=TERM1+TERM2+TERM3
      RETURN
      END
```

APPENDIX IX

Output of Program MODSEP2A

	E (eV)	n	$L\Delta\nu/c$
b = 2 eV			
	1.2401E 00	3.3178E 00	1.1587E-01
	1.2551E 00	3.3337E 00	1.0728E-01
	1.2701E 00	3.3495E 00	1.0690E-01
	1.2851E 00	3.3651E 00	1.0670E-01
	1.3001E 00	3.3803E 00	1.0658E-01
	1.3151E 00	3.3953E 00	1.0654E-01
	1.3301E 00	3.4099E 00	1.0656E-01
	1.3451E 00	3.4242E 00	1.0664E-01
	1.3601E 00	3.4381E 00	1.0677E-01
	1.3751E 00	3.4517E 00	1.0696E-01
	1.3901E 00	3.4648E 00	1.0720E-01
	1.4051E 00	3.4776E 00	1.0749E-01
	1.4201E 00	3.4899E 00	1.0784E-01
	1.4351E 00	3.5018E 00	1.0825E-01
	1.4501E 00	3.5132E 00	1.0871E-01
	1.4651E 00	3.5243E 00	1.0923E-01
	1.4801E 00	3.5348E 00	1.0976E-01
	1.4951E 00	3.5449E 00	1.1403E-01
	1.5101E 00	3.5517E 00	1.1991E-01
b = 3 eV			
	1.2401E 00	3.3056E 00	1.1789E-01
	1.2551E 00	3.3208E 00	1.0895E-01
	1.2701E 00	3.3359E 00	1.0838E-01
	1.2851E 00	3.3509E 00	1.0807E-01
	1.3001E 00	3.3657E 00	1.0788E-01
	1.3151E 00	3.3802E 00	1.0777E-01
	1.3301E 00	3.3944E 00	1.0772E-01
	1.3451E 00	3.4084E 00	1.0773E-01
	1.3601E 00	3.4219E 00	1.0779E-01
	1.3751E 00	3.4352E 00	1.0790E-01
	1.3901E 00	3.4481E 00	1.0806E-01
	1.4051E 00	3.4606E 00	1.0827E-01
	1.4201E 00	3.4728E 00	1.0853E-01
	1.4351E 00	3.4846E 00	1.0883E-01
	1.4501E 00	3.4960E 00	1.0917E-01
	1.4651E 00	3.5070E 00	1.0955E-01
	1.4801E 00	3.5177E 00	1.0983E-01
	1.4951E 00	3.5280E 00	1.1384E-01
	1.5101E 00	3.5350E 00	1.1981E-01

APPENDIX X

Computer Program
Program MODSEP2B

```
      PROGRAM MODSEP2B
      DIMENSION XWL(130),XR(130),XE(130),CXE(1700),CXR(1700),Y(1700),
     1THETA(120),RN(120),DRN(120)
C READ TABULATED DATA, WAVELENGTH XWL AND REFLECTANCE XR
      READ (60,10) (XWL(I),XR(I),I=2,120)
   10 FORMAT(12F6.3)
C CONVERTING WAVELENGTH INTO ENERGY
      DO300I=2,120
      XE(I)=1.24/XWL(I)
  300 CONTINUE
C SOME CONSTANTS
      DE=0.015
      CXE(1)=XE(46)
      CXR(1)=XR(46)
      NF=1.0+(XE(120)-XE(46))/DE
C CALL SUBROUTINE LAGINT FOR INTERPOLATION
      DO111I=1,NF
      CALL LAGINT(XE,XR,CXE(I),CXR(I),120)
      CXE(I+1)=CXE(I)+DE
  111 CONTINUE
      A=CXE(5)
      C=CXE(18)
      D=CXE(31)
      CA=(C+A)/(C-A)
      DA=(D+A)/(D-A)
      A1=ALOG(CA)
      A2=ALOG(DA)
C READ UPPER LIMITS OF INTEGRATION
      WRITE(61,77)
   77 FORMAT(#1#,33X,#OUTPUT#////)
  555 READ(60,11) NJ
   11 FORMAT(I4)
      IF(EOF(60)) GOTO55
      B=CXE(NJ)
      BC=(B+C)/(B-C)
      BD=(B+D)/(B-D)
      B1=ALOG(BC)
      B2=ALOG(BD)
      DET=A1*B2-A2*B1
