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LA THÈSE A ÉTÉ
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ABSORPTION COEFFICIENT OF HEAVILY DOPED GALLIUM ARSENIDE

by

Wichit SRITRAKOOL

Submitted to the School of Graduate Studies
in partial fulfillment of the requirements
for the degree of Ph.D. in Physics

University of Ottawa
Department of Physics
Ottawa, Canada

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UNIVERSITÉ D'OTTAWA
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ABSTRACT

In this thesis we evaluate the screening, the Fermi energy and the absorption coefficient in a heavily doped semiconductor. The specific case of a heavily doped n and p type GaAs is considered because of GaAs's relative simplicity and because experiments and other calculations are available for testing the results. The present calculations are based on the quantum mechanical theory of the density of electron states (DOS) in the energy band tail region of heavily doped semiconductors developed by Sa-yakanit. This theory provides the DOS and the wave functions (harmonic) of the localized electrons in the band tail. A method of determining these and the screening length self-consistently was developed by Sa-yakanit and Glyde (SG). These properties, the DOS, the wave functions and the screening provide the essential input to the evaluation of absorption.

We, firstly, test SG's DOS by calculating, self-consistently, the screening constant and the Fermi energy of heavily doped n type GaAs. We present some numerical results for the SG DOS and include some higher order correction terms to improve the DOS at higher energies. We compare SG's DOS with the only direct measurement of the DOS by Mahan and Conley. The calculated DOS agrees well with experiment.

Next, we calculate self-consistently the screening constant and the Fermi energy for heavily doped n and p type GaAs. These are needed in the calculation of absorption. The doping concentrations are chosen to be the same as those used by Casey et al in their experiments and by

Casey and Stern in their calculations so that comparisons with experiments and other calculations can be made. The screening constant is used in the DOS determination and the Fermi energy is used in the absorption coefficient calculation.

By making use of the SG DOS and the localized harmonic wave function from the SG theory, we create a new wave function for heavily doped semiconductors. It is in the form of a Bloch function modulated by a localized harmonic wave function. We then establish a matrix element of transition and find its asymptotic values. The absorption coefficients of both n and p type GaAs are determined using SG's DOS and the matrix element with and without the bandgap shrinkage due to many-body effects. The bandgap shrinkage is determined using Casey and Stern's empirical formula, and using Inkson's more fundamental Thomas-Fermi approximation. Our results need approximately a factor of 1.45 to bring it into agreement with experiment. Our overall absorption coefficients are also very similar to those of Casey and Stern. This suggests that, while several features of the present calculation are more fundamental, the agreement with experiment is not significantly better than obtained by Casey and Stern.

The sensitivity of the absorption coefficient to several physical quantities used in the calculation is also tested. We find that it is sensitive to the DOS and the bandgap shrinkage; with the latter quantity playing the most important role in the absorption process.

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CHAPTER 1

Introduction

With the development of Esaki diodes and semiconductor lasers, the heavily doped semiconductor has become a sensitive and active part of a device. Much attention has been paid to the transport and optical properties of heavily doped semiconductors. In this thesis, we consider only the absorption near the band edges in heavily doped GaAs crystal since it is the semiconductor which has the most available absorption experimental data. The basic theory of heavily doped semiconductors are given by Bonch Bruevich(1966) and Fistul(1969). By definition, a heavily doped semiconductor is formed when an impurity band and a parent band are merged. From a microscopic point of view, it is formed when the overlapping of electronic wave functions is large compared to impurity separations.

It has been well known since the last two decades that an absorption tail is observed when a semiconductor is heavily doped [Pankove (1965)]. In 1975, Casey et al(1975) presented a set of experimental absorption coefficients for heavily doped GaAs. Their n type data showed an appreciable shift to higher photon energies when the doping concentration is increased. This shift is called the Burstein shift. Their p type data showed larger absorption tails when the doping concentration is increased. In the following year, Casey and Stern(1976) proposed a theory to predict the absorption coefficients in which the initial and final wave functions were in the form of a Bloch function superimposed by a hydrogen-like envelope function. In their theory, they

scaled the Kane(1963) analytic expression for the density of states (DOS) to fit the Halperin and Lax(1966) tail DOS which was derived using a full quantum mechanical approach. Casey and Stern's absorption coefficients were, however, too small compared to experiments.

A few years later, Sa-yakanit (1979) used Feynman's path integration method and Halperin and Lax's ideas to create a new theory and was able to get an analytic expression for the DOS instead of that given in numerical tables of Halperin and Lax. In the following year, Sa-yakanit and Glyde (1980a,b) applied Lloyd and Best(1975)'s variational principle to Sa-yakanit's theory to increase the accuracy. We [Sritrakool, Glyde, and Sa-yakanit (1982)] tested the Sa-yakanit and Glyde DOS by calculating the Fermi energies and the screening constants of heavily doped n type GaAs with different compensation ratios. We [Sa-yakanit, Sritrakool, and Glyde (1982)] also presented some numerical results and included more higher order correction terms in the calculations. The only direct experiment available for the DOS is from the Schottky junction tunnelling experiments done by Mahan and Conley(1967). Takeshima (1983) compared his DOS, which was derived from the Green function method, with that experiment. It fitted the experiment quite well. We also show in this thesis that the Sa-yakanit and Glyde DOS does also fit the experiment. We point out that the difference cannot be observed by comparing with this experiment which is given in linear scales.

Here we mainly use the one-electron approximation. We restrict ourselves to the photon energy range from 1.35 to 1.55 eV. This range

covers transitions between band edges of heavily doped GaAs only since a pure GaAs crystal has a direct bandgap of 1.424 eV at room temperature. A simple parabolic band can then be assumed instead of its complicated band structure because of the small energy range being considered. All impurities are assumed to be shallow, i.e. totally ionized at room temperature, so that the number of free carriers can be estimated from donor and acceptor concentrations. The approximation used in determining the screening constant Q is the Thomas-Fermi approximation which requires a slowly varying potential field. The absorption coefficient is determined within a simplified band structure and, the one-electron approximation. Many-body effects manifest themselves in this calculation through the bandgap shrinkage mechanism.

We make a calculation of the absorption coefficient similar to that of Casey and Stern by using the DOS from the Sa-yakanit and Glyde theory [eq.(3-1)] and by creating new initial and final wave functions for an absorption transition by means of the localized harmonic wave function which comes out simultaneously with the DOS. The asymptotic value of our matrix elements [eq.(5-31)] is investigated and found to approach the matrix element for two plane waves correctly. The absorption coefficient is calculated with and without the bandgap shrinkage due to many-body effects. We evaluate the bandgap shrinkage using Inkson's Thomas-Fermi calculation and using Casey and Stern's empirical formula in order to see the effect of the shrinkage on the absorption coefficient. We find that bandgap shrinkage must be included to obtain good agreement with the observed absorption coefficient. The bandgap shrinkage, therefore, plays an important role in the absorption process. We also test the

sensitivity of the absorption coefficient to some physical quantities used in our calculation, e.g. the DOS, the effective mass, and some parameters involved.

In the next chapter, we review the basic theory for the absorption. Some reviews on the DOS for the band tail and the Sa-yakanit and Glyde theory will be described in chapter 3. The DOS for heavily doped GaAs and a comparison with experiment is also presented. In chapter 4, the method of calculating the screening constant Q for the DOS and the Fermi energy for the absorption self-consistently within the Thomas-Fermi approximation is explained. Some results for heavily doped n type GaAs and the results for the absorption calculation will be presented. In chapter 5, we describe some available matrix elements of transition and our present matrix element. In the last chapter, we present and compare our calculations for the absorption coefficients to experiments and those of Casey and Stern. The bandgap shrinkage will be discussed. Finally, in the Epilogue, conclusion to this work is given.

CHAPTER 2

Basic Theory of Absorption

2.1 Introduction

There are many excellent reviews of the basic theory of absorption in semiconductors from both a microscopic and macroscopic point of view. These are given by, for example, Stern(1963), Bassani(1966), Johnson(1967), Pankove(1971), Ziman(1972), Abeles(1972), Wooten(1972), Bassani et al(1975), and Abram et al(1978). The macroscopic theory describes the absorption using Maxwell's classical theory of electromagnetic waves to explain how waves propagate through a medium; while the microscopic theory begins with an electron in that medium then uses a quantum mechanical approach to describe the behavior of the electron under the time-dependent perturbation of the incoming electromagnetic wave. The decay of the propagating waves in a medium is directly related to the absorption of that medium. The absorption coefficient is defined as the fractional decrease in incident intensity with distance in the absorbing medium.

2.2 Macroscopic Theory

Various materials have different optical properties. Some are transparent and electromagnetic waves can pass through. Some are opaque and electromagnetic waves can only partially pass through. By means of classical Maxwell's equations, the electromagnetic waves propagating through a medium with dielectric function ϵ and magnetic susceptibility μ can be described by the four well-known Maxwell's equations :

$$\nabla \times \vec{H} = \frac{\epsilon_1}{c} \frac{\partial \vec{E}}{\partial t} + \frac{4\pi\sigma}{c} \vec{E} \quad (2-1 a)$$

$$\nabla \times \vec{E} = -\frac{\mu}{c} \frac{\partial \vec{H}}{\partial t} \quad (2-1 b)$$

$$\nabla \cdot \vec{H} = 0 \quad (2-1 c)$$

$$\nabla \cdot \vec{E} = 0 \quad (2-1 d)$$

where σ is the conductivity and c is the speed of light. Since we will not consider any magnetic effects, we take $\mu = 1$. A solution for the electric field from above equations is

$$\vec{E} = \vec{E}_0 \exp[i(\vec{K} \cdot \vec{r} - \omega t)] \quad (2-2)$$

where $\vec{K}$ is the complex propagation wave vector defined by $\vec{K} = \vec{K}_1 + i\vec{K}_2$ which is related to the angular frequency ω by the relation $\vec{K} \cdot \vec{K} = \omega^2 \epsilon / c^2$. The dielectric function ϵ can be complex. It is defined in terms of the real part ϵ_1 and the conductivity σ by $\epsilon = \epsilon_1 + i\epsilon_2 = \epsilon_1 + i4\pi\sigma/\omega$. In the medium, the refractive index N is also complex and defined as $N = n + ik = \epsilon^{1/2}$ where n is the real refractive index and k is the imaginary refractive index which is the so-called extinction coefficient. The latter quantity describes the absorption of electromagnetic waves by the medium. The relationship between these physical quantities is :

$$\epsilon_1 = n^2 - k^2 \quad (2-3)$$

$$\epsilon_2 = 4\pi\sigma/\omega = 2nk \quad (2-4)$$

$$K = (n\omega/c) + i(k\omega/c) = K_1 + iK_2 \quad (2-5)$$

Inserting K into eq.(2-2) and taking only the z component gives the solution for the electric field to be

$$\vec{E} = \vec{E}_0 \exp[i\omega(nz/c - t)] \exp(-kz/c) \quad (2-6)$$

The phase velocity of the wave is reduced to c/n and the wave is attenuated by the factor $\exp(-kz/c)$. The absorption coefficient which describes the fractional decrease in intensity with distance, is defined in the z direction as

$$\alpha = - \frac{1}{I} \frac{dI}{dz} \quad (2-7)$$

where I is the intensity. Since the intensity is proportional to the wave amplitude squared, we find from eqs.(2-6) and (2-7) that

$$\alpha = 2\omega k/c = \omega \epsilon_2 / nc \quad (2-8)$$

The absorption coefficient is a function of the incident wave frequency. We conclude that the absorption and other physical characters of the medium are functions of the frequency of the incident electromagnetic wave.

2.3 Microscopic Theory

In this section the quantum mechanical theory of absorption will be reviewed. The interaction between a radiation field and the electrons in a medium will be studied using standard quantum mechanics. Some basic approximations needed will be mentioned first.

2.3.1 Basic Approximations

The kinetic energy of a system of N electrons in the presence of an electromagnetic field is

$$\sum_{i=1}^N \left[\frac{1}{2m} \left(\vec{p}_i + \frac{e\vec{A}(\vec{r}, t)}{c} \right)^2 \right] \quad (2-9)$$

where $\vec{p}_i^2/2m$ is the kinetic energy an individual free electron, e is the absolute value of the electronic charge and $\vec{A}$ is the vector potential of the electromagnetic field. The choice of the Coulomb gauge implies that $\nabla \cdot \vec{A} = 0$. Furthermore all terms non-linear in the vector potential are also neglected. The Hamiltonian describing the interaction of the electrons with the radiation field is then

$$H' = \frac{e}{mc} \sum_{i=1}^N \vec{A}(\vec{r}_i, t) \cdot \vec{p}_i \quad (2-10)$$

This term is treated as a time-dependent perturbation on the electronic states and will cause electrons to make transitions between occupied bands and empty bands. From the transition probability rate, the relationship between the electronic structure and optical constants can be derived.

Basic approximations used since the beginning are the adiabatic scheme, the one-electron approximation, Koopmans' theorem, and the effective mass approximation. These approximations can simplify the complicated many-body problem into a solvable eigenvalue equation. Many-body effects resulting from electron-electron interactions are not treated rigorously in this work. Rather emphasis will be on the one-electron approximation which is a good approximation provided the electron-electron interaction can be incorporated into an effective single electronic potential. Since the pure GaAs crystal has a direct bandgap and we consider only a small range of photon energies which covers transitions only between band edges, the indirect transitions and other transitions will be disregarded here.

2.3.2 Quantum Theory of Absorption

If the perturbation term is $L \exp(\pm i\omega t)$ and the time-dependence is completely contained in the exponent, the transition probability per unit time from the initial state $|i\rangle$ with energy E_i to the final state $|j\rangle$ with energy E_j is

$$P' = (2\pi/\hbar) |\langle j|L|i\rangle|^2 \delta(E_j - E_i \pm \hbar\omega) \quad (2-11)$$

The perturbation $L \exp(-i\omega t)$ induces a transition with absorption of a photon of energy $\hbar\omega$ while $L \exp(i\omega t)$ induces a transition with emission of a photon of energy $\hbar\omega$. The Dirac delta function indicates the conservation of energy. Since we consider the absorption only, we will neglect the emission term from now on.

We now limit ourselves to transitions from the valence band to the conduction band. The ground state of the electronic system can be written as a Slater determinant composed of all one-electron states in the valence band. When the interaction Hamiltonian (2-10) is introduced it is assumed that only one electron goes to an excited state in the conduction band. The Slater determinant describing the excited state will therefore consist of $(N-1)$ one-electron states in the valence band and only one one-electron state in the conduction band. Hence the matrix element of transition from the ground state to the excited state due to the radiation field is just the transition from a one-electron state in the valence band to a one-electron state in the conduction band. If we define ψ_{kv} and ψ_{kc} to be one-electron wave functions in the valence and conduction bands respectively where k 's are their corresponding wave vectors, then we have the matrix element of the transition

$$\langle j|H'|i\rangle = (e/mc)\langle \psi_{kc}|\vec{A}\cdot\vec{p}|\psi_{kv}\rangle_{sv,sc} \delta \quad (2-12)$$

where sv and sc label the spins of the two wave functions respectively. From now on we will ignore the spins and treat the energy state as a single state. Spin will be re-introduced when we arrive at the final expression for the absorption coefficient. The vector potential can be written in terms of the frequency and the polarization vector $\hat{e}$ which is in the direction of the field as

$$\vec{A}(\vec{r},t) = A_0 \hat{e} \exp[i(\vec{q}\cdot\vec{r} - \omega t)] + \text{c.c.} \quad (2-13)$$

where $\vec{q}$ is the wave vector of the radiation and c.c. is the complex conjugate of the previous term. As before we will not consider the c.c. which is the emission term. The transition probability per unit time is now

$$P' = (2\pi/\hbar)(eA_0/mc)^2 |\langle \psi_{kc}|e^{i\vec{q}\cdot\vec{r}}\hat{e}\cdot\vec{p}|\psi_{kv}\rangle|^2 \delta(E_c - E_v - \hbar\omega) \quad (2-14)$$

where E_v and E_c are the corresponding energies to the states for the valence and conduction bands respectively. The magnitude of a typical photon wave vector is small compared to the magnitude of the wave vectors for the electronic wave functions whose magnitude is of the order of 10^8 cm^{-1} . Thus the exponential term in eq.(2-14) becomes unity and

$$P' = (2\pi/\hbar)(eA_0/mc)^2 |\hat{e}\cdot\vec{M}_{cv}(\vec{k}_c, \vec{k}_v)|^2 \delta(E_c - E_v - \hbar\omega) \quad (2-15)$$

where $\hat{e}\cdot\vec{M}_{cv}(\vec{k}_c, \vec{k}_v) = \langle \psi_{kc}|\hat{e}\cdot\vec{p}|\psi_{kv}\rangle$. The magnitude of $\vec{M}_{cv}$ in the $\hat{e}$ direction is

$$M_{cv} = \hat{e} \cdot \int_{\Omega} \psi_{kc}^*(\vec{k}_c, \vec{r}) (-i\hbar\nabla) \psi_{kv}(\vec{k}_v, \vec{r}) d\vec{r} \quad (2-16)$$

We now keep in mind that E_c is a function of $\vec{k}_c$ and E_v is a function of $\vec{k}_v$. To obtain the rate of the transition per unit volume $W(\omega)$, we must sum eq.(2-15) over all possible states in the unit volume, i.e. we must sum over all wave vectors $\vec{k}_c$ and $\vec{k}_v$ (and over spin degeneracy). If there is more than one valence band or more than one conduction band we must also sum over all those bands. Since $\vec{k}_c$ and $\vec{k}_v$ are confined to the first Brillouin zone with a density $\Omega/(2\pi)^3$ (Ω being the volume of the crystal), the transition rate per unit volume is

$$W(\omega) = (2\pi/\hbar)(eA_0/mc)^2 \Omega \int_{BZ} \frac{d\vec{k}_c}{(2\pi)^3} \int_{BZ} \frac{d\vec{k}_v}{(2\pi)^3} M_{cv}^2 \delta(E_c - E_v - \hbar\omega) \quad (2-17)$$

The absorption coefficient is also defined as the energy absorbed in unit time and in unit volume divided by the energy flux. The average energy density u in a medium of radiation field described by the vector potential in eq.(2-13) is related to the optical constants by the relation

$$u = n^2 A_0^2 \omega^2 / 2\pi c \quad (2-18)$$

This is also the energy density associated with a single photon of energy $\hbar\omega$. If we ignore the dispersion of the index of refraction n , the product of the average energy density u and the velocity of the propagation in the medium c/n is the energy flux [see Stern(1963) p.309]. Hence the absorption coefficient is simply written in terms of $W(\omega)$ as

$$\alpha(\omega) = \hbar\omega W(\omega) / u(c/n) \quad (2-19)$$

$$\text{or } \alpha(\omega) = \frac{4\pi^2 e^2 \Omega}{m^2 c n \omega} \int_{BZ} \frac{d\vec{k}_c}{(2\pi)^3} \int_{BZ} \frac{d\vec{k}_v}{(2\pi)^3} M_{cv}^2 \delta(E_c - E_v - \hbar\omega) \quad (2-20)$$

In heavily doped semiconductors, translational symmetry is broken by the random impurity potentials and the wave vector can no longer be regarded as a good quantum number. Thus the integration over all wave vectors must be converted to the integration over all energies. Using one of the definitions of the density of states $\rho(E) = (1/8\pi^3) d\vec{k}/dE$ and a property of the delta function, one can rewrite eq.(2-20) as

$$\alpha(\omega) = \frac{4\pi^2 e^2 \Omega}{m^2 c n \omega} \int_{-\infty}^{\infty} dE \rho_v(E) \rho_c(E + \hbar\omega) M_{cv}^2 \quad (2-21)$$

This shows that the absorption coefficient depends upon the density of states at the initial energy, the density of states at the mapping energy, and also the matrix element linking the initial and the final states through the interaction Hamiltonian (or momentum operator in another words). Therefore there are two basic physical quantities needed for the determination of the absorption coefficient of heavily doped semiconductors; the density of states and the matrix element of transition.

It should be noted that eq.(2-21) is valid at absolute zero temperature only. This means that all the valence band states are occupied and all the conduction band states are empty and there is no thermal excitation. The experimental data given by Casey et al (1975) and the work done by Casey and Stern(1976) are both for heavily doped GaAs at room temperature. In order to compare our results with theirs, the thermal factor which describes the occupancy at that temperature must also be introduced to the expression for the absorption coefficient. This thermal factor is also called the occupancy factor and it is defined in terms of the Fermi function as

$$f(E)[1-f(E+\hbar\omega)]-f(E+\hbar\omega)[1-f(E)] = f(E)-f(E+\hbar\omega) \quad (2-22)$$

Multiplying the integrand in eq.(2-21) by this factor gives

$$\alpha(\omega) = \frac{4\pi^2 e^2 \Omega}{m^2 c n \omega} \int_{-\infty}^{\infty} dE \rho_v(E) \rho_c(E+\hbar\omega) M_{cv}^2 [f(E)-f(E+\hbar\omega)] \quad (2-23)$$

There is another factor inside the Fermi function that must be established. This is the chemical potential known as the Fermi level or the Fermi energy in semiconductor physics. The Fermi energy can be determined self-consistently with another quantity called the screening constant Q which describes how the impurity potential decays in the medium. One of the methods available for this is Thomas-Fermi approximation. This method can give a reasonable result within certain limits. The details will be described in the next chapter. This screening constant is also needed to determine the densities of states for both bands.

Finally, it should be noted that the spin degeneracy of each single state must be included in the DOS's used in the final expression for the absorption coefficient [eq.(2-23)].

CHAPTER 3

The Density of States

3.1 Overview

A review on the electronic density of states (DOS) of a heavily doped semiconductor will be described. This consists of the parabolic DOS of an undoped semiconductor, Kane's DOS, Halperin and Lax's DOS [HL's DOS], and the recent Sa-yakanit and Glyde DOS [SG's DOS] which we pay more attention to in the present work. SG's DOS is essentially the DOS in the deep tail energies plus Kane's DOS at high energies. A mathematical representation for it will be given by eq.(3-1). More details on these DOS's will be given in following sections.

It is well known that a heavily doped semiconductor is a disordered system composed of randomly located impurities in a host medium which is assumed to have a constant static dielectric function. An electron in the semiconductor is then in a potential created by the overlapping of those impurity potentials. This random overlapping is referred to as the potential fluctuation. To study how the heavy doping affects the physical properties, one usually starts with the DOS since it can be used to calculate most physical quantities.

For an undoped semiconductor, an electron is assumed to be in an averaged crystal potential within the framework of the effective mass approximation. Electrons in the valence and the conduction bands have their $E-\vec{k}$ dispersion relations like free electrons with different effective masses so that the densities of electronic states vary as the

square root of energy. When the crystal is doped, the impurity sites in the doped crystal are assumed to be located randomly throughout the system. The distribution function selected to describe the randomness depends upon how high the doping concentration is. In heavily doped semiconductors, the impurity concentration is so high that the impurity band merges with the parabolic energy band of the unperturbed crystal, thus an energy band tail is formed.

The DOS associated with energy band tailing has been studied for years by many workers using different approaches. The perturbation approach fails to explain the states near the band edges because the impurity disorder cannot be regarded as small. A better description is to allow for charge carriers to respond more completely to the impurity random potentials than appears to be possible with perturbation methods. Kane(1963) and Bonch-Bruевич (1963, 1966a,b) independently developed a semi-classical theory of the band. Since the semi-classical theory does not take into account the kinetic energy of localization properly, it overestimates the tail DOS. A quantum mechanical theory which includes the kinetic energy of localization was developed by Halperin and Lax(1966,1967). Their first paper describes all the main ideas of the theory, while the second one focusses on higher order corrections. Since the theory is valid in the very deep energy tail region only and gives the DOS in numerical tables as a function of the potential fluctuation, it leads to some difficulties in practical use.

In 1974 Samathiyakanit [or Sa-yakanit] used essentially the same ideas as Halperin and Lax but exploited Feynman's path integration

formalism to attack the problem and could set up an equation for the DOS for the whole range of energies. Sa-yakanit(1979) studied the specific example of a disordered system having a gaussian or screened Coulomb impurity potential and included the Lloyd and Best(1975) variational principle which was especially proposed for the disordered system. The expression for the DOS at the tail region was established and some analyses were made and compared to those given by Halperin and Lax. Sa-yakanit and Glyde(1980a,b) devoted their work to the DOS of heavily doped semiconductors and could set up an analytic expression which was valid in the whole range of energies. An analytic expression for the tail DOS was also derived from the full expression for the DOS. Their numerical value of the tail DOS gives a little better result at higher energies than that of Halperin and Lax, and it also crosses Kane's semi-classical DOS. Although Sa-yakanit and Glyde have set up the full expression for the DOS of heavily doped semiconductors, it has not been possible to evaluate the full expression exactly at all energies because of many built-in essential singularities. Efforts are underway to evaluate the full expression of the DOS for a better result.

We [Sa-yakanit, Sritrakool, and Glyde] use that theory to evaluate the tail DOS for heavily doped semiconductors at four different values of potential fluctuations. We simplify the variational expression for the variational parameter by writing it in terms of the well known incomplete gamma function. Some higher correction terms are included in the tail DOS expression. Our present numerical results are compared to previous methods. The chosen DOS for all energies is thus our tail DOS, $\rho_1(E)$, matched with Kane's DOS, $\rho^K(E)$, in higher energies, i.e.

$$\rho(E) = \rho_1(E)[1-H(E-E')] + \rho^K(E)H(E-E') \quad (3-1)$$

where E' is the energy at which $\rho_1(E)$ crosses $\rho^K(E)$ and $H(x)$ is the heaviside step function equal to 1 for $x > 0$ and equal to 0 for $x < 0$. Since the idea of matching is first made by Sa-yakanit and Glyde(1980a), the DOS in eq.(3-1) is simply called the SG DOS. The DOS will be used in our calculation for the optical absorption coefficient.

3.2 Free Electron DOS

In a perfect crystal, an electron sees the same potential everywhere provided the potential variation is so small that the potential can be smeared out and be represented by a single mean value. The potential variation is considered to be the second order effect to the electronic states. The $E-\vec{k}$ dispersion relation of the electron is like a free electron with different effective mass depending on the crystal structure. The number of states having energy up to E can be obtained by summing all possible wave vectors which label the states. For a large system with volume Ω the number of states $N(E)$ is

$$N(E) = \frac{\Omega}{(2\pi)^3} \int d\vec{k} \quad (3-2)$$

This leads to the DOS which defined as the number of (single spin) states per unit energy per unit volume, i.e.

$$\rho(E) = \frac{1}{\Omega} \frac{dN(E)}{dE} = \frac{m^*{}^{3/2}}{\sqrt{2} \pi^2 \hbar^3} E^{1/2} \quad (3-3)$$

Thus the free electron DOS varies as the square root of energy. Using Thomas-Fermi approximation, eq.(3-3) can be generalized to be

$$\rho(E) = \frac{m^*{}^{3/2}}{\sqrt{2} \pi^2 \hbar^3} (E-V)^{1/2} \quad (3-4)$$

where V is a slowly-varying potential. The DOS has a parabolic shape with V as a reference energy level so that it is always called the "parabolic" DOS.

3.3 Kane's Theory

For a heavily doped semiconductor, a high density of impurities is expected to create an impurity band tail in the bandgap (the low energy region) and the DOS is expected to remain nearly free electron like higher in the band (the high energy region). The tail of the DOS is anticipated to decay exponentially as a function of energy. After perturbation approaches [Parmenter(1955), Wolff(1962a,b), Bonch-Bruevich and Miranov(1962)] failed to explain this tailing phenomena in disordered systems, Kane(1963) and Bonch-Bruevich (1963, 1966a,b) independently developed a semi-classical theory to attack this problem. Bonch-Bruevich has given a formal mathematical description of the method, but in this section we adopt the physical intuitive view of Kane.

Kane's theory is a semi-classical treatment of an electron in a disordered system. The main idea is to assume each electron to have the same kinetic energy everywhere in the system independent of the local potential $V(\vec{r})$. The DOS is simply proportional to the square root of $E - V(\vec{r})$ by means of the free electron theory. Since the local potential is random in position, the DOS for the system must be averaged over the random potential. Since it is assumed that scatterers are weak and dense, the probability distribution function is then a gaussian function. Sa-yakanit and Glyde(1980a,b) wrote the averaged result of

the DOS in terms of the parabolic cylinder function $D_p(z)$ [see Appendix B] as

$$\rho^K(E) = \frac{f}{2\sqrt{2}} \xi^{1/2} e^{-1/2(E-V_0)^2/\xi} D_{-3/2}[-(E-V_0)/\sqrt{\xi}] \quad (3-5)$$

with $f \equiv \frac{m^*3/2}{\sqrt{2} \pi^2 \hbar^2}$. (3-6)

Here V_0 is the averaged potential, and ξ is the potential fluctuation which has the unit of energy squared [$\xi = \frac{2\pi e^2 \bar{N}}{Q \epsilon_0^2}$ with $\bar{N}$ being impurity concentration, see definition in eq.(4-7)]. For large E , eq.(3-5) approaches the limit of free electrons, i.e. Kane's DOS varies as the square root of energy. The Kane DOS at very deep tail region where $E-V_0$ is large and negative is a function of $\exp(-E^2)$.

It should be noted that the validity of Kane's theory depends upon the assumption of weak and dense scatterers. The Kane DOS may be written in a different form from his original paper. The linkage between them has been verified by Sa-yakanit and Glyde(1980b). We will mention eq.(3-5) as the Kane DOS.

3.4 Halperin and Lax's Theory

Halperin and Lax(1966) presented a quantum mechanical theory for the tail states. Their method is only valid for deep tail states even though the kinetic energy of localization is properly included. The main idea of the theory is to include the response of the electrons under the potential fluctuations. In the regions of deep and narrow potential wells the electrons will be highly localized and the kinetic energy will

be large. Including the kinetic energy of localization, the total electronic energy will be larger than in Kane's theory where the kinetic energy variations are neglected. Thus the DOS for the band tail region in this theory is expected to be smaller than in the semi-classical theory.

Basically, Halperin and Lax find the DOS by counting the number of allowed energy states in a unit volume and averaging the DOS over all random potentials V , i.e.

$$\rho(E) = \frac{1}{\Omega} \int \langle \delta(E - E_i(V)) \rangle_V \quad (3-7)$$

where $E_i(V)$ are the exact energy states of the electrons under the potential V . Since the determination of E_i is very complicated, only the main ideas will be discussed and then the final DOS will be presented. To treat the states quantum mechanically, they use a variational method in which the eigenvalue is optimized with respect to an assumed real and normalized trial wave function.

Halperin and Lax assume that an eigenstate of the system may be associated with each local energy minimum. At these minima, the energy is close to but greater than the energy of the true eigenstate. Since the trial function gives a higher energy than the true eigenvalue, the DOS is expected to be smaller than the true value. Therefore the best trial function must be chosen to maximize the DOS. The maximization leads to a Hartree-Fock like equation from which the trial function can be solved if the impurity potential is assumed.

Halperin and Lax use the screened Coulomb potential in their explicit calculation of the tail DOS. The result, expressed in terms of the dimensionless energy $\nu = (V_0 - E)/E_Q$ where $E_Q = \hbar^2 Q^2 / 2m^*$ is the energy associated with the screened Coulomb potential, is

$$\rho(\nu) = \frac{Q^3}{E_Q \xi'^2} a(\nu) \exp[-b(\nu)/2\xi'] \quad (3-8)$$

Here

$$\xi' \equiv \frac{\xi}{E_Q} = \frac{8\pi \bar{N} m^* Z^2 e^4}{\hbar^4 Q^5 \epsilon_0^2} \quad (3-9)$$

with Z being the impurity charge compared to the perfect crystal, $\bar{N}$ being the impurity concentration, and ϵ_0 being the static dielectric function of the medium. The $a(\nu)$ and $b(\nu)$ are universal dimensionless functions given numerically by Halperin and Lax(1966). These two functions are not dependent on any other physical quantity except energy. It can be seen from eq.(3-8) that HL's DOS also decays exponentially as a function of energy. Generally speaking, it decays as a function of $\exp(-E^n)$ with n varies from 1/2 (for short-range potential with large Q) to 2 (for long-range potential with small Q).

3.5 Sa-yakanit and Glyde's Theory

Even though Halperin and Lax presented a better tail DOS than the the semi-classical Kane DOS, there are two disadvantages in practical uses. Firstly, the DOS is given in numerical tables and secondly the theory is valid only in the energy tail region and cannot be extended to higher energies. To obtain a DOS at all energies, an interpolation between HL's DOS and the parabolic DOS is usually made [Hwang(1970a,b), Hwang and

Brews(1971)]. To obtain an analytic expression, the only potential fluctuation parameter in Kane's theory may be scaled until the tail DOS fits to Halperin and Lax's result [Stern(1971), Casey and Stern(1975)], or Halperin and Lax's result may be fitted by a single simple (but rough) analytic expression [Zee(1979)].

Sa-yakanit(1974,1979) developed a new theory based upon the Feynman path integration formalism which could successfully explain the polaron problem [Feynman(1955)]. Sa-yakanit and Glyde(1980a,b) derived an explicit expression for the DOS especially for heavily doped semiconductors using the theory developed by Sa-yakanit, again using the path integration method. Reviews and applications of the Feynman path integration methods are given in Feynman's original paper [Feynman(1948)] and in some textbooks [Feynman and Hibbs(1965), Feynman(1972), Schulman(1981)].

The model used by Sa-yakanit is like that in Halperin and Lax's theory. The main idea of his theory is also to include the response of the electrons under potential fluctuations. The potential fluctuations form non-local potential wells and each well is modelled by a single harmonic well. The shape of the harmonic well is of the form characterized by a variational parameter which must be determined by a variational principle. Sa-yakanit and Glyde(1980a,b) employ the Lloyd and Best(1975) variational principle for a disordered system to determine the variational parameter.

In the Feynman path integration method, a retarded propagator $G(\vec{r}_2, \vec{r}_1; t)$ describing the propagation of an electron from position $\vec{r}_1$ to

position $\vec{r}_2$ and at time t can be found by summing over all possible paths joining the two positions. This can be written in Feynman's notation of infinite integration $D(\vec{r}(\tau))$ as

$$G(\vec{r}_2, \vec{r}_1; t) = \int D(\vec{r}) e^{(i/\hbar) S_\ell} \quad (3-10)$$

where S_ℓ is the action defined as

$$S_\ell = \int_0^t d\tau \left[\frac{m^*}{2} \dot{\vec{r}}^2(\tau) - V_0 - V(\vec{r}(\tau)) \right] \quad (3-11)$$

The DOS can be related to the diagonal elements of the propagator G through the relation [Sayakanit(1974), Schulman(1981)] :

$$\rho(E) = \frac{1}{\pi \hbar} \operatorname{Re} \int_0^\infty dt e^{iEt/\hbar} \langle G(\vec{r}_1, \vec{r}_1; t) \rangle_V \quad (3-12)$$

To find the diagonal elements, one must average the retarded propagator in eq.(3-10) and reduce it for the diagonal elements. We define random averaging by

$$\begin{aligned} \bar{G} &\equiv G(\vec{r}_2, \vec{r}_1; t) = \int_{\vec{\Omega}} d\vec{R}_1 \dots \int_{\vec{\Omega}} d\vec{R}_N G(\vec{r}_2, \vec{r}_1; t) \\ &= \int D(\vec{r}(\tau)) e^{(i/\hbar) S} \end{aligned} \quad (3-13)$$

where for a gaussian random potential the action is

$$S = \int_0^t d\tau \left\{ \frac{m^*}{2} \dot{\vec{r}}^2(\tau) - V_0 + \frac{i}{\hbar} \int_0^t d\tau' W(\vec{r}(\tau) - \vec{r}(\tau')) \right\} \quad (3-14)$$

To proceed, the full action S in eq.(3-13) is modelled by a nonlocal harmonic trial action

$$S_0 = \int_0^t d\tau \left\{ \frac{m^*}{2} \dot{\vec{r}}^2(\tau) - \frac{m^* \omega^2}{4t} \int_0^t d\tau' |\vec{r}(\tau) - \vec{r}(\tau')|^2 \right\} \quad (3-15)$$

Essentially, the correlation function is modelled by a single nonlocal harmonic well with the steepness of the well characterized by the variational parameter ω . By writing eq.(3-13) in terms of S_0 , one obtains

$$\begin{aligned}\bar{G} &= \int D e^{(i/\hbar)S_0} \left[\frac{\int D e^{(i/\hbar)(S_0+(S-S_0))}}{\int D e^{(i/\hbar)S_0}} \right] \\ &= \bar{G}_0 \left\langle e^{(i/\hbar)(S-S_0)} \right\rangle_{S_0}\end{aligned}\quad (3-16)$$

where the average is made with respect to the trial action. Making a cumulant expansion of eq.(3-16) and keeping only the first cumulant gives the first order approximation of $\bar{G}$ as

$$\bar{G}_1 = \bar{G}_0 \left[\exp \left((i/\hbar) \langle S-S_0 \rangle_{S_0} \right) \right] \quad (3-17)$$

For the case of gaussian-random screened Coulomb potentials, $\bar{G}_1$ can be evaluated exactly [Sa-yakanit(1979)] and the diagonal elements can be found. This leads to the full expression for the DOS which is valid for all energies

$$\begin{aligned}\rho_1(E) &= \frac{1}{\pi\hbar} \operatorname{Re} \int_0^t dt \left[\left(\frac{m^*}{2\pi i\hbar t} \right)^{1/2} \left(\frac{\omega t}{2 \sin \omega t} \right) \right]^3 \exp \left[-\frac{i}{\hbar} (V_0 - E) t \right] \\ &\quad - \frac{1}{2\hbar^2} \frac{\xi Q t}{\sqrt{\pi}} \int_0^t dx \int_0^\infty dy y e^{-Q^2 y} j(x,y)^{-3/2} \left[\frac{3}{2} \frac{\omega t \cot \omega t - 1}{2} \right]\end{aligned}\quad (3-18)$$

$$\text{where } j(x,y) = y + \frac{i\hbar}{m^*\omega} \left[\frac{\sin \omega x}{2} \frac{\sin \omega(t-x)}{2} \frac{1}{\sin \omega t} \right] \quad (3-19)$$

The subscript "1" in the DOS in eq.(3-18) denotes that only the first cumulant expansion is used. It is the full expression for the DOS which cannot be evaluated exactly at the moment because there are many built-in essential singularities especially in the cotangent term.

The asymptotic limit of eq.(3-18) valid in the tail region can be found by taking t to infinity [Feynman and Hibbs(1965)]. By writing it in terms of the dimensionless energy as Halperin and Lax, the result is

$$\rho_1(v,z) = \frac{Q^3}{E_Q \xi^{5/4}} \frac{a(v,z)}{b(v,z)} e^{-b(v,z)/4\xi'} D_{3/2}(\sqrt{b(v,z)/\xi'}) \quad (3-20)$$

where $z=(2E_Q/\hbar\omega)^{1/2}$ is now a new variational parameter, $a(v,z)$ and $b(v,z)$ are universal dimensionless functions defined by Sa-yakanit and Glyde(1980a,b) as

$$a(v,z) = (T+v)^{3/2} / [8\pi\sqrt{2} z^6 \exp(z^2/2) D_3^2(z)] \quad (3-21)$$

$$\text{and } b(v,z) = (T+v)^{2\sqrt{\pi}} / [2\sqrt{2} \exp(z^4/4) D_3(z)] \quad (3-22)$$

with $T=(3/4)\hbar\omega/E_Q=3/2z^2$ being the electronic kinetic energy of localization in units of E_Q . To see the correspondence between this theory and Halperin and Lax's, we consider the asymptotic expansion of the parabolic cylinder function for large x [see Appendix B]

$$D_p(z) = e^{-x^2/4} x^p \left[1 - \frac{p(p-1)}{2} \frac{1}{x^2} + \dots \right] \quad (3-23)$$

For the very deep tail limit with large $b(v,z)/\xi'$, we ignore the term in $1/x^2$ and get

$$\rho_1(v,z) = \frac{Q^3}{E_Q \xi'^2} a(v,z) \exp[-b(v,z)/2\xi'] \quad (3-24)$$

which is in the same form as eq.(3-8) in Halperin and Lax's theory.

The DOS in eq.(3-20) also approaches Kane's semi-classical limit if we take t to zero [Feynman and Hibbs(1965)], i.e.

$$\rho_1^{SC}(\nu) = \frac{1}{8\sqrt{2}\pi^2} \xi^{9/4} e^{-\nu^2/4\xi} D_{3/2}(\nu/\sqrt{\xi}) \quad (3-25)$$

or in the real energy notation as

$$\rho_1^{SC}(E) = \frac{f}{2\sqrt{2}} \xi^{1/4} e^{-(E-V_0)^2/4\xi} D_{3/2}[-(E-V_0)/\sqrt{\xi}] \quad (3-26)$$

It should be noticed that the semi-classical DOS is independent of the variational parameter z . Eq.(3-26) has also the same asymptotic values as Kane's DOS in the high and low energy limits. It behaves at high energies like the parabolic DOS.

To determine the variational parameter z , Halperin and Lax maximized the DOS but Sa-yakanit(1979), and Sa-yakanit and Glyde(1980a,b) used the Lloyd and Best(1975) variational principle which was especially suited for this kind of disordered system. Lloyd and Best considered a many-Fermion problem in which the single-particle eigenstates of interest are filled up to some Fermi energy. They wrote the pressure of the system as a function of the DOS

$$\begin{aligned} P(E, z) &= \int_{-\infty}^E dE' \int_{-\infty}^{E'} dE'' \rho_1(E'', z) \\ &= \int_{-\infty}^E (E-E') \rho_1(E', z) dE' \end{aligned} \quad (3-27)$$

$$\text{or} \quad P(\nu, z) = -E_Q^2 \int_{\nu}^{\infty} (\nu-\nu') \rho_1(\nu', z) d\nu' \quad (3-28)$$

and proposed that this pressure should be maximized instead of the DOS. They reasoned that the actual many-Fermion system has a fixed chemical

potential, temperature (zero) and volume so that the thermodynamic potential to be minimized is that of the grand canonical ensemble, namely $-P\Omega$, and this leads to the pressure P to be maximized. Maximizing the pressure with respect to z gives the variational equation for z

$$\int_v^\infty dv' (v-v') a(v', z) e^{-b(v', z)/2\xi'} \left[\left[\frac{2D_{-4}(z)}{D_{-3}(z)} - \frac{1}{z} \left(\frac{T}{T+v'} + 2 \right) \right] \right. \\ \left. - \frac{b(v', z)}{2\xi'} \left[\frac{D_{-4}(z)}{D_{-3}(z)} - \frac{2z^{-3}}{(T+v')} \right] \right] = 0 \quad (3-29)$$

If only the DOS is maximized, the variational equation reduces to setting the terms in the curly brackets equal to zero. It should be noted that the variational equation (3-29) results from using the DOS in eq.(3-24) which is obtained from using only the leading term in the expansion of the parabolic cylinder function [see Appendix B] in eq.(3-23).

3.6 Numerical results for the tail DOS

The expression in eq.(3-24) for the tail DOS has been derived using two approximations to the full expression of DOS, retaining only the contribution from the electronic ground states and using only the leading term in the expansion of the parabolic cylinder function [see Appendix B]. We [Sa-yakanit, Sritrakool, and Glyde(1982)] refer the result as the "deep tail approximation". We also simplify the variational expression in eq.(3-29) by writing it as a function of the well-known incomplete gamma function $\Gamma(a, y)$ as

$$\left[\frac{2}{z} - \frac{1}{4} \frac{D_4(z)}{D_3(z)} \right] \Gamma\left(\frac{7}{4}, y\right) + \left[\frac{3}{4} \frac{D_4(z)}{D_3(z)} - \frac{2}{z} - \frac{z^{-3}}{T+v} \right] \Gamma\left(\frac{5}{2}, y\right) = 0 \quad (3-30)$$

$$\text{where } y = b(v, z)/2 \xi' \quad (3-31)$$

$$\text{and } \Gamma(a, y) = \int_y^\infty ds s^{a-1} e^{-s} \quad (3-32)$$

In that paper we used the DOS in eq.(3-20) instead of (3-24) and included the term x^{-2} in the $D_p(x)$ expansion. The new variational equation for this case is

$$\begin{aligned} & \left[\frac{2}{z} - \frac{1}{4} \frac{D_4(z)}{D_3(z)} \right] \int_x^\infty dx' x' e^{-x'^2/4} D_{3/2}(x') \\ & + \left[\frac{3}{4} \frac{D_4(z)}{D_3(z)} - \frac{2}{z} - \frac{z^{-3}}{T+v} \right] \int_x^\infty dx' e^{-x'^2/4} D_{3/2}(x') = 0 \end{aligned} \quad (3-33)$$

$$\text{with } x = [b(v, z)/\xi']^{1/2} \quad (3-34)$$

We compare our result which will be called "the full ground-state DOS" to the results of the "deep tail approximation" and of Halperin and Lax in Fig.3.1 for a fixed potential fluctuation $\xi'=0.5$. Comparison numerical results for four values of ξ' are given in Tables 3.2 to 3.5. We can see from Fig.3.1 that our tail DOS is just a little higher than the previous result. This DOS will be joined with Kane's result at higher energies and the total DOS will be referred as SG's DOS in the future use.