      DO110I=89,92
      E0=CXE(I)
      R1=CXR(I)
      DO100J=5,NJ
      EJ=CXE(J)
      R2=CXR(J)
      IF(J.EQ.I) GOTO15
      Y(J)=(ALOG(R2/R1))/(EJ*EJ-E0*E0)
      GOTO100
   15 Y(J)=(CXR(J+1)-CXR(J-1))/4./DE/CXE(J)/CXR(J)
  100 CONTINUE
      ESUM=0.0
      OSUM=0.0
      NF2=NJ-1
      DO50M=2,NF2,2
   50 ESUM=ESUM+Y(M)
C CALCULATING INTEGRAL USING SIMPSON RULE
      THETA(I)=(E0/3.14159)*(DE/3.)*(Y(5)+4.*ESUM+2.*OSUM+Y(NJ))
  110 CONTINUE
      TC=THETA(18)-(0.5/3.1416*ALOG(CXR(18)))*(A1+B1)
      TD=THETA(31)-(0.5/3.1416*ALOG(CXR(31)))*(A2+B2)
      IF(DET.EQ.0.0)STOP
      AA=(TD*B1-TC*B2)/DET
      BB=(TC*A2-TD*A1)/DET
C NUMERICAL DIFFERENTIATION AND NORMALIZED FREQUENCY SPACING
      DO330I=89,92
      E0=CXE(I)
      AR1=(E0+A)/(E0-A)
      AR2=(B+E0)/(B-E0)
      F=0.5/3.1416*ALOG(CXR(I))
      THETA1=(AA-F)*ALOG(AR1)
      THETA3=(BB-F)*ALOG(AR2)
      THETAT=THETA1+THETA(I)+THETA3
      DENOM=1.+CXR(I)-2.*SQRT(CXR(I))*COS(THETAT)
      RN(I)=(1.-CXR(I))/DENOM
  330 CONTINUE
      I=90
      DRN(I)=(RN(I+1)-RN(I-1))/(2.*DE)
      SEPMOD=0.5/(RN(I)+CXE(I)*DRN(I))
      WRITE(61,70) CXE(NJ),SEPMOD
   70 FORMAT(2E17.4)
      GOTO555
   55 STOP
      END
      SUBROUTINE LAGINT(X,Y,XA,YA,N)
      DIMENSION X(130),Y(130)
      DO8I=46,N
      IF(XA-X(I))9,9,8
    8 CONTINUE
    9 TERM1=(XA-X(I))*(XA-X(I+1))*Y(I-1)/((X(I-1)-X(I))*(X(I-1)-X(I+1)))
      TERM2=(XA-X(I-1))*(XA-X(I+1))*Y(I)/((X(I)-X(I-1))*(X(I)-X(I+1)))
      TERM3=(XA-X(I-1))*(XA-X(I))*Y(I+1)/((X(I+1)-X(I-1))*(X(I+1)-X(I)))
      YA=TERM1+TERM2+TERM3
      RETURN
      END
```

APPENDIX XI

Output of Program MODSEP2B

b (eV)	$L\Delta\nu/c$
2.0201E 00	1.0696E-01
3.0401E 00	1.0790E-01
4.0301E 00	1.0880E-01
5.0501E 00	1.0969E-01
6.0401E 00	1.1036E-01
7.0301E 00	1.1075E-01
8.0501E 00	1.1101E-01
9.0401E 00	1.1109E-01
1.0030E 01	1.1104E-01
1.2040E 01	1.1081E-01
1.4050E 01	1.1054E-01
1.6030E 01	1.1021E-01
1.8040E 01	1.0982E-01
2.0050E 01	1.0941E-01
2.2030E 01	1.0911E-01
2.4040E 01	1.0887E-01

APPENDIX XII

Upper Integration Limit Data

In program MODSEP2B, CXE represents the interpolated photon energy E and NJ the subscript corresponding to the point CXE(NJ). In other words b = CXE(NJ). The following table gives the values of NJ and the corresponding values of b.

NJ	b (eV)
133	2
201	3
267	4
335	5
401	6
467	7
535	8
601	9
667	10
801	12
935	14
1067	16
1201	18
1335	20
1467	22
1601	24

Note--For program MODSEP2A only the first two values of NJ were needed.