3.7 DOS of Heavily Doped GaAs

Since Sa-yakanit and Glyde(1980a) have shown that their tail DOS crosses Kane's DOS, the DOS chosen for our work is the combination of these two DOS's. A mathematical representation is given by eq.(3-1).

For a pure GaAs crystal, the DOS's of the conduction and valence bands are assumed to be parabolic and to be separated by the energy gap E_g . Usually we set the valence band edge at $E_v=0$ and the conduction band edge at $E_c=E_g$. Hence the DOS's of the two bands are

$$\rho_c(E) = f_c (E-E_g)^{1/2} H(E-E_g) \quad (3-35)$$

and
$$\rho_v(E) = f_v (-E)^{1/2} H(-E) \quad (3-36)$$

where f_c and f_v are constants defined by eq.(3-6) with effective masses for the conduction and valence bands, respectively.

When GaAs becomes heavily doped the two band edges change to E'_v and E'_c because there is a rigid shift due to the average impurity potential. The reference points used for the determination of the DOS for this case are not the same as the zero points of the undoped case. Since the relative shift of both bands due to the averaged impurity potential is still unchanged [Fig.6.7A,B], we can use the band edges in case of the pure crystal as the reference points. In fact, the energy shift, E_x , is due not only to the average impurity potential but also the many-body interactions. This energy causes the bandgap shrunk to $E_g'=E_g-E_x$. The mechanisms of bandgap shrinkage are discussed by Auverge et al (1975), Berggren and Sernelius (1981) etc. Bandgap shrinkage is the effect of unequal shifts of energy bands. The valence band is assumed to be fixed

and the shift occurs only at the conduction band [Fig.6.7C]. The energy E_x for this case can be found only approximately. A rigorous treatment of many-body effects must be taken into account to get a better value of E_x . Another fact is that, we are considering an interband absorption attributed to the relative energy between the two bands thus the absorption will change only if the band separation is changed. For these reasons we will use the band edges for the pure crystal as our reference points.

To obtain the DOS of heavily doped GaAs, we must calculate self-consistently the screening constant Q (and the Fermi energy) for a given doping concentration. In our work we choose concentrations similar to those used by Casey and Stern(1976) to determine the DOS's in both bands for the absorption calculation. In fact, there are three degenerate valence bands, the heavy-hole band, the light-hole band and the split-off band. The last one is ignored because of the small contribution it makes to the absorption in the energy range being considered. The light-hole band is claimed by many authors to contribute about one third but actually the contribution depends upon the energy range being considered. In Figs.3.2 and 3.3 we display the DOS's for the conduction and valence bands using Sa-yakanit and Glyde's theory compared to the parabolic bands. The value of Q is obtained from a self-consistent calculation.

3.8 Comparison of the SG DOS to Experiment

It is well known that the only experiment that directly reflects the DOS of heavily doped GaAs is deduced from Schottky junction tunnelling

experiment done by Mahan and Conley (1967). As far as we know, since Halperin and Lax (1966) published their paper, there has been only one comparison made with theoretical prediction [Takeshima (1983)]. Takeshima compared his DOS which was derived using the Green function method with the experiment. It seems to be a fairly good fit although his DOS is shown to be greater than the Kane DOS which is well known to overestimate the tail DOS.

We calculate self-consistently the value of the screening constant for $p = 9.9 \times 10^{18} \text{ cm}^{-3}$ at $T = 4.2 \text{ K}$, which is the temperature at which the experiment was done, using a parabolic DOS. It will be seen later in chapter 4 that the Q value is not very sensitive to the choice of a DOS used. If we need to obtain an accurate value of the Fermi energy, we should use the DOS with a tail rather than the parabolic DOS. This can be seen from our results tabulated in Tables 4.2 to 4.7. We also determine the Q value at room temperature in order to see a reasonable value compared to those calculated at room temperature [Table 4.1]. The Q values and other quantities involved for $p = 9.9 \times 10^{18} \text{ cm}^{-3}$ at $T = 4.2 \text{ K}$ and 297 K are shown in Table 3.1.

SG's and the parabolic DOS's in arbitrary units are compared to Mahan and Conley's experimental one in Fig. 3.4. We may wonder why the SG DOS give similar results to that of Takeshima which is much larger than the Kane one. We explain this by including the Kane DOS in to Fig. 3.4 and plotting in a semilog graph [Fig. 3.5]. It can be seen in Fig. 3.5 that the difference between Kane's DOS and SG's DOS can be observed in a very deep tail region only. This difference, of course, cannot easily be seen

in linear scales. We may conclude that when Q is smaller (less screening) SG's, Kane's, and Takashima's DOS's should approach to the same limit.

CHAPTER 4

Screening Constant and Fermi Energy

4.1 Overview

An increase in the impurity doping concentration is obviously accompanied by an increase in the number of free charge carriers. The interaction between them can be significant. One of the effects is the screening of the fields of the impurity atoms by the free charges. The potentials of the impurity atoms become short-range. The screening effect is generally characterized by the screening constant Q which increases with increasing impurity concentration. Wolff(1962a,b) has shown that the electron-electron interaction can be ignored provided the impurity potential is to be screened by all charges in the system. The electron-electron interaction included into the screening constant which characterizes the decay of the Coulomb potential of an impurity.

It is well known for an intrinsic semiconductor that its chemical potential at absolute zero temperature is in the middle of its energy gap. When the semiconductor becomes extrinsic, by having a number of impurities, the Fermi energy will adjust itself to a new equilibrium value. Donor impurities which have positive ions compared to the host medium tend to increase the Fermi energy while acceptor impurities tend to lower the Fermi energy. Therefore the Fermi energy as well as the screening constant vary as the impurity concentration. The screening is assumed to be linear, i.e. the potential at any position is given by a superposition of individually screened impurity potentials. Thomas-Fermi

approximation is then used to obtain the screening constant and the Fermi energy self consistently. This approximation is valid provided that the potential fluctuation is small compared to the Fermi energy [Halperin and Lax (1966)].

Since SG's DOS is a little larger than HL's DOS, we [Sritrakool, Glyde, and Sa-yakanit (1982)] use SG's DOS to calculate the Fermi energy and the screening constant for n type GaAs as a function of net doping concentrations in order to see if the results differ greatly from Hwang(1970a,b)'s calculation which is obtained using HL's DOS. Our results turn out to agree well with his results and do not show much difference. We notice that the Fermi energy and the screening constant in n type GaAs are not sensitive to the band tail DOS.

Casey et al (1975) reported some experimental results for absorption coefficients for both n type and p type GaAs and in the following year Casey and Stern(1976) tried to work out a theoretical prediction to fit the experimental results. They used HL's DOS to determine the absorption coefficient. Since Halperin and Lax's DOS was given by a numerical table which was not convenient in the absorption coefficient calculation, they then employed Kane's DOS but adjusted the Kane single parameter until the Kane DOS fitted to HL's DOS in the deep tail region. The prediction resulted with unsatisfactory results for p type and fair results for n type.

Since we want to use SG's DOS to determine theoretically the same thing as what Casey and Stern did, the screening constant needed for the DOS must be determined first. We use the values of doping

concentrations given by Casey and Stern in our calculation in order to compare our results with theirs at the end. The linear screening suggested by Halperin and Lax is employed in this calculation. We use two sets of effective masses, one is the same as used by Casey and Stern and the other is from Ehrenreich(1963)'s work, in order to see the variation in effective masses chosen. The results are compared with those calculated using Kane's DOS and using parabolic DOS in order to see the variation on the DOS used.

In the following sections we will explain the model used, the Thomas-Fermi approximation for linear screening, the self consistent calculation for the Fermi energy and the screening constant, our results for n type GaAs, and lastly the results needed for the absorption coefficient calculation. 

4.2 The Model

Heavily doped semiconductors are a specific example of a disordered system. A heavily doped semiconductor is composed of a pure semiconductor crystal and high concentration of donors and/or acceptors which are assumed to be randomly distributed throughout the pure crystal whose medium has a constant static dielectric function. Donor ions have positive charges relative to the host medium while acceptors ions have negative charges. An electron sees this random impurity potential field. When the impurity concentration is high, the potential fluctuations will be large and must be taken into account. The potential fluctuations can form non-local potential wells so that there exists some localized states in these wells. These localized states are the states in the energy band tail.

Many basic approximations made at the beginning are the Born-Oppenheimer approximation, the adiabatic scheme, Koopmans' theorem, and the one-electron approximation. The details of these approximations are described in many standard textbooks. Many-body effects such as correlation and exchange interactions are taken care of by the screening effect. The system is simplified by the one-electron approximation and the Hamiltonian for the electron with effective mass m_e in the conduction band is

$$H = -\frac{\hbar^2 \nabla^2}{2m_e} + E_c + E_0 + V(\vec{r}) \quad (4-1)$$

where E_c is the conduction band edge of a pure semiconductor, $V(\vec{r})$ is the potential fluctuation at $\vec{r}$ about the average potential energy E_0 . $V(\vec{r})$ is the total impurity potential, measured away from its average value, i.e.

$$V(\vec{r}) = \sum_i v(\vec{r}-\vec{R}_i) - E_0 \quad (4-2)$$

$$\text{with } v(\vec{r}-\vec{R}) = \frac{-e^2}{\epsilon_0 |\vec{r}-\vec{R}|} e^{-Q|\vec{r}-\vec{R}|} \quad (4-3)$$

$\vec{R}$ being an impurity position.

Let us suppose that our semiconductor is doped by N_D donors and N_A acceptors per unit volume. If N_D is larger than N_A , the semiconductor will become n type. We assume that all impurity atoms are completely ionized and compensated. At a finite temperature, electrons and holes will reach an equilibrium and will have a single Fermi energy. This Fermi energy can be determined if the neutrality condition of the system

is known. The electron concentration in the conduction band, n_c , plus the electron concentration in the donor levels, n_D , is equal to the electron concentration at $T = 0K$, $N_D - N_A$, plus empty states (or holes) in the valence band, p_v , and in the acceptor levels, p_a , i.e.

$$n_c + n_D = N_D - N_A + (p_v + p_a) \quad (4-4)$$

Since in heavily doped semiconductors, the impurity levels merge with their host bands, we may rewrite eq.(4-4) to be

$$N_D - N_A = n - p \quad (4-5)$$

where n is the electron concentration in the conduction band including its band tail, and p is the hole concentration in the valence band including its band tail. For a semiconductor with large energy gap, $E_g \gg k_B T$, minority carriers are small and negligible. Since GaAs has $E_g = 1.424 \text{ eV}$ at room temperature which is considered very large compared to the value .025 eV of $k_B T$, we approximate

$$n = N_D - N_A \quad (4-6 a)$$

$$\text{and } p = N_A - N_D \quad (4-6 b)$$

if we first assume N_A is greater than N_D . These are the neutrality conditions used to determine the Fermi energy.

For randomly distributed, statistically independent impurities, Halperin and Lax(1966) have shown that the mean square fluctuation in $V(\vec{r})$ reduces to

$$\xi \equiv \langle V(\vec{r}) V(\vec{r}) \rangle = (N_A + N_D) \int_{\Omega} \frac{d\vec{R}}{\Omega} [V(\vec{r} - \vec{R})]^2$$

$$= \frac{2\pi e^2}{Q \epsilon_0^2} (N_A + N_D) \quad (4-7)$$

and the average potential E_0 can be written as

$$E_0 = \frac{4\pi e^2}{\epsilon_0 Q^2} (N_A - N_D) \quad (4-8)$$

Since it is clear that impurity ions change the value of potential seen by an electron, the average impurity potential will cause a rigid shift of DOS's in both bands in such a way that the energy gap remains unchanged. The shift was depicted by Panish and Casey(1967), for instance. However, the many-body interaction among electrons can cause the DOS shift as well but it is not taken into account in our work.

4.3 Thomas-Fermi Approximation

The screening has taken care of both exchange and correlation interactions. Our system is treated as an electron gas in the screened Coulomb potential fields of the impurity ions and embedding in their host medium which has a constant static dielectric function. The system is then assumed to have a new dielectric function which is the effect of the perturbation of the impurity ions and the many-body interactions. The new dielectric function as a function of the wave vector and the frequency of the perturbation can be determined by the well-known Lindhard's expression. After considering only the effect of a static perturbation and assuming the perturbing wave vector $\vec{q}$ go to zero, we have the dielectric function at zero frequency to be [Ziman(1972)]

$$\epsilon(\vec{q}, \omega=0) = 1 + \frac{4\pi e^2}{\epsilon_0 q^2} \int_{-\infty}^{\infty} \rho(E) \left(-\frac{\partial f(E)}{\partial E} \right) dE \quad (4-9)$$

(4-10)

where $f(E)$ is the Fermi-Dirac distribution function. Hence the screening constant Q satisfies the equation

$$Q^2 = \frac{4\pi e^2}{\epsilon_0} \int_{-\infty}^{\infty} \rho(E) \left(-\frac{\partial f(E)}{\partial E} \right) dE \quad (4-11)$$

It should be noted that the spin degeneracy must also be included in the DOS. The expression (4-9) is obtained using perturbation theory. The same result can be found using Thomas-Fermi approximation which first takes into account the change of the local electron density due to the perturbing potential. The change in the local electron density will give rise to a local potential which must satisfy Poisson's equation. This local potential turns out to be the screened Coulomb potential provided the ions are assumed to behave like point charges. Therefore this approximation is obviously not valid at a very high impurity concentration where the ions are too close together to be assumed to be point charges. Halperin and Lax(1966) describe the condition for the validity in terms of the difference of the Fermi energy and the potential fluctuation. Since both physical quantities are functions of doping concentration, the validity can then be described as a function of the doping concentration.

4.4 Determination of Screening Constant and Fermi Energy

Since the screening constant Q is a function of the DOS which in turn depends upon the screening constant, Q must be determined self consistently with the density of states. For an n-type semiconductor, we use the neutrality equation in eq.(4-6) and find the number of electrons per unit volume by integrating over all possible states in the conduction band, namely

$$N_D - N_A = \int_{-\infty}^{\infty} \rho_c(E) f(E) dE \quad (4-12)$$

A similar equation can be written for a p-type semiconductor [see eq.(4-15)]. The Fermi-Dirac distribution function can be written explicitly as

$$f(E) = \frac{1}{1 + \exp \left[(E - E_F) / k_B T \right]} \quad (4-13)$$

where E_F is the Fermi energy and $k_B T$ is the thermal energy.

We have to solve eqs.(4-11) with $\rho(E) = \rho_c(E)$ and (4-12) self-consistently for the screening length Q . We first assume a trial value of Q and then solve eq.(4-12) for the Fermi energy and use the Fermi energy to solve for a new Q by eq.(4-11). Q_0 is firstly assumed to be the value obtained by using the parabolic conduction band, namely

$$Q_0^2 = \frac{4\pi e^2}{\epsilon_0 \hbar^2} \left[\frac{3(N_D - N_A)}{\pi} \right]^{1/3} \quad (4-14)$$

The new Q is then re-entered as Q_0 and the process will be repeated until Q is equal to Q_0 in a certain accuracy needed. For a p-type semiconductor, the number of holes satisfies the equation

$$N_A - N_D = \int_{-\infty}^{\infty} \rho_v(E) f_h(E) dE \quad (4-15)$$

where $f_h(E)$ is the Fermi function for holes defined by

$$f_h(E) = 1 - f(E) \quad (4-16)$$

If we now consider the valence and the conduction bands simultaneously, the total screening contributed by carriers in all bands is just the sum of the contribution from each band. Halperin and Lax(1966) give a relation for the total screening constant Q to be

$$Q^2 = \sum_j Q_j^2 \quad (4-17)$$

where Q_j is the contribution from band j , calculated according to the formula (4-11). Since GaAs has a single conduction band and three degenerate valence bands, a heavy-hole band, a light-hole band and a split-off band, there are three bands altogether to consider except the split-off band. The split-off band contributes very little to the absorption. Using the neutrality condition in eq.(4-6), we simply have the number of holes per unit volume

$$p = \sum_i \int_{-\infty}^{\infty} \rho_{vi}(E) f_h(E) dE \quad (4-18)$$

where i indicates all valence bands being considered. Similarly, the equation for the screening constant contributed by holes is

$$Q_h^2 = \sum_i \frac{4\pi e^2}{\epsilon_0} \int_{-\infty}^{\infty} \rho_{vi}(E) \left(-\frac{\partial f_h(E)}{\partial E} \right) dE \quad (4-19)$$

Eqs.(4-18) and (4-19) must be solved self-consistently for Q and E_F .

4.5 Results for N Type GaAs

We [Sritrakool, Glyde, and Sa-yakanit (1982)] determined the screening constant Q and the Fermi energy E_F of GaAs using eqs.(4-11) and (4-12). The DOS used in the calculation is in eq.(3-1) but $\rho_i(E)$ was chosen to be eq.(3-24) which is valid in the deep tail region only. The purpose was to test SG's DOS if it could affect those two physical quantities greatly and to compare with the result with non-compensation of Hwang(1970a,b). The calculation was done at three temperatures, 20K, 77K, and 300K, and for three compensation ratios, 0.0, 0.2, and 0.4. The compensation ratio is defined as N_A/N_D for n-type semiconductors, and N_D/N_A for p-type semiconductors.

The results for Fermi energies as a function of net carrier concentration at those three different temperatures, compared with the results using Kane's DOS alone, are displayed in Figs.4.1 to 4.3 for three compensation ratios. Since Thomas-Fermi approximation is valid only when the potential seen by an electron is slowly-varying (or small potential fluctuation) compared to the Fermi energy, the result at each temperature is valid above the root mean square of the potential fluctuation which is represented by a dotted line. From these figures, we may determine a minimum net concentration at each temperature at which $\xi^2 = E_F - E_c$. The minimum net concentration at each temperature and at each compensation ratio is tabulated in Table 4.1. The results for screening lengths as a function of net carrier concentration at those three temperatures, compared with the classical Debye screening length

$$Q^{-1} = \left(\frac{\epsilon_0 k_B T}{4\pi e^2} \right)^{1/2} (N_A - N_D)^{-1/2} \quad (4-20)$$

are depicted in Figs.4.4 to 4.6 for three compensation ratios.

When the net carrier concentration is kept constant while the compensation ratio changes, the DOS's for valence and conduction bands vary as a function of total doping concentration. Since the DOS in the tail region increases as a function of doping concentration [Serre et al (1981)], Fermi energies (at the same temperature and same net carrier concentration) may be lowered when the compensation ratio is increased. This variation of the Fermi energy on the compensation ratio may be observed by comparing Figs.4.1 4.2 and 4.3. For instance, at $N_D - N_A = 10^{17} \text{ cm}^{-3}$ and at 20K, the Fermi energy is lowered when the

compensation ratio increases. The variation of $\bar{Q}^{-1}$ on compensation ratios can also be seen from those figures. It is easy to see that the screening length $\bar{Q}^{-1}$ is varied as a function of compensation ratio. The relation between E_F and Q is given in the expression for Thomas-Fermi screening constant given in eq.(4-11). Since, at $T=0K$, the derivative of Fermi function $\partial f/\partial E$ becomes a Dirac delta function and Q is a function of DOS evaluated at the Fermi energy, Q is decreased as a function of compensation ratio. Thus the screening length $\bar{Q}^{-1}$ is increased as a function of compensation ratio.

4.6 Results Needed for Absorption Coefficient

We isolate these results from above because they are later found using a little different DOS and different doping concentrations. The doping concentrations are chosen the same as those used by Casey and Stern(1976) in their work on absorption coefficient of heavily doped GaAs. The purpose is to compare our absorption coefficient results with theirs.

The DOS used in our calculation is again eq.(3-1) but $\rho_1(E)$ is now the full ground state DOS given by eq.(3-20) instead of the deep tail DOS in eq.(3-24). Eq.(3-20) is valid at higher energies than the eq.(3-24) since higher terms have been included. The calculation is done for both p and n type GaAs using SG's DOS [eq.(3-1)], Kane's DOS [eq.(3-26)], and parabolic DOS [eq.(3-4)]. We also do calculations for two sets of effective masses in order to see the variation on chosen effective masses. The first set is the same as that chosen by Casey and Stern, namely $m_e=0.066$, $m_{hh}=0.55$, and $m_{hl}=0.085$ in the unit of free

electron mass. They are the effective masses for an electron in the conduction band, for a heavy hole, and for a light hole respectively. The other set is taken from Ehrenreich(1963)'s result. They are $m_e=0.072$, $m_{hh}=0.68$, and $m_{hl}=0.12$.

The results are presented in Tables 4.2 to 4.7 for different DOS's and for different effective masses. The Fermi energy is measured with respect to the conduction band edge E_c in n type GaAs and to the valence band edge E_v in p type GaAs. Since the calculation in p type GaAs is done for empty states, the energy scale must be reversed when the Fermi energy is used in the absorption calculation. The value of potential fluctuation, ξ^k , is also tabulated for each pair of doping concentration. v_F is the dimensionless Fermi energy defined the same way as v , i.e. $v_F = (E_c - E_F)/E_Q$ in n type GaAs or $(E_v - E_F)/E_Q$ in p type GaAs.

CHAPTER 5

Matrix Element of Transition

5.1 Overview

The matrix element of transition defined in eq.(2-12) is obviously a function of the interaction Hamiltonian and the wave functions of initial and final states. Since the real wave function of an electron in a solid may not be found exactly, it is always evaluated using a model. Even for a GaAs crystal, the band structure is complicated and the DOS's of both valence and conduction bands do not have perfect parabolic shapes as in the theory. The interband absorption calculated by assuming the two parabolic bands is just an approximate result. For a better interband absorption calculation one must take into account the band structure.

Before the advent of heavily doped semiconductors, people were interested in lightly doped semiconductors and studied the matrix element of transition between a single localized state to a delocalized state. The localized state for an acceptor level in GaAs was first assumed by Eagles(1960) in a hydrogenic form. This form was used by Dumke(1963) for both donor and acceptor levels. This simple matrix element of transition obviously cannot be applied to a more complicated problem like heavily doped semiconductors. Our interest is focused on finding a matrix element of transition which is physically reasonable in order to predict the absorption coefficient correctly.

The wave function of an electronic state near a band edge is written as a Bloch periodic function at that energy band edge modulated by a slowly varying wave function, an envelope function, by means of the effective mass theory given by Kohn(1957). This idea is well-known and has been used by many authors [Lasher and Stern(1964), Stern(1971), Casey and Stern(1976)]. The matrix element of transition can then be split independently into two parts. One consists of initial and final Bloch functions with the momentum operator and the other is composed of initial and final envelope functions without any operator. The first one is known as Kane's matrix element which is well known and almost constant for most III-V semiconductors. The latter is then called the envelope matrix element. The momentum operator appears only in Kane's matrix element because of the slowly varying assumption of the envelope function. This matrix element between p-like and s-like Bloch periodic functions has been obtained by Kane(1957) in his work on InSb crystal. Casey and Stern assumed an envelope function of hydrogenic form and with it they could determine the matrix element of transition for heavily doped GaAs analytically.

We assume an envelope function of gaussian form since the DOS is determined using harmonic wells and the ground state wave function of a harmonic well is a gaussian wave function [see Appendix A]. We can find a simple analytic expression for the transition matrix element which can be reduced to the matrix element between two delocalized states correctly. The parameter z used in our envelope function is determined directly from the variational calculation done in the DOS calculation and cannot be freely adjusted. The localized parameter used by Casey

and Stern for the hydrogenic envelope function was determined by a judgement of counting the number of states.

In the following sections, we will briefly review the basic concept of finding the matrix element of transition for heavily doped semiconductors; the matrix elements given by Kane, Eagles, Casey and Stern. Lastly, our matrix element will be presented and discussed.

5.2 Basic Concept

It has been shown by Kohn(1957) that a state near a band extremum can be written as a Bloch periodic function at the extremum modulated by a slowly varying envelope function provided there is only one extremum. This can be applied to the case of GaAs crystal which has one conduction band minimum and one valence band minimum at $\vec{k}=0$ direction. An impurity state, either a donor or an acceptor state, for a heavily doped GaAs can then be written as the modulation between the Bloch periodic function at $\vec{k}=0$, $u_0(\vec{r})$, and the envelope function, $\phi(\vec{r})$

$$\psi(\vec{r}) = \phi(\vec{r})u_0(\vec{r}) \quad (5-1)$$

with normalizations

$$\frac{1}{\Omega} \int |u_0(\vec{r})|^2 d\vec{r} = 1 \quad (5-2)$$

and

$$\int |\phi(\vec{r})|^2 d\vec{r} = 1 \quad (5-3)$$

If we have a transition from a state in the valence band to a state in the conduction band, and if both states can be represented by wave functions like eq.(5-1), the matrix element of transition which is essentially the overlap of the two wave functions by the momentum operator is

$$M = \frac{1}{\Omega} \int \phi_c^*(\vec{r}) u_c^*(\vec{r}) \nabla [\phi_v(\vec{r}) u_v(\vec{r})] d\vec{r} \quad (5-4)$$

where c and v indicate the conduction and valence bands respectively. The subscript "0" of $u_0(\vec{r})$ has been ignored for our writing convenience. The integration in eq.(5-4) can be split out into two integrals. By assuming that the envelope functions are slowly varying, they can be taken out of the integrals. The summation over all impurity sites is then approximated by an integral over all crystal. This gives the expression

$$M = \int \phi_c^*(\vec{r}) \phi_v(\vec{r}) d\vec{r} \cdot \frac{1}{\Omega} \int u_c^*(\vec{r}) \nabla u_v(\vec{r}) d\vec{r} + \int \phi_c^*(\vec{r}) \nabla \phi_v(\vec{r}) d\vec{r} \cdot \frac{1}{\Omega} \int u_c^*(\vec{r}) u_v(\vec{r}) d\vec{r} \quad (5-5)$$

Using the fact that $u_c(\vec{r})$ and $u_v(\vec{r})$ are orthogonal in III-V semiconductors, the last term in eq.(5-5) vanishes and eq.(5-5) can then be written as

$$M = M_b M_{env} \quad (5-6)$$

by defining

$$M_b = \frac{1}{\Omega} \int u_c^*(\vec{r}) \nabla u_v(\vec{r}) d\vec{r} \quad (5-7)$$

$$\text{and } M_{env} = \int \phi_c^*(\vec{r}) \phi_v(\vec{r}) d\vec{r} \quad (5-8)$$

5.3 Kane's Matrix Element

Kane(1957) derived a matrix element of interband transition between p-like and s-like Bloch functions in his work on InSb using his well known k.P theory. The matrix element M_b mentioned earlier here is the Kane matrix element at $\vec{k}=0$ direction. In order to use the matrix element in eq.(5-6) with the absorption coefficient calculation, we square and average it over all spins and directions to get

$$\langle M^2 \rangle = |M_{env}^2| \langle M_b^2 \rangle \quad (5-9)$$

$$\text{with } \langle M_b^2 \rangle = m_e^2 P^2 / 6\hbar^2 = \frac{m_0^2 E_g}{12m_e} \left[\frac{E_g + \Delta}{E_g + 2\Delta/3} \right] \quad (5-10)$$

where P is the interband matrix element given by Kane(1957), E_g is the energy gap and Δ is the spin-orbit splitting. The approximate value in eq.(5-10) was first derived for a pure InSb crystal. For GaAs at room temperature, $E_g = 1.424\text{eV}$, $\Delta = 0.33\text{eV}$.

In order to see the role of the envelope matrix element, we keep $\langle M_b^2 \rangle$ constant and consider the envelope matrix element M_{env}^2 in many cases.

5.4 Eagles' Matrix Element

Eagles(1960) assumed the envelope function of an acceptor in a hydrogenic form

$$\phi_v(\vec{r}) = (\pi a^3)^{-1/2} e^{-|\vec{r}-\vec{r}_i|/a} \quad (5-11)$$

where a is the effective Bohr radius of the acceptor and $\vec{r}_i$ is the center of an acceptor.

The envelope matrix element between the localized acceptor state and a delocalized state in the conduction band is equivalent to a Fourier transform of that localized state, i.e.

$$M_{\text{env}} = \frac{1}{\Omega^{\frac{1}{2}}(\pi a^3)^{\frac{1}{2}}} \int e^{-|\vec{r}-\vec{r}_i|/a} e^{i\vec{k}_c \cdot \vec{r}} d\vec{r} \quad (5-12)$$

$$|M_{\text{env}}|^2 = \frac{64\pi a^3 \Omega^{-1}}{(1+a^2 k_c^2)^4} \quad (5-13)$$

When the k-dependent term is neglected the rest of the matrix in eq.(5-13) is referred to as a "constant matrix element" which has the order of magnitude about a sphere with radius of a.

5.5 Casey and Stern's Matrix Element

Stern(1971) studied the optical absorption of amorphous Si and proposed an envelope function for all states of the form

$$\phi(\vec{r}) = (\beta^3/\pi)^{\frac{1}{2}} \exp(i\vec{k} \cdot \vec{r}) \exp(-\beta|\vec{r}-\vec{r}_i|) \quad (5-14)$$

to determine the matrix element of interband transitions using the same idea mentioned in section 5.2. The energy-dependent parameter, β and k , are determined in an arbitrary manner for each band. Consider the conduction band as an example. Let $\rho_{\text{pc}}(E)$ be the parabolic DOS of a pure crystal. For each state at energy E' in a heavily doped semiconductor there is an associated state in a pure crystal at energy E^* , which satisfies

$$\int_{E_c}^{E^*} \rho_{\text{pc}}(E) dE = \int_{-\infty}^{E'} \rho_c(E) dE \quad (5-15)$$

Then k is assigned the value in the doped case of

$$\frac{\hbar^2 k^2}{2m_e} = E^* - E_c \quad (5-16)$$

and β is determined by the apparent lowering of the conduction band state due to disorder by

$$\frac{\hbar^2 \beta^2}{2m_e} = \lambda(E^* - E') \quad (5-17)$$

where $\hbar^2 \beta^2 / 2m_e$ is the kinetic energy of localization of the deep tail states and λ is a parameter which assures that the kinetic energy coincides with the kinetic energy obtained by Halperin and Lax at the energy where $\rho_c(E)$ is fitted to their DOS. Casey and Stern's envelope matrix element is

$$|M_{env}|^2 = (64\pi b/3)(t^4 - q^4)^{-5} [(b^4 - 5b^2 B^2 + 5B^4)(3t^4 + q^4)(t^4 - q^4)^2 + 8b^2 B^2 t^2 (3b^2 - 10B^2)(t^8 - q^8) + 16b^4 B^4 (5t^8 + 10t^4 q^4 + q^8)] \quad (5-18)$$

where $B = \beta_c \beta_v$, $b = \beta_c + \beta_v$, $t^2 = b^2 + k_c^2 + k_v^2$ and $q^2 = 2k_c k_v$. The subscripts c and v again denote the conduction and valence bands respectively.

5.6 Present Matrix Element

If the envelope wave functions for both bands are assumed to be plane-wave, i.e.

$$\phi_{kc}(\vec{r}) = \frac{1}{\Omega^{1/2}} e^{i\vec{k}_c \cdot \vec{r}} \quad (5-19)$$

$$\text{and } \phi_{kv}(\vec{r}) = \frac{1}{\Omega^{1/2}} e^{i\vec{k}_v \cdot \vec{r}} \quad (5-20)$$

the envelope matrix element is

$$M_{env}^2 = \frac{(2\pi)^3}{\Omega} \delta(\vec{k}_c - \vec{k}_v) \quad (5-21)$$

which implies direct interband transitions with momentum conservation.

Since SG's DOS is obtained by modelling impurity-fluctuation wells by harmonic wells and the model gives gaussian wave functions [see Appendix A], our envelope function is assumed to be of a gaussian form instead of a hydrogenic form. The envelope functions for the valence and conduction bands are

$$\phi_v(\vec{k}_v, \vec{r}) = (2\alpha/\pi)^{3/4} e^{i\vec{k}_v \cdot \vec{r}} e^{-\alpha |\vec{r} - \vec{r}_i|^2} \quad (5-22)$$

$$\phi_c(\vec{k}_c, \vec{r}) = (2\beta/\pi)^{3/4} e^{i\vec{k}_c \cdot \vec{r}} e^{-\beta |\vec{r} - \vec{r}_j|^2} \quad (5-23)$$

where the localization parameters α and β are related to the variational parameters z_v and z_c by the relations $\alpha = Q^2/2z_v^2$ and $\beta = Q^2/2z_c^2$. The only energy dependent parameter is the wave vector $\vec{k}$. The envelope matrix element using the definition in eq.(5-8), is then

$$M_{env} \sim \int e^{-i(\vec{k}_c - \vec{k}_v) \cdot \vec{r}} e^{-\alpha |\vec{r} - \vec{r}_i|^2} e^{-\beta |\vec{r} - \vec{r}_j|^2} d\vec{r} \\ \sim \left(\frac{\pi}{\alpha + \beta}\right)^{3/2} e^{-(\alpha \vec{r}_i^2 + \beta \vec{r}_j^2)} e^{[i(\vec{k}_c - \vec{k}_v) + 2(\alpha \vec{r}_i + \beta \vec{r}_j)]^2 / 4(\alpha + \beta)} \quad (5-24)$$

where the normalized factors of the envelope functions are temporarily ignored. The centers of the envelope functions are assumed to be at different positions, $\vec{r}_i$ and $\vec{r}_j$. The result in eq.(5-24) is obtained by using the integration formula

$$\int_{-\infty}^{\infty} e^{ax^2 + bx} dx = (\pi/-a)^{1/2} e^{-b^2/4a} \quad (5-25)$$

The magnitude of M_{env} squared is

$$|M_{\text{env}}|^2 \sim \left(\frac{\pi}{\alpha+\beta}\right)^3 e^{-\frac{(\vec{k}_c - \vec{k}_v)^2}{2(\alpha+\beta)}} e^{-\frac{2\alpha\beta}{\alpha+\beta} (\vec{r}_i - \vec{r}_j)^2} \quad (5-26)$$

Since we are concerned with a random system, we must average the result over all random positions $\vec{r}_i$ and $\vec{r}_j$. If $A(\vec{r}_i, \vec{r}_j)$ is the quantity to be averaged, the average will be

$$\langle A(\vec{r}_i, \vec{r}_j) \rangle_{\vec{r}_i, \vec{r}_j} = \int_{\Omega} \frac{d\vec{r}_i}{\Omega} \int_{\Omega} \frac{d\vec{r}_j}{\Omega} A(\vec{r}_i, \vec{r}_j) \quad (5-27)$$

The result after averaging eq.(5-26) is

$$\langle |M_{\text{env}}|^2 \rangle_{\vec{r}_i, \vec{r}_j} \sim \frac{1}{\Omega} \left(\frac{\pi}{\alpha+\beta}\right)^3 e^{-\frac{(\vec{k}_c - \vec{k}_v)^2}{2(\alpha+\beta)}} \left[\frac{\pi(\alpha+\beta)}{2\alpha\beta} \right]^{3/2} \quad (5-28)$$

The orientations of wave vector $\vec{k}_c$ and $\vec{k}_v$ are random and the angle between them is assumed to be θ . We must also average over this angle or practically over the cosine of this function, i.e.

$$\langle |M_{\text{env}}|^2 \rangle_{\vec{r}_i, \vec{r}_j, \cos\theta} = \frac{1}{2} \int_{-1}^1 d\cos\theta \langle |M_{\text{env}}|^2 \rangle_{\vec{r}_i, \vec{k}_j} \quad (5-29)$$

$$\sim \frac{1}{\Omega} \left(\frac{\pi}{\alpha+\beta}\right)^3 \left(\frac{\pi(\alpha+\beta)}{2\alpha\beta}\right)^{3/2} e^{-\frac{(k_c^2 + k_v^2)}{2(\alpha+\beta)}} \left(\frac{\alpha+\beta}{k_c k_v}\right) \sinh\left(\frac{k_c k_v}{\alpha+\beta}\right) \quad (5-30)$$

We re-introduce the normalization factors into eq.(5-30) and call the left hand side as

$$\bar{M}_{\text{env}}^2 = \frac{1}{\Omega} \left(\frac{2\pi}{\alpha+\beta}\right)^{3/2} \left(\frac{\alpha+\beta}{k_c k_v}\right) \sinh\left(\frac{k_c k_v}{\alpha+\beta}\right) e^{-\frac{(k_c^2 + k_v^2)}{2(\alpha+\beta)}} \quad (5-31)$$

This is the envelope matrix element used in our work.

To see the asymptotic behavior of $\bar{M}_{\text{env}}^2$ when both localized parameters, α and β , approach zero, we write $\sinh$ in an exponential form and take the limits for α and β to zero:

$$\lim_{\alpha, \beta \rightarrow 0} \bar{M}_{\text{env}}^2 = \lim_{\alpha, \beta \rightarrow 0} \frac{1}{\Omega} \left(\frac{2\pi}{\alpha+\beta}\right)^{3/2} (1 + e^{-2k_c k_v / (\alpha+\beta)}) e^{-\frac{(k_c - k_v)^2}{2(\alpha+\beta)}}$$

$$= \frac{2\pi^2 \delta(k_c - k_v)}{\Omega k_c k_v} \quad (5-32)$$

One of many delta function representations [Baym(1973)]

$$\delta(k_c - k_v) = \lim_{\alpha, \beta \rightarrow 0} (2\pi(\alpha + \beta))^{-1/2} e^{-(k_c - k_v)^2 / 2(\alpha + \beta)} \quad (5-33)$$

has been used to get the above result. The delta function $\delta(k_c - k_v)$ can be related to $\delta(\vec{k}_c - \vec{k}_v)$ by the relation [Jackson(1975)]

$$\delta(\vec{k}_c - \vec{k}_v) = \frac{1}{k_c^2} \delta(k_c - k_v) \delta(\phi - \phi') \delta(\cos\theta - \cos\theta') \quad (5-34)$$

If the distributions of $\vec{k}_c$ and $\vec{k}_v$ are spherically symmetric, we simply have

$$\delta(\vec{k}_c - \vec{k}_v) = \frac{4\pi}{k_c^2} \delta(k_c - k_v) \quad (5-35)$$

under the integration over all either $\vec{k}$ space. This leads the matrix $\bar{M}_{env}^2$ to

$$\lim_{\alpha, \beta \rightarrow 0} \bar{M}_{env}^2 = \frac{(2\pi)^3}{\Omega} \delta(\vec{k}_c - \vec{k}_v) \quad (5-36)$$

which is the case when we have only plane-wave states. The result is exactly the same as that given in eq.(5-11).

To see the limit of our matrix element when a localized state ($\alpha \neq 0, k_v = 0$), reverts to a delocalized state ($\beta = 0, k_c \neq 0$), $\bar{M}_{env}^2$ is reduced to

$$\bar{M}_{env}^2 = \frac{1}{\Omega} \left(\frac{2\pi}{\alpha}\right)^{3/2} e^{-k_c^2 / 2\alpha} \quad (5-37)$$

If the k dependence in eq.(5-37) is removed, the matrix will be

$$\bar{M}_{env}^2 = \frac{1}{\Omega} \left(\frac{2\pi}{\alpha}\right)^{3/2} = \frac{1}{\Omega} 64\pi \pi^{1/2} (z_v / 2Q)^3 \quad (5-38)$$

and can be compared to Eagles' matrix element given in eq.(5-13).

5.7 Determination of Needed Parameters

The problem left is how to determine k_c and k_v correctly. According to Anderson(1958)'s theory of localization and the recent theory of Phillips(1983), the change of localized states to delocalized in disordered systems is sudden instead of continuous. This means that both kinds of states are separated by a conventional energy level called the "mobility edge". At the "mobility edge" we suppose the wave vector k to start from 0. If we have a transition from a localized state to a delocalized state we will have the matrix element

$$\bar{M}_{env}^2 = \frac{1}{\Omega} \left(\frac{2\pi}{\alpha+\beta} \right)^{3/2} \quad (5-39)$$

characterized by the two localized parameters only. However, the "mobility edge" is still a very difficult quantity to determine exactly so that we will use the "mobility edge" as an adjusting parameter when we determine the absorption coefficient.

In this work we assume that the "mobility edges" of conduction and of valence bands are at their band edges before doping, namely E_c and E_v respectively. The states in the band tails are all localized, shaded areas in Fig.5.1A, and have all k 's equal to zero. The unshaded areas represent all delocalized states that have parabolic $E-k$ dispersion relationships like free electrons [Fig.5.1B].

Since the values of the parameter z calculated from SG's theory are well defined in the tail regions only and they are needed for

calculating the matrix element at high energies, a linear extrapolation is then made for each band by means of the fact that the kinetic energy of localization vanishes at high energies, i.e. z tends to infinity at high energies. The value of z for each band before extrapolation is plotted against the energy in the band tail measured with respect to each corresponding band edge in Fig.5.2. The value of z for each band after extrapolation made is plotted in Fig.5.3.

CHAPTER 6

Optical Absorption

6.1 Overview

In this work, we are interested in the interband absorption near band edges only. The photon energy range used in our calculation is between 1.35 to 1.55 eV. This range covers the energy gap of a pure GaAs crystal of 1.424 eV at room temperature. Some experimental work on absorption coefficient has been done by Moss and Hawkins(1961), Sturge(1962). The theoretical work has been done by Callaway(1964). It has been shown that the absorption coefficient is dependent on the square root of the difference of the incoming photon energy and the energy gap, $(E_p - E_g)^{1/2}$, provided in the transition the momentum is conserved. This is, in fact, proportional to the joint DOS between the DOS's of two bands. In some cases like amorphous semiconductors, there is no periodicity and k cannot label all states, and in the transition the momentum is transferred through lattice vibration. The absorption coefficient is dependent on the square of $E_p - E_g$ [Mott and Davis(1979)] because the momentum is not conserved in the transition. More precisely, the momentum is conserved but the transition is phonon assisted.

When a GaAs crystal becomes heavily doped, some periodicity of the system is destroyed by substitutional impurities. Therefore the system is partially translationally invariant and the wave vector cannot label all states from the bottom of a band. The transitions between these bands are then expected to have a partial momentum conservation in the

sense mentioned above, i.e. we expect to have the absorption coefficient proportional to $(E_p - E_g)^s$ where s is between 1/2 and 2.

Experimental work on heavily doped semiconductors has been done by many workers [e.g. Hill(1964), Pankove(1965), Casey et al(1975)]. Stern(1971) assumed an envelope function of a hydrogenic form and determined successfully the absorption coefficient of amorphous Si. Casey and Stern(1976) applied this idea to heavily doped GaAs to predict its absorption coefficient and luminescence peak. The results for p type GaAs were unsatisfactory because at large energy their absorption coefficient was still a factor of 1.6 below the experimental value. The results for n type GaAs showed the Burstein shift correctly but the magnitude of each curve was still too small compared to the experimental result. In their calculation the Kane DOS was scaled until it fitted to HL's tail DOS.

Since the localized wave function from Sa-yakanit and Glyde's theory can be found simultaneously as the DOS at a particular energy, the matrix element can be obtained within the model. We want to test the dependence of $\alpha(\omega)$ on DOS and also to test whether the wave function that follows from Sa-yakanit and Glyde's theory in the matrix element leads to a reasonable $\alpha(\omega)$ on effective masses, bandgaps, and the "parameter" k determined by counting the number of occupied states [Casey and Stern(1976)] and by arbitrary choices of "mobility edges".

It should also be mentioned here that the bandgap shrinkage in a doped semiconductor due to many-body effects can shift the absorption coefficient greatly to the low photon energy side. Therefore a correct

value of a bandgap shrinkage is needed for a better prediction of an absorption coefficient curve. This bandgap shrinkage is well known as the shift due to exchange energy since the Coulomb interaction between electrons and impurity ions cause a rigid shift and the band separation remains the same [Halperin and Lax(1966), Panish and Casey(1967), Kane(1972), Inkson(1973)]. Bandgap shrinkage mechanism have been reviewed by many authors [Mahan(1980), Berggren and Sernelius(1981), etc.].

In the next section, we will briefly review the absorption with momentum conservation. Our work with and without the bandgap shrinkage will be presented and compared with experimental results in following sections. Effects of wave vector k and variational parameter z will be presented and discussed. Another section will be devoted to the discussion on bandgap shrinkage. Present absorption coefficient will be summarized. Lastly, an overall discussion will be given in the Epilogue.

6.2 Momentum Conserved Absorption

The matrix element for the transition with momentum conservation is the Dirac delta function of $(\vec{k}_c - \vec{k}_v)$ in eq.(5-21). If we substitute the matrix element of this special case into the expression for $\alpha(\omega)$ in eq.(2-23), we can have simply

$$\alpha(\omega) = \frac{4\pi^2 e^2}{m^2 c n \omega} \rho(\hbar\omega) [f(E_v) - f(E_v + \hbar\omega)] \langle M_b^2 \rangle \quad (6-1)$$

where $\rho(\hbar\omega)$ is the joint DOS linking a state with energy E_v and momentum $\vec{k}_v$ to a state with energy $E_c = E_v + \hbar\omega$ and momentum $\vec{k}_c = \vec{k}_v$. The interband absorption coefficient computed using eq.(6-1) is complete provided M_b^2 takes care the $\vec{k}$ dependence.

The transitions now occur at the same $\vec{k}$ obtained from the energy conservation relation

$$\hbar\omega = E_c(\vec{k}_c) - E_v(\vec{k}_v) \quad (6-2)$$

For a perfect crystal the DOS can be determined by finding the volume in $\vec{k}$ space divided by the volume occupied by a single state, i.e.

$$\rho(E) = k^2/2\pi^2(dE/dk) \quad (6-3)$$

By differentiating eq.(6-2) and using eq.(6-3) we can express the joint DOS in terms of the DOS's at initial and final energies

$$\rho(\hbar\omega) = [1/\rho_c(E_v + \hbar\omega) + 1/\rho_v(E_v)]^{-1} \quad (6-4)$$

If the dispersion relations for both bands are parabolic the joint DOS and k are found to be

$$\rho(\hbar\omega) = \frac{1}{\sqrt{2}\pi^2} (2m_v/\hbar\omega)^{3/2} (\mu/m_v)^{1/2} (\hbar\omega - E_g)^{1/2} \quad (6-5)$$

$$k^2 = 2\mu(\hbar\omega - E_g) \quad (6-6)$$

Here m_v is hole's effective mass and μ is the joint effective mass defined by

$$1/\mu = 1/m_e + 1/m_v \quad (6-7)$$

The total absorption coefficient must be summed over all degenerate bands and multiplied by a factor "2" to include the spin degeneracy, i.e.

$$\alpha(\omega) = 2 \sum_j \alpha_j(\omega), \quad j = \text{all degenerate bands} \quad (6-8)$$

It is simple to see that the $\alpha(\omega)$ in eq.(6-1) is dependent on $(\hbar\omega - E_g)^{1/2}$. Thus we can conclude that if parabolic bands are assumed, a parabolic absorption coefficient will be obtained.

6.3 Absorption without Bandgap Shrinkage

To calculate the $\alpha(\omega)$ from eq.(2-23) we need to know the DOS's of the valence and the conduction bands [eqs.(3-35) and (3-36)], the matrix element [eq.(5-31)], and the Fermi energy from a self-consistent calculation. Eqs.(5-18) and (5-13) are the matrix elements given by Casey and Stern and by Eagles respectively. The values needed to determine first for the GaAs DOS is the screening constant Q from a self consistent calculation. The Fermi energy is also obtained simultaneously from the calculation. In this work the two equations to solve are eqs.(4-11) and (4-12) for n type GaAs [eqs.(4-15) and (4-19) for p type GaAs]. To determine the matrix element in eq.(5-31) the localization parameters, α and β , and the "parameters" k_c and k_v must be determined first. From SG's theory α and β are obtained simultaneously with the DOS for the band tail. However, they cannot be found at high energies. Simple linear extrapolation are made to find the two parameter above the band tail by means of a physical idea that localization energy approaches zero above the band tail. k_c and k_v may be determined either by counting the number of states [eqs.(6-11) and (6-12)] or by arbitrary choices of "mobility edges" described in section 5.7.

In this section we will ignore the bandgap shrinkage due to many-body effects. The doping concentrations chosen are the same as used by Casey and Stern(1976). Numerical values of the screening length and the Fermi

energy calculated self consistently are tabulated in Tables 4.2 to 4.7. Physical quantities used in this calculation are $\epsilon_0 = 13.13$ [Hwang(1970a,b)], $n = 3.6$ [Johnson(1967)], $m_e = 0.066m_0$, $m_{hh} = 0.55m_0$, $m_{hl} = 0.085m_0$ [Casey and Stern(1976)]. SG's DOS is mainly used in all calculations. Since SG's DOS is very complicated and lengthy in computer time, we then first generate the DOS point by point with an interval of 6 milli eV and make an interpolation to regenerate the DOS for all energies.

The matrix element used here is given by eq.(5-31). The values of k_v , α , and β are determined using the method described in section 5.7. The matrix elements for heavily doped p type GaAs with net hole concentration $p = 1.2 \times 10^{18} \text{ cm}^{-3}$ [$N_A = 1.5 \times 10^{18} \text{ cm}^{-3}$ and $N_D = 3 \times 10^{17} \text{ cm}^{-3}$] at three photon energies, 1.37 eV, 1.42 eV, 1.55 eV, are plotted as a function of energy measured away from E_v in Fig.6.1. The full lines are for heavy holes and the dotted lined are for light holes. The curves are slowly varying at low photon energies and are gaussian like at high photon energies. In Fig.6.2, the present calculated absorption coefficient is compared with that using Eagles' constant matrix element [eq.(5-13) with $k_c = 0$] and that from parabolic bands mentioned in section 6.2. The Eagles matrix element is expected to overestimate the absorption coefficient [Casey and Stern(1976)].

We also vary the position of E_{mc} [Fig.3.2A] by 10% of E_g in order to investigate the sensitivity of the number of localized states in the band tail while the valence band is kept constant. The two results are shown in Fig.6.3 compared to the experimental result. Curve A is

calculated when the "mobility edge" in the conduction band is at E_g , and curve B is calculated using the "mobility edge" at $E + 0.1E_g$. In both cases the "mobility edge" in the valence band remains at E_v . The results show that the absorption coefficient is not very sensitive to the choice of "mobility edge" at low photon energies, i.e. at absorption tail region which we are interested in. The results for heavily doped p type GaAs at three net hole concentrations are plotted in Fig.6.4. It is seen that the absorption coefficient is shifted to the high energy side at higher doping. This is because the Fermi energy penetrates into the valence band at higher doping concentrations and the bandgap shrinkage is not taken into account here [Figs.6.5A,B]. The $\alpha(\omega)$ for n type GaAs are depicted in Fig.6.6. The Burstein shift can be seen but again all absorption curves are small compared to the experimental results like Casey and Stern's results.

6.4 Absorption with Bandgap Shrinkage

If the bandgap shrinkage is taken into account, the band separation will be smaller if the doping is higher. The effect of the band shrinkage on the absorption coefficient will be compensated for by the penetration of the Fermi energy into the valence band [Fig.6.5C]. It is not necessary for a heavier doped semiconductor to have a larger absorption coefficient at low energies. This depends on the compensation of the two physical quantities mentioned above.

It should be mentioned here again that when a pure crystal is doped by donors (or acceptors) the allowed energy levels will appear in the bandgap close to the conduction (or valence) band [Fig.6.7A]. When the

crystal becomes heavily doped, the positive donor ions will cause a rigid band shift down by an amount of E_0 [Fig.6.7B] but the band separation remains the same. E_0 is dependent on the doping concentration. An explicit expression has been given by Halperin and Lax(1966). If the many-body effects are taken into account, the band separation will be smaller by an amount of E_x [Fig.6.7C]. The new bandgap will be $E_g' = E_g - E_x$. The bandgap shrinkage due to many-body effects is sometimes assumed to be contributed by the exchange interaction only because the correlation interaction is small [e.g. Hwang(1970a,b), Hwang and Brews(1971), Auverge et al (1975), Serre et al (1981)]. Thus the bandgap shrinkage is represented by E_x . It is understood that the E_x has the same meaning as $|\Delta E_g|$ in this work.

We should also mention how Casey and Stern(1976) found the parameter k in their work. If we have a transition from a state E in the valence band to a state E' in the conduction band [Fig.6.8A], the wave vector associated to the energy E' (or E) can be found by counting the number of states down to the bottom of the band and filling up to energy E' in the parabolic conduction (or valence) band [Fig.6.8B]. All the above can be represented by the following equation

$$\int_{-\infty}^{E'} \rho_c(E) dE = \int_{E_c}^E \rho_{pc}(E) dE \quad (6-9)$$

and similarly for the state E in the valence band. The parabolic bands shown in Fig.6.8B have parabolic $E-k$ relationship as shown in Fig.6.8C or explicitly

$$E = \frac{\hbar^2 k^2}{2m_e} \quad (6-10)$$

We use eqs.(6-9) and (6-10) to determine k for the matrix element. The k value for the conduction band is

$$k_c = \left[6\pi^2 \int_{-\infty}^{E'} \rho_c(E) dE \right]^{1/3} \quad (6-11)$$

and similarly for the valence band

$$k_v = \left[6\pi^2 \int_E^{\infty} \rho_v(E) dE \right]^{1/3} \quad (6-12)$$

To consider the bandgap shrinkage due to exchange energy one may consider a heavily doped semiconductor as a very dense electron gas which has the exchange energy proportional to $n^{1/3}$ (in n type) [Wolff(1962a,b)]. Hwang and Brews(1971) wrote this exchange energy as

$$E_x = \left(\frac{4}{\alpha \pi b} \right) \left(\frac{m_e e^4}{2 \epsilon_0^2 \hbar^2} \right) \quad (6-13)$$

with $b = (3/4\pi n a^3)^{1/3}$ and $\alpha = (4/9\pi)^{1/3}$. Eq.(6-13) is true when $b \ll 1$ or the average separation is lower than the Bohr radius, i.e. $n^{1/3} a \gg 1$. This is only applicable for heavily doped semiconductors.

The bandgap shrinkage due to many-body effects may be determined using the self-energy formalism of many-body theory [Hedin and Lundqvist (1969)]. Inkson(1976) used the self-energy formalism to calculate the change of the bandgap of a semiconductor due to an electron gas which occupies a part of the conduction band. He examined the relative movement of the bottom of the conduction band and the top of the valence band. His method is, therefore, a two-band approach. He derived an expression for the change in the bandgap of a semiconductor due to high

doping in the limit where the free carriers form a degenerate gas. The change in the bandgap is found to be

$$\Delta E_g = - \frac{2e^2 k_F}{\pi \epsilon_0} \left[1 + \frac{Q}{k_F} \left(\frac{\pi}{2} - \tan^{-1}(k_F/Q) \right) \right] \quad (6-14)$$

where Q is the screening constant calculated from the Thomas-Fermi approximation and k_F is the Fermi wave vector given in terms of n by

$$k_F = (3\pi^2 n)^{1/3} \quad (6-15)$$

Since Inkson used the Thomas-Fermi approximation to find the screening constant, the bandgap shrinkage found by eq.(6-14) is then called Inkson's Thomas-Fermi bandgap shrinkage. There are some other better methods to determine the shrinkage but also more complicated. We will give more details of these methods in section 6.6.

There is also a simple empirical formula written by Casey and Stern (1976) for the bandgap shrinkage in p type heavily doped GaAs at 297K. The bandgap shrinkage is dependent on the cube root of the hole concentration. This is similar to the case of free electron mentioned above. The explicit empirical expression is

$$\Delta E_g = -1.6 \times 10^{-8} [p \text{ in cm}^{-3}]^{1/3} \text{ eV} \quad (6-16)$$

We use the bandgap shrinkage given by Inkson [eq.(6-14)] and by Casey and Stern [eq.(6-16)] to calculate the absorption coefficient for both heavily doped n type and p type GaAs. The results for the p type using Inkson's bandgap shrinkage are plotted in Fig.6.9. The solid lines are calculated using the method to calculate k and z described in section

5.7 . The broken lines are computed using k by counting the number of states [eqs.(6-11) and (6-12)]. The latter results seem to be smaller than the first one because of the decay of the matrix element due to the k dependence. The envelope matrix elements calculated using k 's from Casey and Stern's method for $p=1.2 \times 10^{18} \text{ cm}^{-3}$ are shown in Fig.6.10 . The results for the n type are shown in Fig.6.11 in similar fashion to the p type. They show similar decay due to the k dependence. The Burstein shifts of both sets of results are also observed.

When the empirical formula of Casey and Stern is taken into account, our $\alpha(\omega)$ for the p type [Fig.6.12] are almost the same as the $\alpha(\omega)$ obtained by Casey and Stern except our curve for $p=2.4 \times 10^{18} \text{ cm}^{-3}$ does not cross over the curve for $p=1.2 \times 10^{18} \text{ cm}^{-3}$. The experimental $\alpha(\omega)$ for the p type [Casey et al(1975)] is shown in Fig.6.13. Casey and Stern's absorption coefficients for the p type are depicted in Fig.6.14. One of their curves with $p=1.2 \times 10^{18} \text{ cm}^{-3}$ needs a factor of 1.6 to be closer to the experimental one [Fig.6.15]. Their matrix element calculated from eq.(5-18) at three photon energies is also demonstrated in Fig.6.16. Our $\alpha(\omega)$ needs a factor of about 1.45 to make our result close to the experimental one [Fig.6.17]. However the overall results for the p type are comparable to those of Casey and Stern even if different methods of determining all relevant parameters are used.

Our $\alpha(\omega)$ for the n type are presented in Fig.6.18. They again show similarity to those of Casey and Stern [Fig.6.19]. However, the $\alpha(\omega)$ are too small compared to the experimental results in Fig.6.20.

All values of $|\Delta E_g|$ used in this work are shown in Fig.6.21 by the "X". All lines shown in Fig.6.21 are free-hand drawn to join all calculated values in this work. It may not be necessary to have the same bandgap shrinkage as these curves at other net concentration. The dotted line is from Casey and Stern's empirical expression for both n and p type. The dot-dash lines are from Inkson's Thomas-Fermi approximation. The curves for the p type and the n type are not the same depending on the Fermi energy and the screening constant.

6.5 Sensitivity of $\alpha(\omega)$ to Some Physical Quantities

The purpose of this section is to test how the absorption coefficient varies with some physical quantities used in this calculation, e.g. the DOS, the effective mass, and the "mobility edge".

In order to see the change of $\alpha(\omega)$ on a choice of DOS, we calculate $\alpha(\omega)$ using SG's DOS and Eagles' matrix element [eq.(5.13)] and compare the result with that using Kane's DOS and the same matrix element. The Eagles matrix element is chosen since we cannot find the localization parameters, α and β , when Kane's DOS is used and if our present matrix element [eq.(5-13)] is employed. The curves for $p=1.2 \times 10^{18} \text{ cm}^{-3}$ with [solid lines] and without [broken lines] bandgap shrinkage determined using Casey and Stern's empirical formula are presented in Fig.6.22. Since the Kane DOS has a larger band tail than the SG DOS, the $\alpha(\omega)$ using Kane's DOS shown in Fig.6.22 are larger than that using SG's DOS. We may conclude that the absorption is sensitive to the DOS.

Since the effective mass is a function of doping concentration [Raymond et al (1979)], we then vary the heavy hole mass m_{hh}^* from 0.55 [Casey and Stern (1976)] to 0.68 [Ehrenreich (1963)] in our calculation to see the variation of $\alpha(\omega)$ on these choices. All other quantities used are fixed. The results are presented in Fig.6.23. The curves differ little; a few percent only. This difference would not account for the difference between the present and Casey and Stern's $\alpha(\omega)$.

The last quantity to test is the choice of "mobility edge" described in section 5.7. The "mobility edge" here is an energy level separating delocalized states from localized states. If it is moved higher in the conduction band, the number of localized states will be increased and the number of delocalized states will be decreased. To see only this effect on $\alpha(\omega)$, we fix the "mobility edge" in the valence band at $E_{mv} = E_v$ and vary the "mobility edge" in the conduction band E_{mc} only. The $\alpha(\omega)$ for $p = 1.2 \times 10^{18} \text{ cm}^{-3}$ with E_{mc} varied up to 15% of E_g are plotted in Fig.6.24. They show appreciable difference at high photon energies. The $\alpha(\omega)$ is saturated for the increase of E_{mc} greater than 15% of E_g . Above this value of E_{mc} all the states in the conduction band become localized within our photon energy range of interest and the absorption coefficient cannot get any greater. We may conclude here that the choice of a "mobility edge" could affect greatly the absorption coefficient especially at high photon energies.

We do not test some other physical quantities in the expression of $\alpha(\omega)$, e.g. the refractive index n and the static dielectric constant ϵ_0 , because all of them do not vary much with photon energy. They are expected to have less effect on the $\alpha(\omega)$.

6.6 Discussion on Bandgap Shrinkage

It has been shown in Fig. 6.4 that the bandgap shrinkage plays an important role in predicting the absorption coefficient correctly. Inkson (1976) employed the self-energy formalism for many-body theory to determine the bandgap shrinkage by considering the effect of free carriers, which were assumed to be a free electron gas, to both the valence and the conduction bands. He used the Thomas-Fermi approximation to find the screening constant Q in his derivation while Abram et al (1978) used the Lindhard dielectric function [Hedin and Lundqvist (1969)] to improve the accuracy. Abram et al also determined the bandgap shrinkage due to the exchange interaction with free carriers without screening. This is called the unscreened exchange calculation. We plot these predictions for the bandgap shrinkage for both p and n type GaAs in Figs. 6.25 and 6.26 respectively [after Abram et al] compared to our calculation using Casey and Stern's empirical formula. Theoretically, the Inkson curve is the largest because the dielectric function used is the semiclassical one. The Lindhard calculation should be the best one because of a better dielectric function. However, the Casey and Stern curve, deduced from Casey et al's experiments at 297K, fits best with the experiments done by Zverev (1977) at 77K [Fig. 6.27]. Since the free carriers in the system are treated as a (degenerate) free electron gas when the bandgap shrinkage is taken into account, the shrinkage should not be very dependent on the temperature range of interest.

It should be noted that there are some excellent papers discussing the bandgap shrinkage due to many-body effects. These are, for examples,

Mahan (1980), Berggren and Sernelius (1981), and Sterne and Inkson (1981).

6.7 Summary

In this work, we calculate the absorption coefficient of heavily doped GaAs using the SG DOS with the envelope matrix element derived using a harmonic wave function from the SG theory. The harmonic wave function is used because in SG's model a non-local harmonic well is assumed to fit a potential-fluctuation well due to disordered effects. The asymptotic value of the present envelope matrix element when the localized parameters, α and β , go to zero is found to approach the limit of momentum-conserved transitions created by two plane waves correctly [eq.(5-36)]. It is also comparable to Eagles' matrix element when the initial state is localized and the final state is delocalized [eq.(5-37)].

We choose the same values of doping concentration as those of Casey and Stern in order to compare our results with theirs. We calculate the absorption coefficients with and without the bandgap shrinkage. The bandgap shrinkage used in our calculations is determined from Casey and Stern's empirical formula and from Inkson's Thomas-Fermi approximation. We find that the effect of the bandgap shrinkage is compensated for by the sinking of the Fermi energy in p type semiconductors. In n type semiconductors, the Fermi energy rises (instead of sinks) if the doping concentration is increased. Since the conduction-band DOS in GaAs is very small compared to the valence-band DOS, the rising of the Fermi energy in heavily doped n type GaAs dominates over the bandgap shrinkage. Thus the Burstein shift is easily observed in n type GaAs.

One of our absorption coefficients [$p=1.2 \times 10^{18} \text{ cm}^{-3}$] needs a factor of 1.45 to be close to the experimental result while Casey and Stern needs a factor of 1.6. Although our factor is smaller, it is hard to say that our result is better. This is because we compare one curve only and the overall results look very similar. We may say that these two sets of results give the same predictions within the calculational errors.

We also test the sensitivity of $\alpha(\omega)$ on the DOS, the effective mass, and the parameters needed for the calculation. Our procedure of determining k and localization parameters is based upon the separation of localized and delocalized states suggested by Phillips (1983). The $\alpha(\omega)$ calculated using this procedure is also compared to that using the counting method used by Casey and Stern.

On the whole the absorption coefficients $\alpha(\omega)$ determined in the present work are of comparable values to those of Casey and Stern but too small compared to the experiments. It is important to point out that the magnitude of the absorption coefficient depends upon the value of Kane's matrix element M_b^2 used in eq.(5-9) for the total matrix element of transition. More detailed studies of GaAs [Chadi et al(1976), Hermann and Weisbuch(1977)] have found the matrix element M to be about 25% larger than the value we use here. This would raise all the absorption coefficients in this work by a factor of 1.25. However, the results would still be smaller by a factor of 1.16 [from $(1.45/1.25)$]. This may be due to the limitation of the approximations used in this calculation.

6.8 Epilogue

In the theory for the DOS, semiconductors must be heavily doped until an impurity band merges with its host band. Physically, the electronic wave functions must be larger than the impurity separations. Mathematically, the ratio between the Bohr radius a and the impurity separation $1/n^{1/3}$ must be larger than unity, i.e. $a n^{1/3} \gg 1$. Even if the doping concentrations we consider in this work do not meet that condition, they are high enough to be degenerate semiconductors which have Fermi energies deep into the host bands. The impurities must have small ionization energies, i.e. shallow. They are all ionized by thermal excitations. It is also assumed that the impurities are randomly distributed in the host crystal and do not perturb the structure.

In the screening process, all other effects are taken care of by the screening constant Q . The screening is assumed linear so that the Thomas-Fermi approximation can be applied. This, however, does not hold when the number of impurities is so high that linearity can no longer be assumed.

The effective mass approximation is used to split off the envelope matrix element from the total matrix element of transition. This leaves the well known Kane's matrix element of transition which is a function of physical quantities which are all known, such as the energy gap, the spin-orbit splitting, and the effective mass. The values of the localization parameters, α and β , and the k values are not well established; whether or not the "mobility edges" are simply selected or k is determined by counting the number of occupied states. The k values

are used to count the number of states only [Tauc(1972)]. The position of a "mobility edge" is still a large problem to deal with. In this work, we locate it at a nominal band edge without any knowledge of its actual position. The localization parameters at some energies are obtained by linear extrapolations with a simple physical idea that the kinetic energy of localization vanishes at higher energies [for conduction band only]. This may not be entirely correct but it should be valid within the photon energy range of interest.

The interband transition we are concerned with is the transition between band edges only. The photon momentum is neglected. The calculation of $\alpha(\omega)$ is still based upon many assumptions [see eq.(2-23)]. It is shown that the $\alpha(\omega)$ at low photon energies is sensitive to the DOS in the tail region and the bandgap shrinkage, and the $\alpha(\omega)$ at high photon energies is sensitive to the mobility edge, i.e. the number of localized states.

The knowledge of the effect of the compensation ratio on the absorption is still not well determined. Herbert et al (1975) and Serre et al (1981) investigated the effect of the compensation ratio on the energy band tailing. Serre et al found that the DOS band tail is increased if the compensation ratio is increased while the net doping concentration is kept fixed. They also found that the effect of electron-impurity scattering could increase the $\alpha(\omega)$ at low photon energies.

We calculate the absorption coefficient at $T=297K$. The temperature effect is not taken into account here. The variation of the $\alpha(\omega)$ at low

photon energies [Urbach tail] should be observed if the temperature is varied.)

We note that a free hole and a free electron as a pair of opposite charges experience a Coulomb attraction. This electron-hole pair, known as an exciton, has a very large hydrogenic orbit compared to a donor (or an acceptor) orbit. This is due to the effective mass of an electron-hole being much smaller. Since its energy states are close to the conduction band edge, the electron-hole Coulomb interaction dominates the shape of the absorption edge especially in a pure GaAs crystal. This effect is weaker in heavily doped materials due to larger screening effects. We restrict ourselves to a degenerate heavily doped semiconductor which has a large number of free carriers to increase the screening effects and reduce the existence of the electron-hole pairs. Consequently the more the screening effects, the less important the electron-hole Coulomb interaction. Theoretically, this interaction is ignored when the Bohr radius of an electron-hole pair is larger than the screening length. However, this effect is included in the experimental results despite of its small contribution. Since this effect only contributes a few percent to the absorption edge of heavily doped GaAs, we do not take it into consideration.

The advantage of our calculation over that of Casey and Stern is that almost all quantities come out from a single theory except Kane's matrix element of transition. These quantities are the localization parameters, the harmonic wave functions used in the envelope matrix element. However, the procedure to determine the k values is still arbitrary and

it needs more physical judgement. Lastly, we may conclude that the absorption coefficient is sensitive to many physical quantities so that it is difficult to predict it correctly given that many approximations must be made.

APPENDIX A

The Harmonic Wave Function from the SG Theory

As mentioned in the text, the envelope matrix element of transition defined in eq.(5-8) is a function of initial and final state wave functions. They may be localized or delocalized. In this appendix we are concerned with localized wave functions since the delocalized wave functions are taken to be plane waves.

It is well known from the Feynman path integration formalism that a propagator can imply direct information about the wave function of the system [Feynman and Hibbs (1965)]. In the SG theory, the average propagator is evaluated exactly up to the first cumulant with the variational parameter determined from the Lloyd and Best variational principle. This propagator is called the first-order propagator. Although, in principle, we should use the first-order propagator to find the wave function; it is, however, well known in quantum mechanics that only the zero-order wave function is sufficient if the first order energy is required.

The zero-order propagator given by Sa-yakanit(1974) is

$$G_0(\vec{x}, t; \vec{x}', t') = \left(\frac{m}{2\pi i \hbar (t-t')} \right)^{3/2} \left(\frac{\omega t}{2 \sin \omega t} \right)^{3/2} \times \exp \left[\frac{i}{\hbar} \frac{m \omega}{4} \cot \omega t \frac{|\vec{x} - \vec{x}'|^2}{2} \right] \quad (A-1)$$

Since this expression is obviously translationally invariant, it contains no information on localized states. In order to obtain localized wave functions, the translational invariance must be broken. The idea of breaking the translational symmetry is similar to that used in the mean field theory [Ashcroft and Mermin (1976), for a brief review].

To understand this problem, it should be noted that eq.(A-1) can be derived by averaging over all directions the propagator of the harmonic oscillator centered at other positions, G_H , i.e.

$$G_0(\vec{x}, t; \vec{x}', t') \sim \int d\vec{R} G_H(\vec{x} + \vec{R}, t; \vec{x}' + \vec{R}, t') \quad (A-2)$$

where

$$G_H(\vec{x} + \vec{R}, t; \vec{x}' + \vec{R}, t') = \int D(\vec{x}(\tau)) \times \exp \left[\frac{i}{\hbar} \int_{t'}^t d\tau \left(\frac{m}{2} \dot{\vec{x}}^2(\tau) - \omega^2 (\vec{x}(\tau) + \vec{R})^2 \right) \right] \quad (A-3)$$

For simplicity, we set $\vec{R}=0$ and obtain the well known result

$$G_H(\vec{x}, t; \vec{x}', t') = \left(\frac{m\omega}{2\pi i \hbar \sin \omega(t-t')} \right)^{3/2} \times \exp \left[\frac{i}{\hbar} \frac{m\omega}{2 \sin \omega(t-t')} \{ (\vec{x}^2 - \vec{x}'^2) \cos \omega(t-t') - 2\vec{x} \cdot \vec{x}' \} \right] \\ = \sum_n \phi_n(\vec{x}) \phi_n^*(\vec{x}') e^{-\frac{i}{\hbar} E_n(t-t')} \quad (A-4)$$

where E_n and ϕ_n are harmonic oscillator energies and wave functions respectively. In order to obtain the localized wave function

corresponding to the SG DOS, we take the limit t to infinity [Feynman and Hibbs (1965)]. Physically, this corresponds to taking the ground-state wave function only, i.e.

$$G_H(\vec{x}, t; \vec{x}', t') = \phi_0(\vec{x}) \phi_0^*(\vec{x}') e^{-\frac{1}{\hbar} \hbar \omega (t-t')} \quad (A-5)$$

where

$$\phi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{3/4} e^{-\frac{m\omega x^2}{2\hbar}} \quad (A-6)$$

The parameter ω that is related to z can be determined variationally from eq.(3-33), or (3-30), or (3-29) depending upon which variational calculation is chosen.

Rewrite eq.(A-6) to be

$$\phi_0(\vec{x}) = \left(\frac{2\alpha}{\pi}\right)^{3/4} e^{-\alpha \vec{x}^2}, \quad \alpha = Q^2/2z^2 \quad (A-7)$$

by means of the relation $m\omega/\hbar = Q^2/z^2$ [Sa-yakanit and Glyde (1980)]. The angular dependence of the wave function in eq.(A-7) can be separated by writing in terms of the zero-order spherical harmonic function, Y_0^0 , i.e.

$$\phi_0(\vec{x}) = \frac{S(r)}{r} Y_0^0 = \frac{1}{\sqrt{4\pi}} \frac{S(r)}{r} \quad (A-8)$$

where $S(r)/r$ is the radial part [Halperin and Lax (1966)]. Equalizing eqs.(A-7) and (A-8) gives

$$Q^{-1/2} S(r) = 2\pi^{-1/2} z^{-3/2} (Qr) e^{-\frac{1}{2}(Qr)^2/z^2} \quad (A-9)$$

In order to compare our $S(r)$ with that of Halperin and Lax, we plot $Q^{-1/2} S(r)$ against Qr [or $S(r)$ against r with $Q=1$] using $z=0.7059$ for $v=10$

[Sa-yakanit, Sritrakool, and Glyde (1982)]. Our calculated $S(r)$ is depicted by a full line in Fig.A.1 compared to that of Halperin and Lax (broken lines). The potential $U(r)/E_Q = (1/2)m\omega^2 r^2/E_Q = (Qr)^2/z^4$ is also plotted on Fig.A.1 with $U(r)$ being measured in E_Q unit.

APPENDIX B

The Parabolic Cylinder Function $D_p(z)$

The parabolic cylinder function $D_p(z)$ has an integral representation written in terms of the gamma function Γ [see Gradshteyn and Ryzhik (1965)] as

$$D_p(z) = \frac{e^{-z^2/4}}{\Gamma(-p)} \int_0^\infty e^{-zx-x^2/2} x^{-p-1} dx, \quad \text{Re } p < 0 \quad (B-1)$$

The asymptotic expansion of $D_p(z)$ for $|z| \gg 1$ and $|z| \gg p$ is

$$D_p(z) \sim e^{-z^2/4} z^p \left[1 - \frac{p(p-1)}{2z^2} + \dots \right] \quad (B-2)$$

One of the recursion formulas is

$$D_{p+1}(z) - z D_p(z) + p D_{p-1}(z) = 0 \quad (B-3)$$

We use eq.(B-1) to generate numerical values of $D_p(z)$ with $\text{Re } p < 0$. We derive, using the recursion formula given in eq.(B-3), an expression for $D_p(z)$ with $\text{Re } p > 0$

$$D_p(z) = \left[z^4 - 3(p-2)z^2 + (p-3)(p-1) \right] D_{p-4}(z) + (p-4)(z^3 - z(2p-3)) D_{p-5}(z), \quad 0 < \text{Re } p < 4 \quad (B-4)$$

The recursion may be repeated to obtain an expression valid at higher values of $\text{Re } p$.

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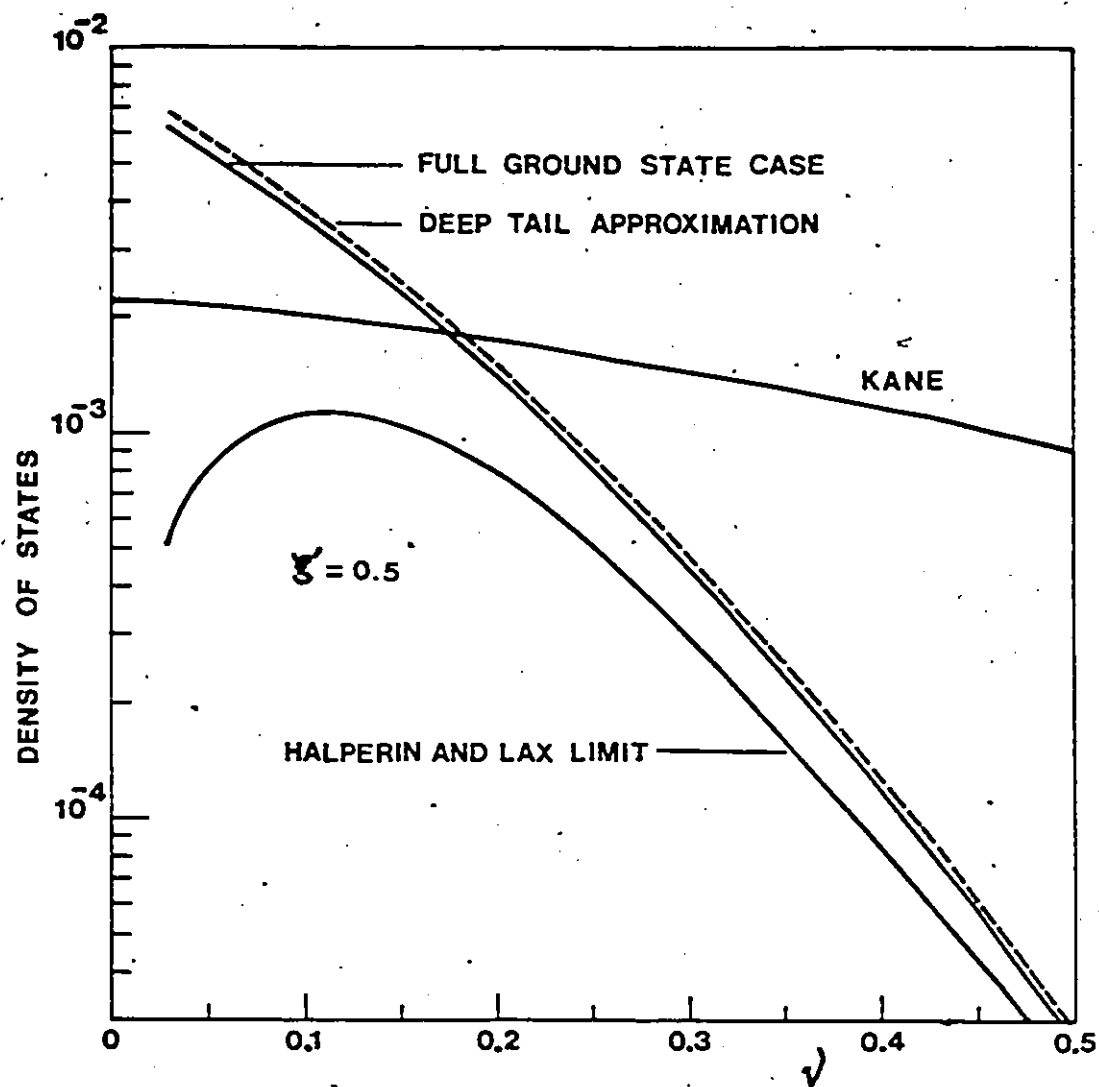


FIGURE 3.1

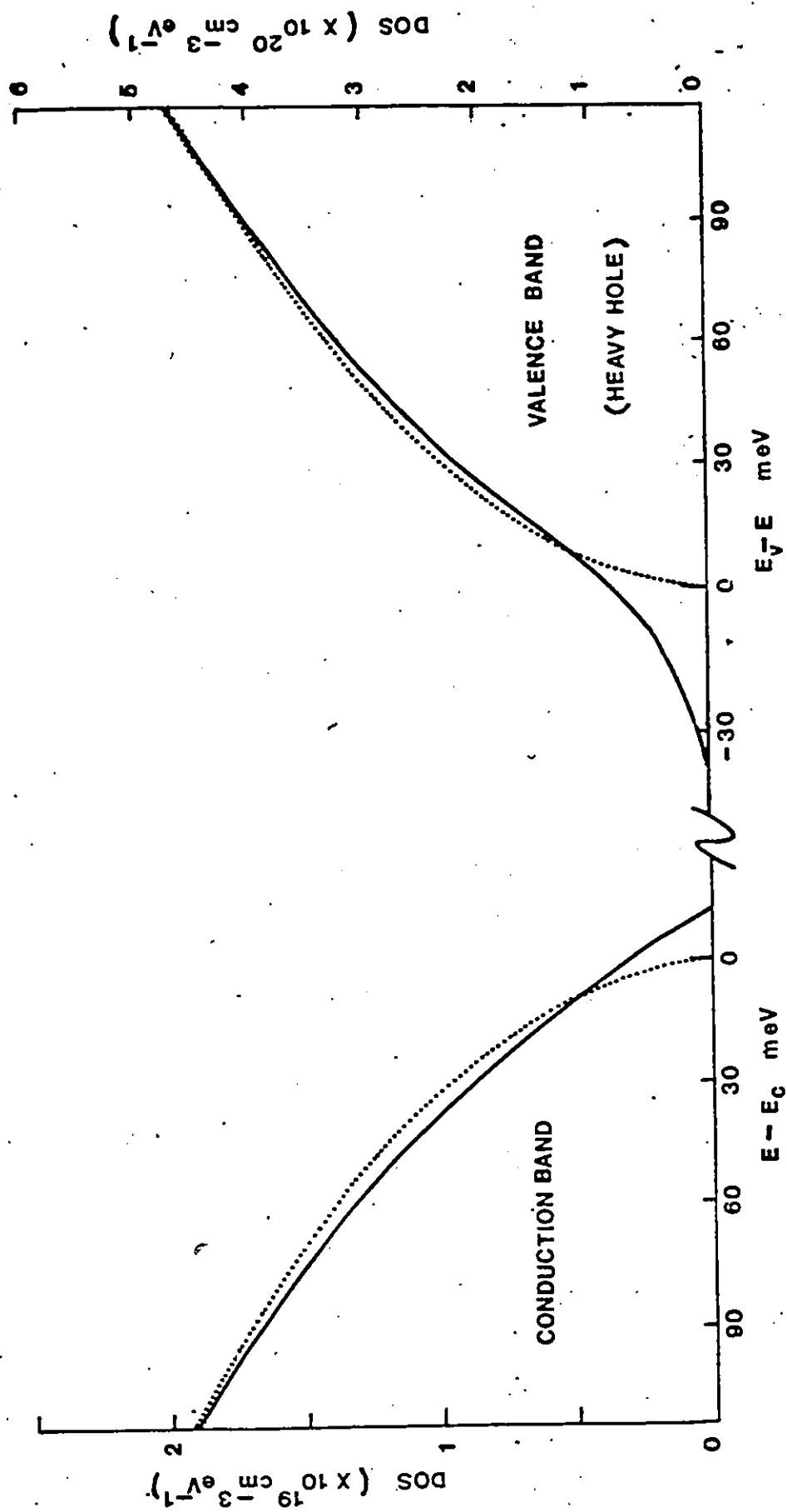


FIGURE 3.2

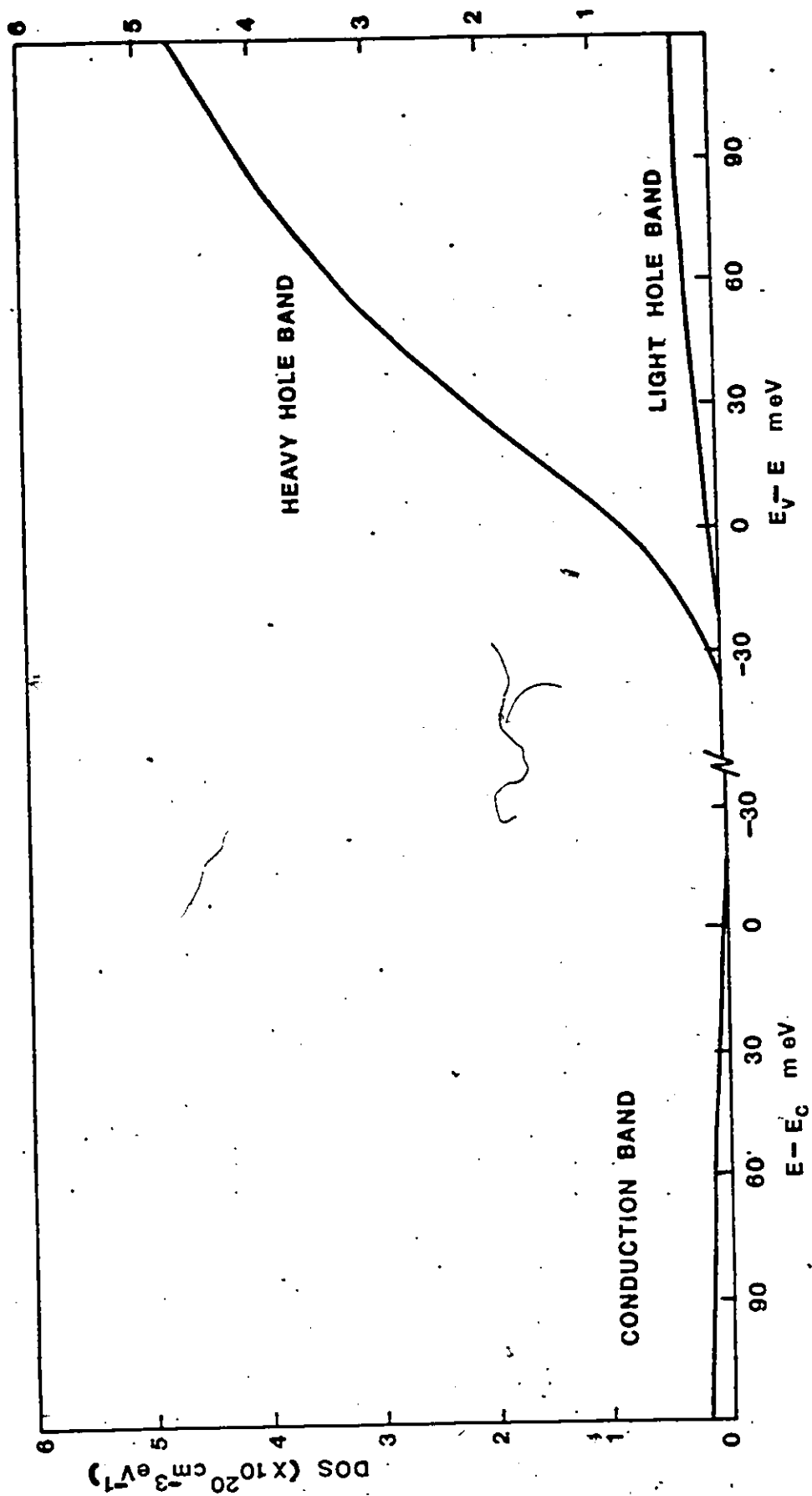


FIGURE 3.3

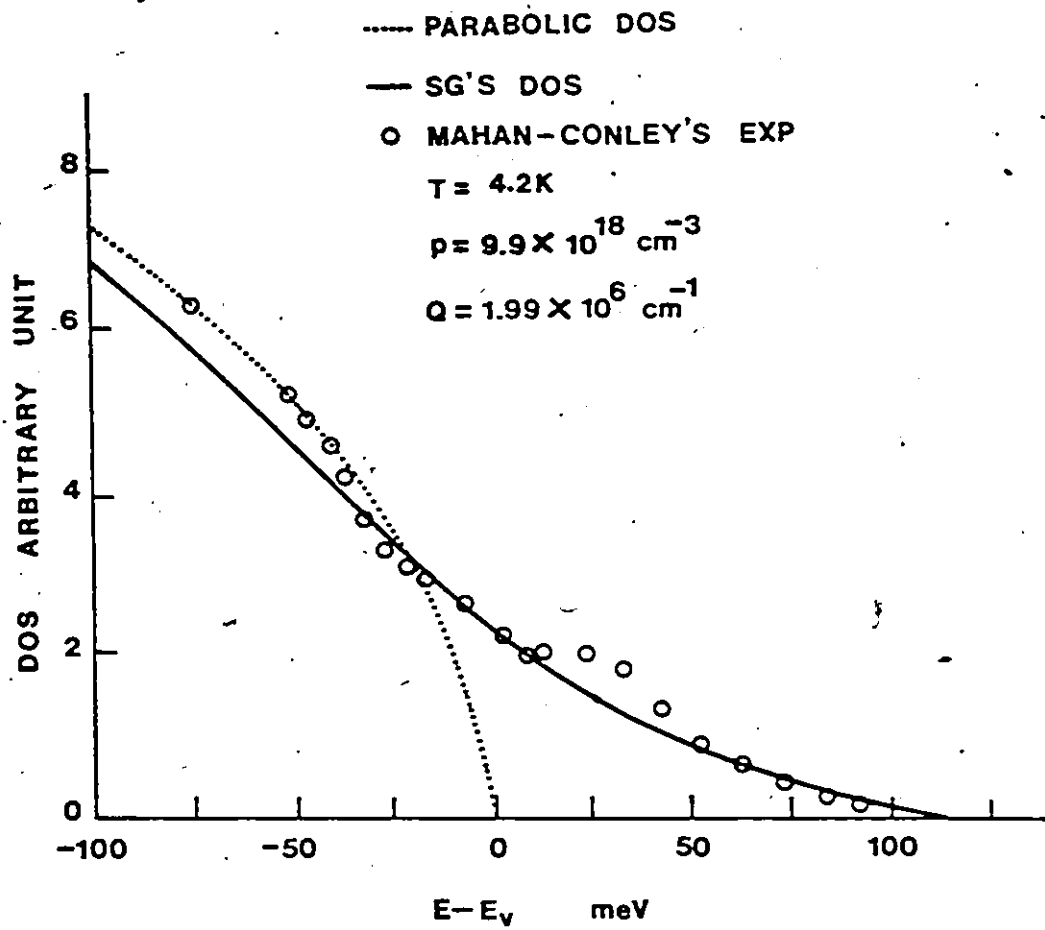


FIGURE 3.4

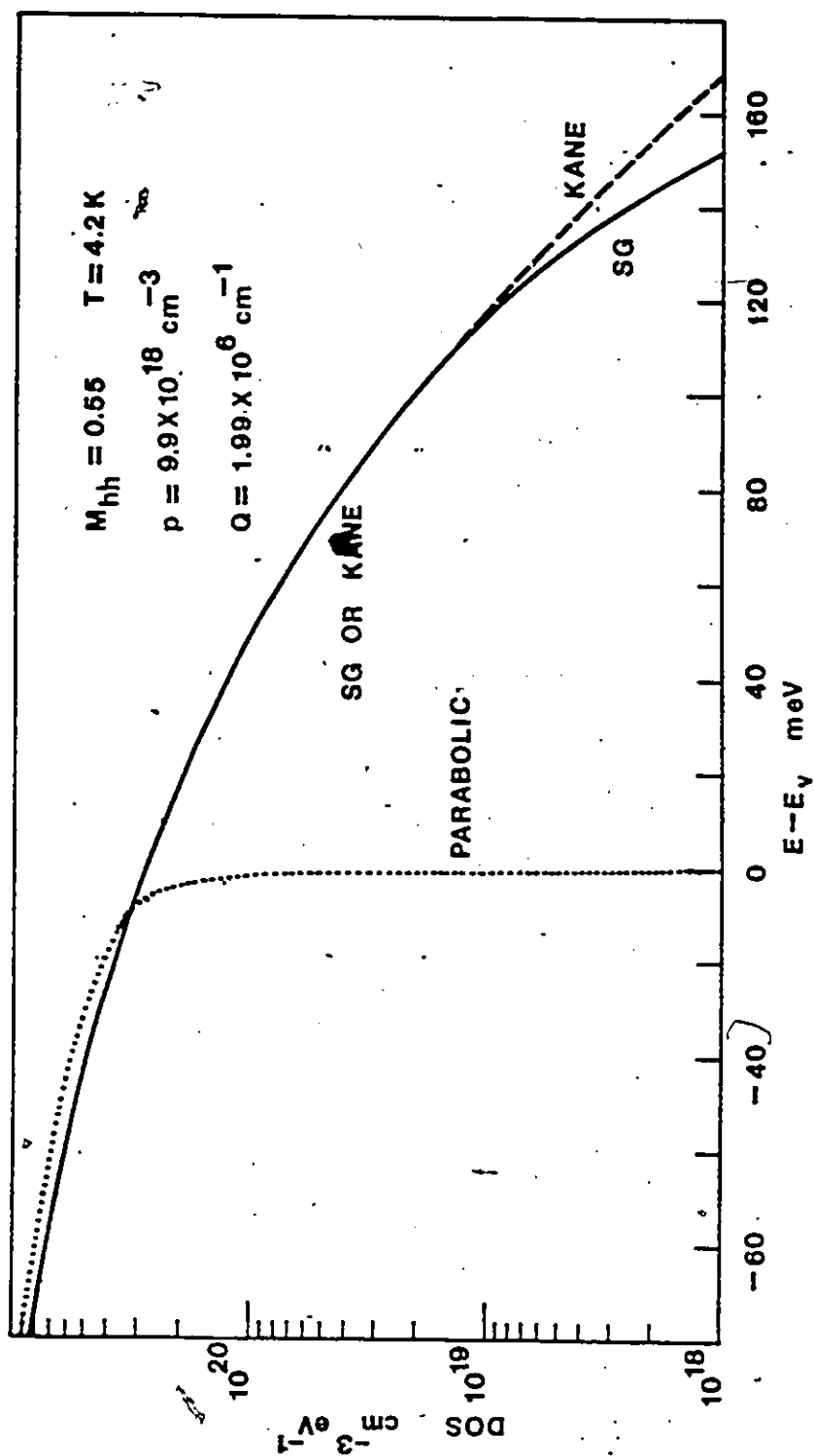


FIGURE 3.5

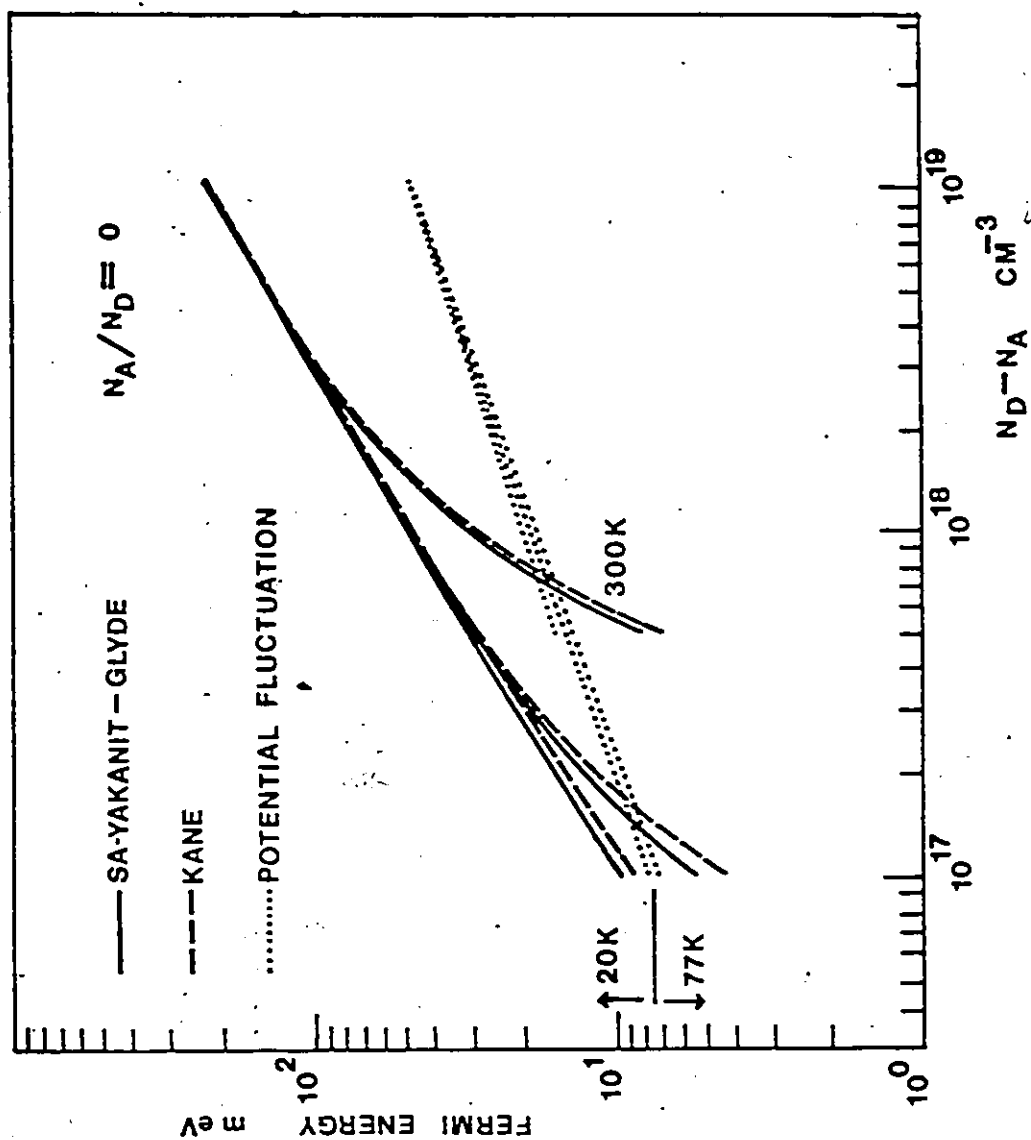


FIGURE 4.1

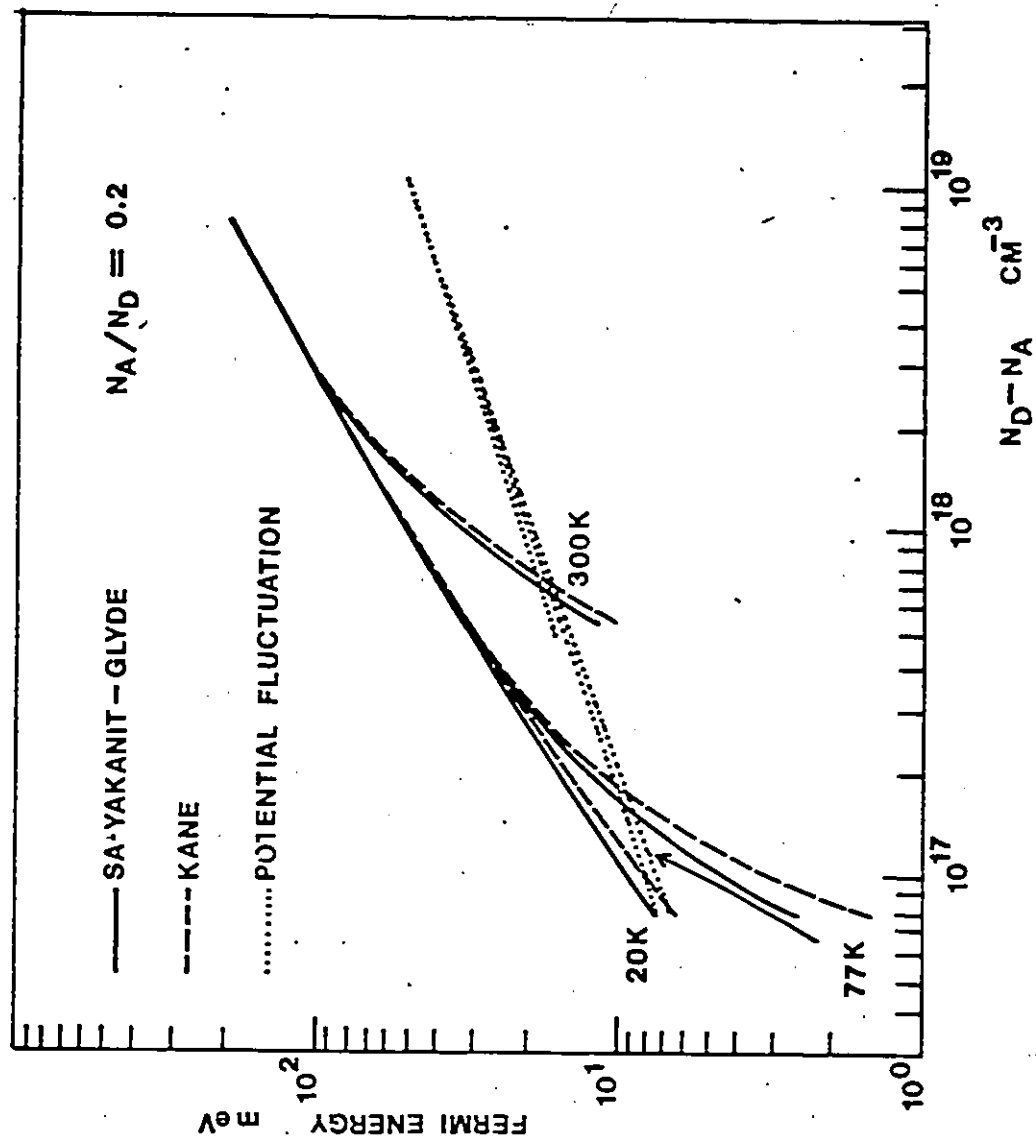


FIGURE 4.2

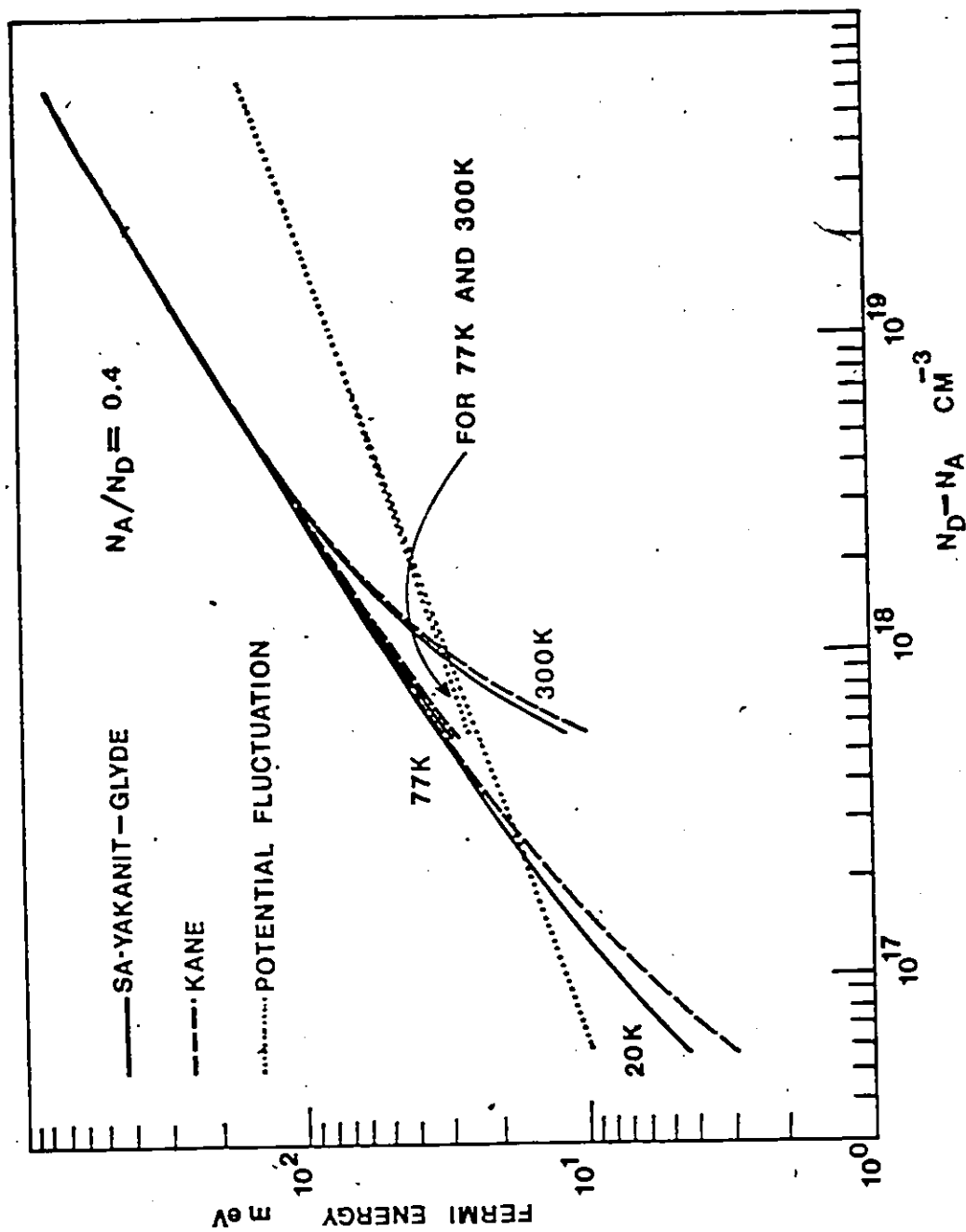


FIGURE 4.3

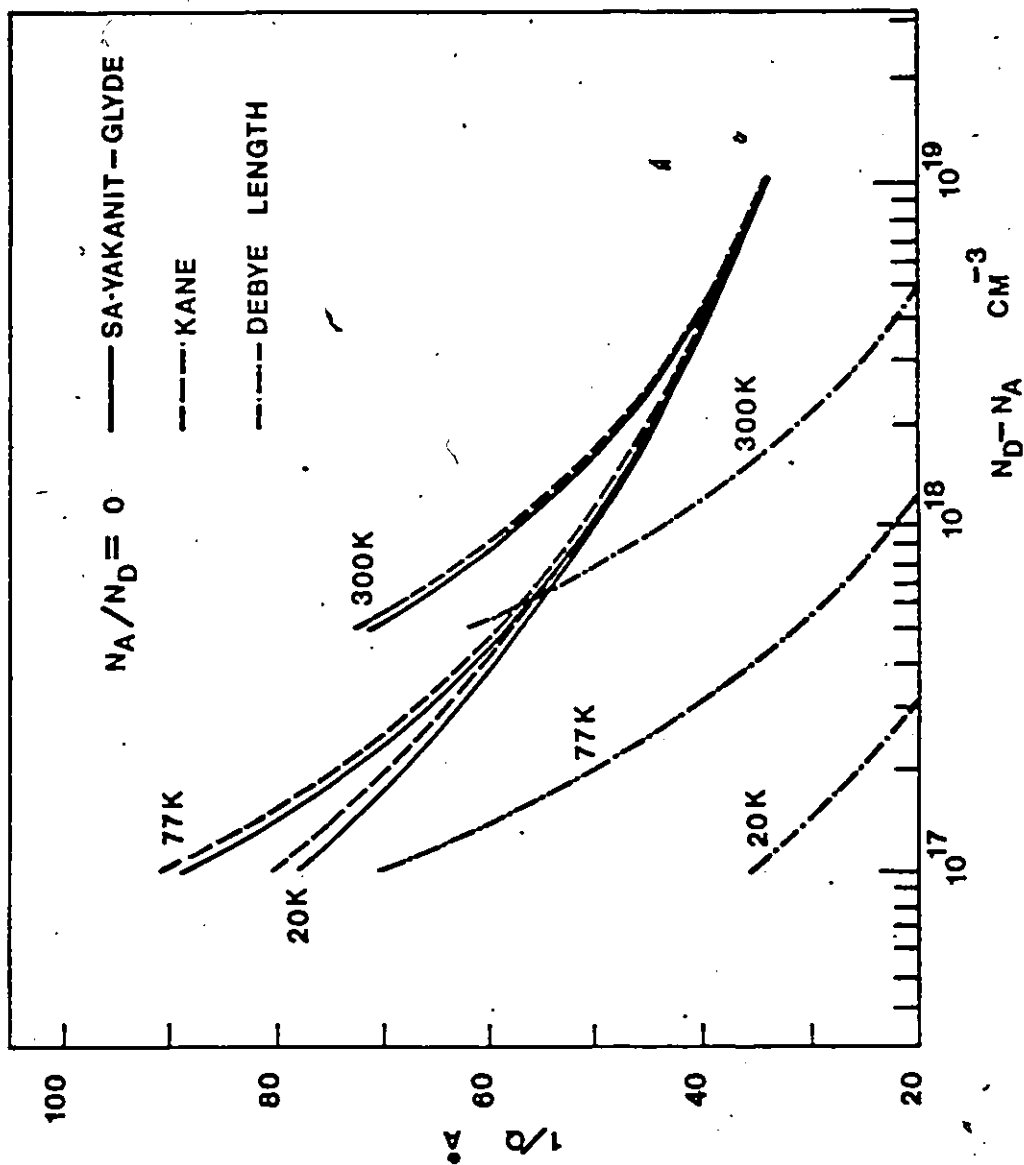


FIGURE 4.4

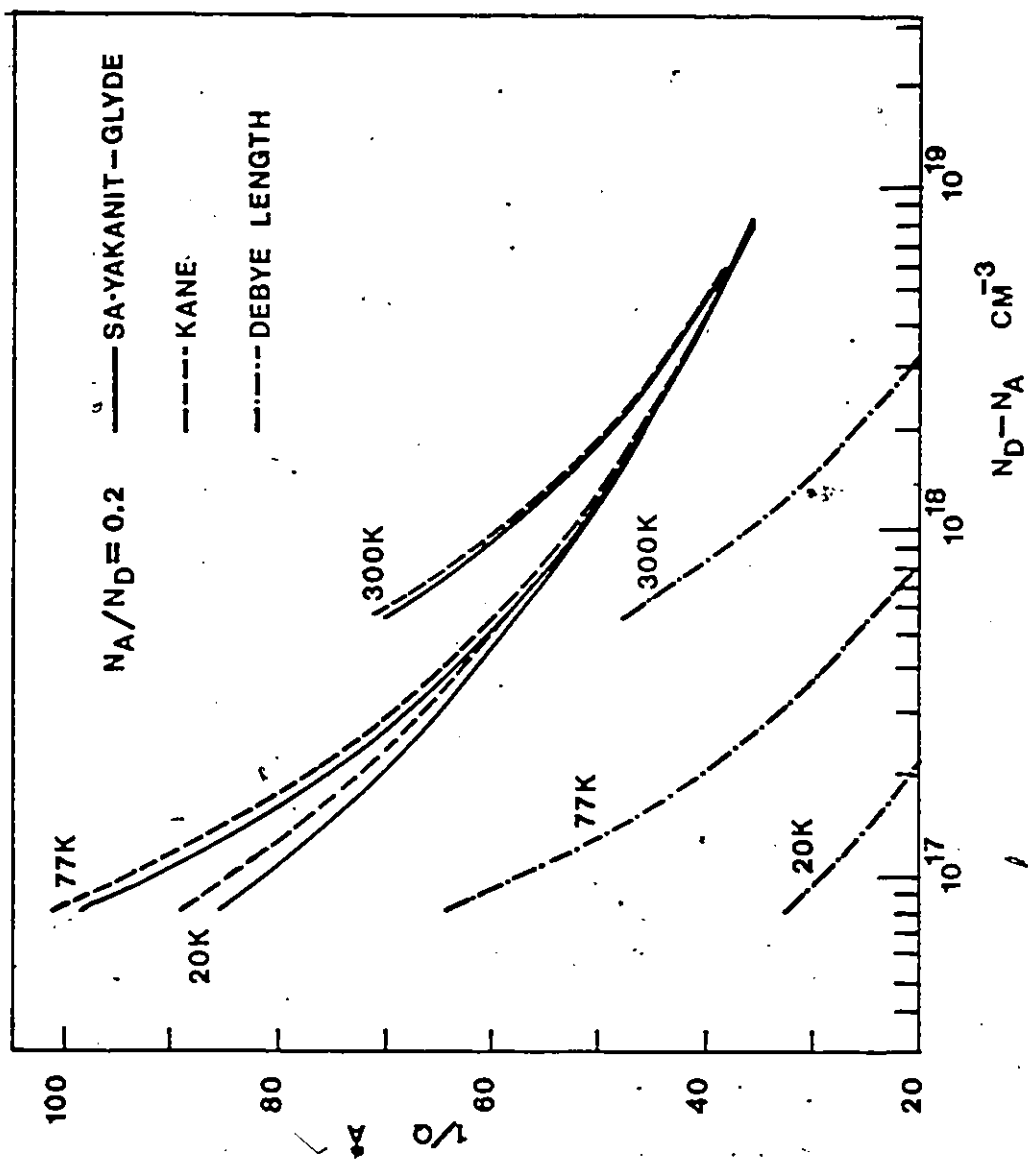


FIGURE 4.5

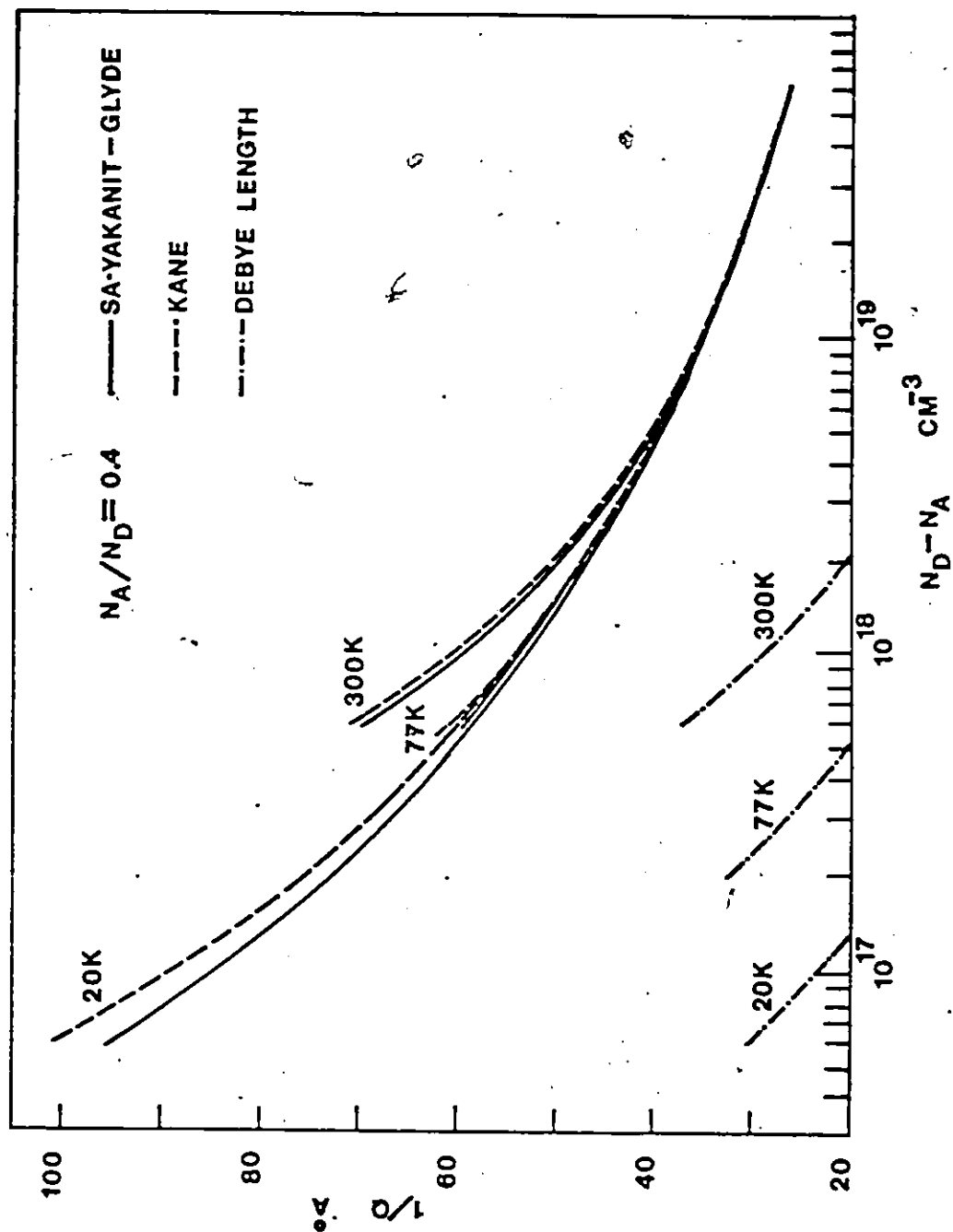


FIGURE 4.6

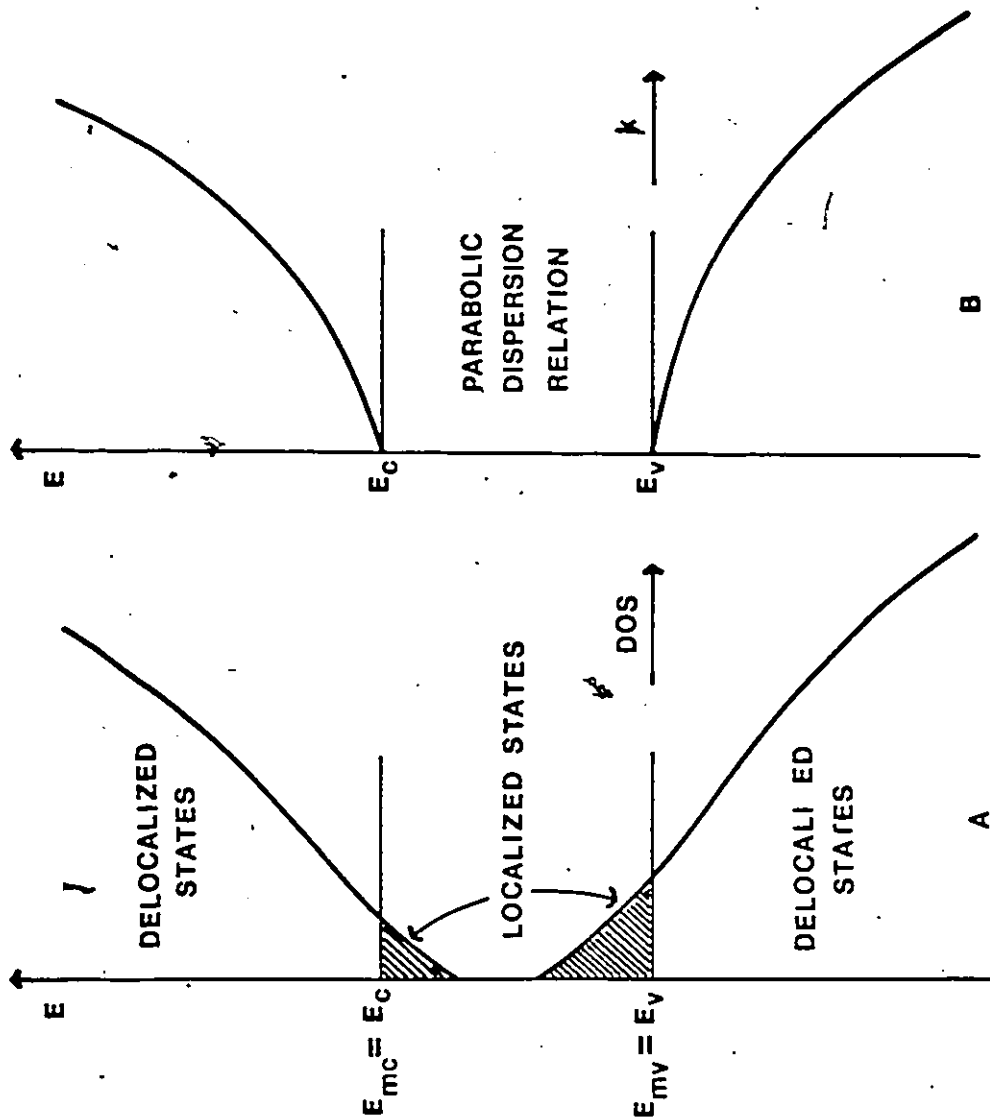


FIGURE 5.1

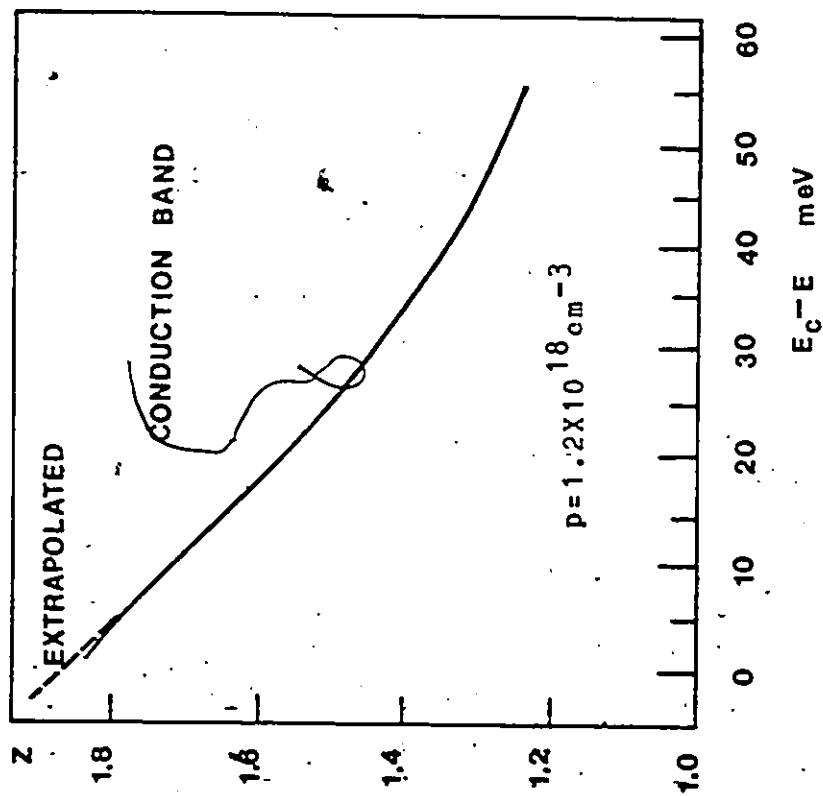


FIGURE 5.2A

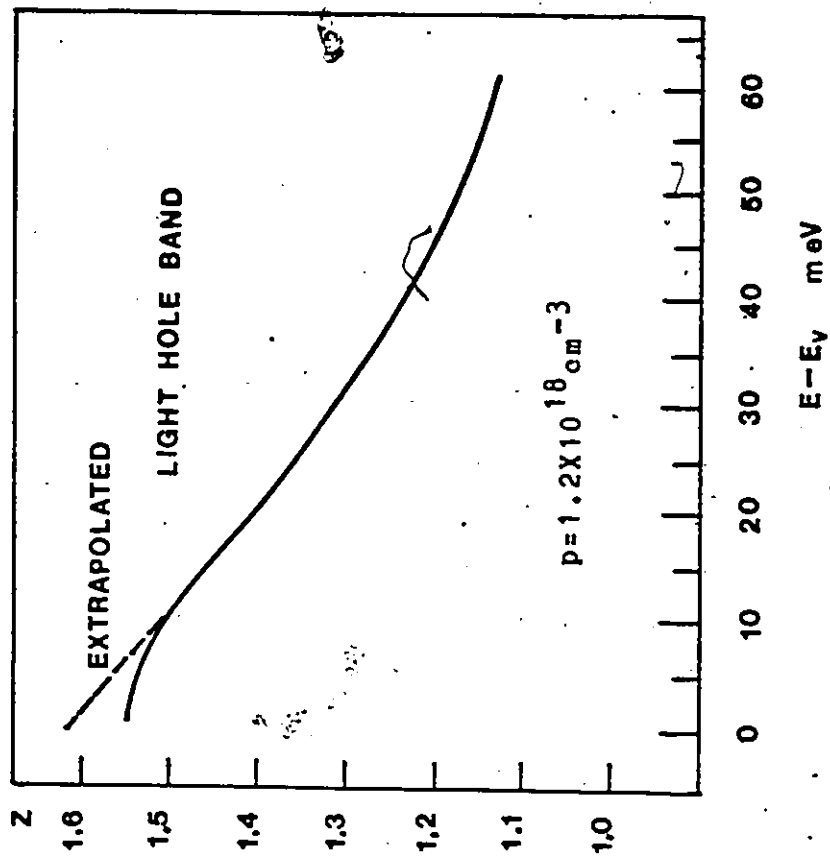


FIGURE 5.2B

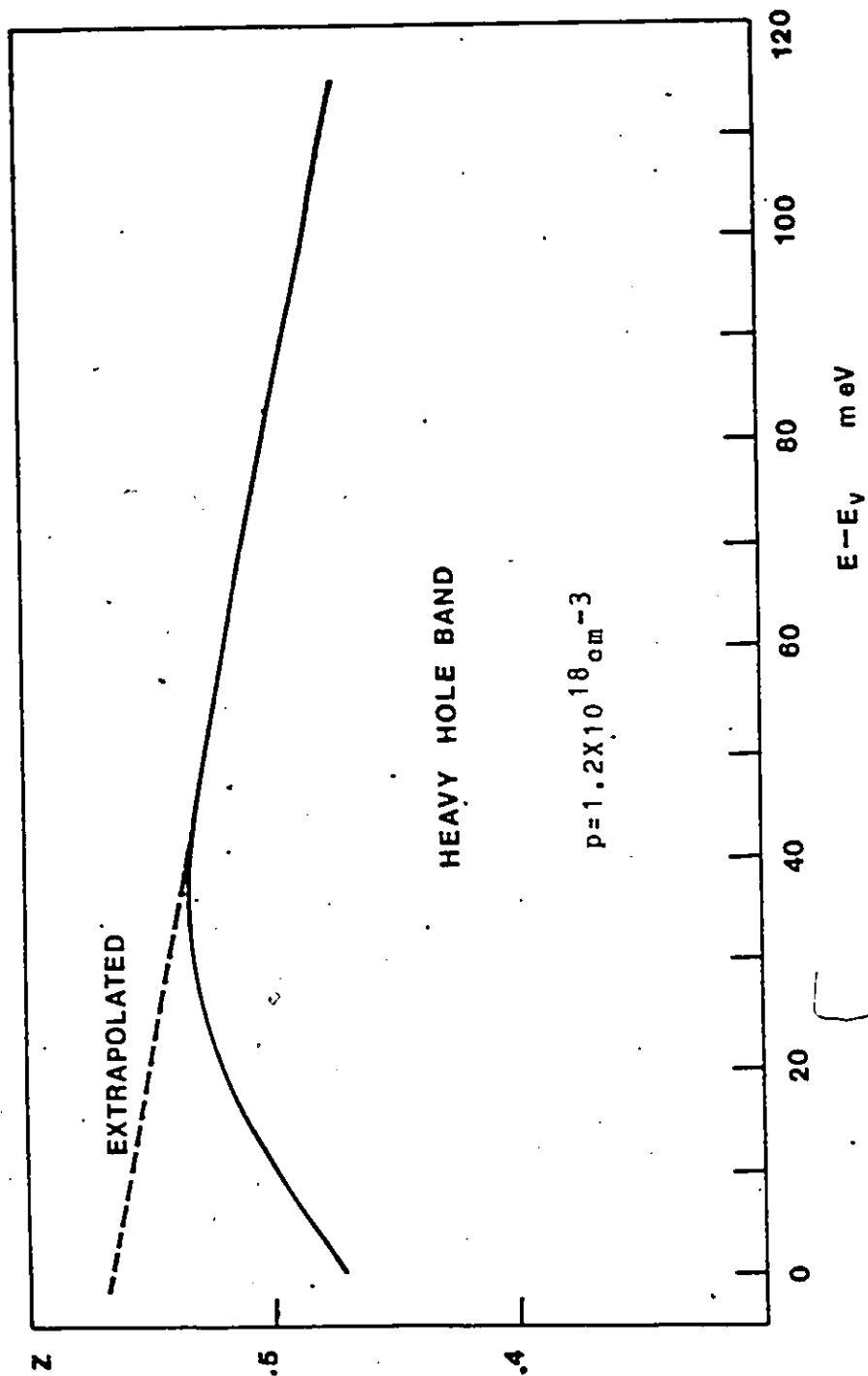


FIGURE 5.2C

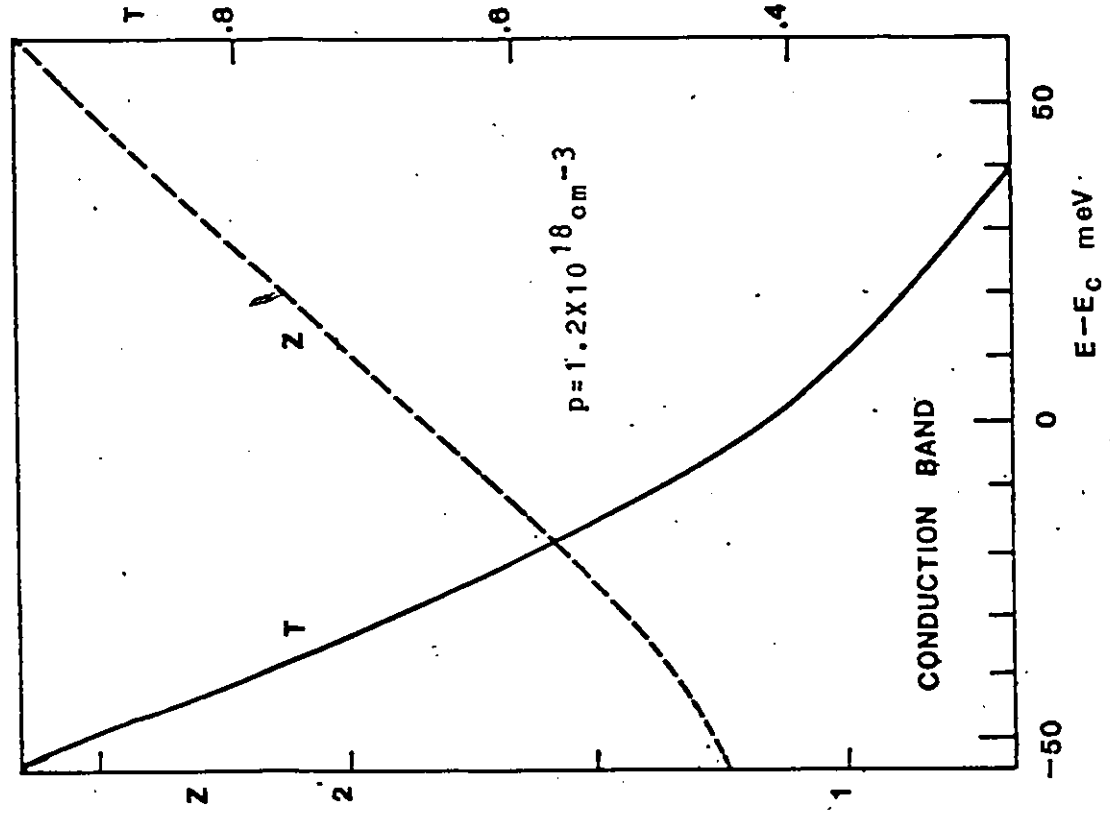


FIGURE 5.3A

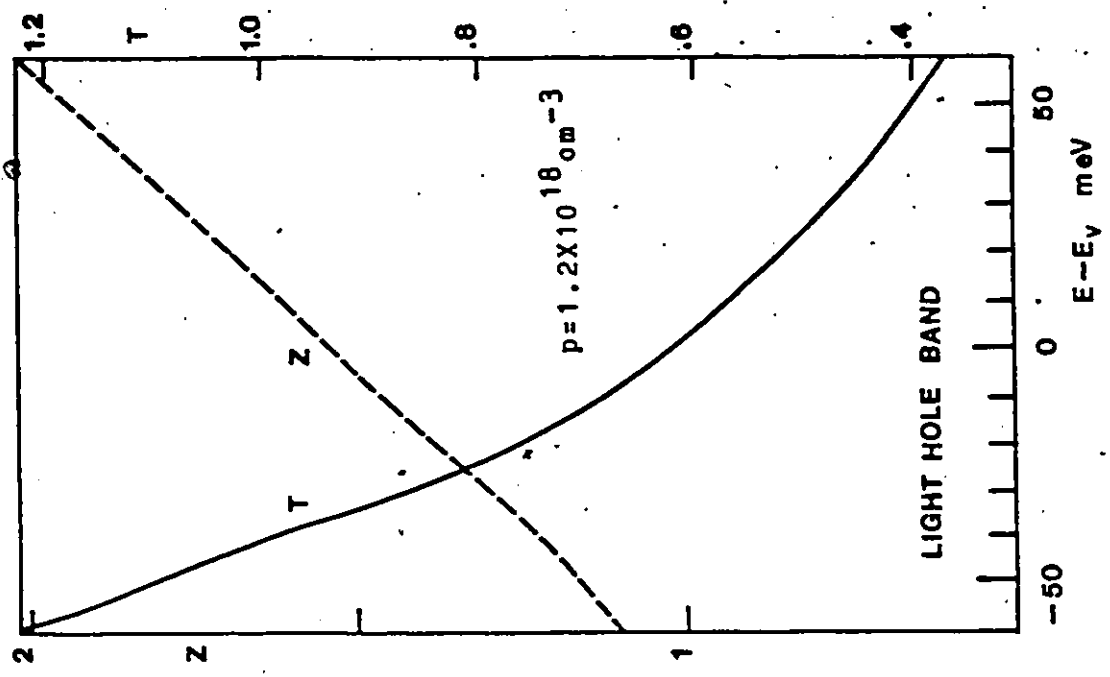


FIGURE 5.3B

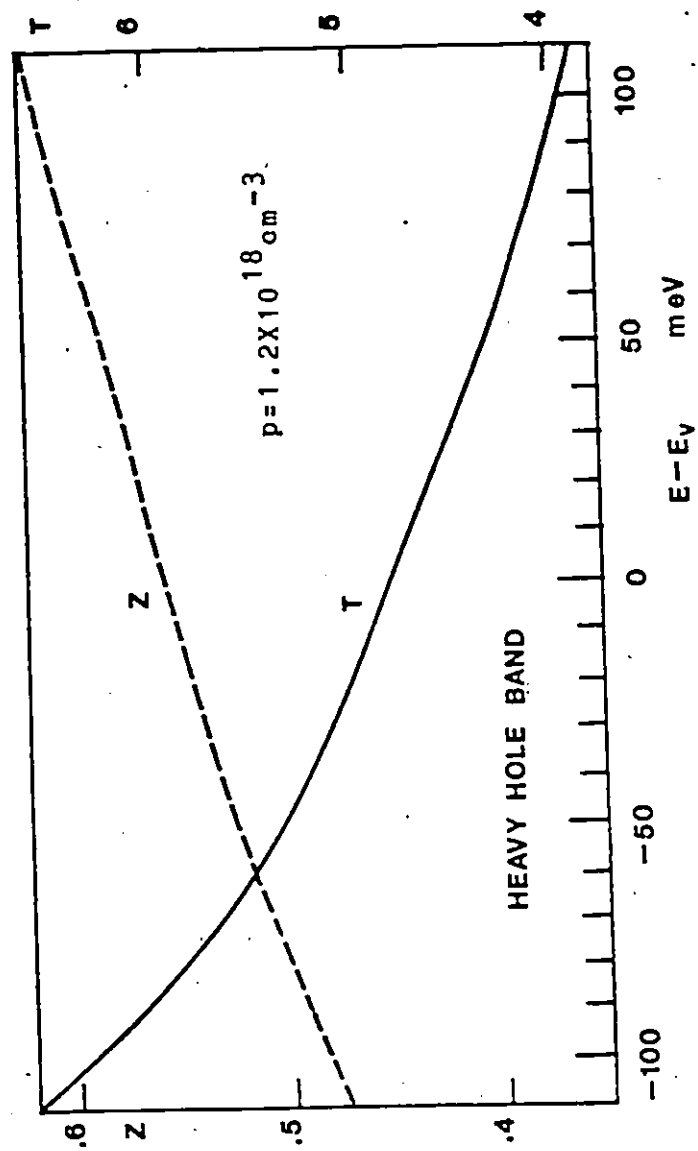


FIGURE 5.3C

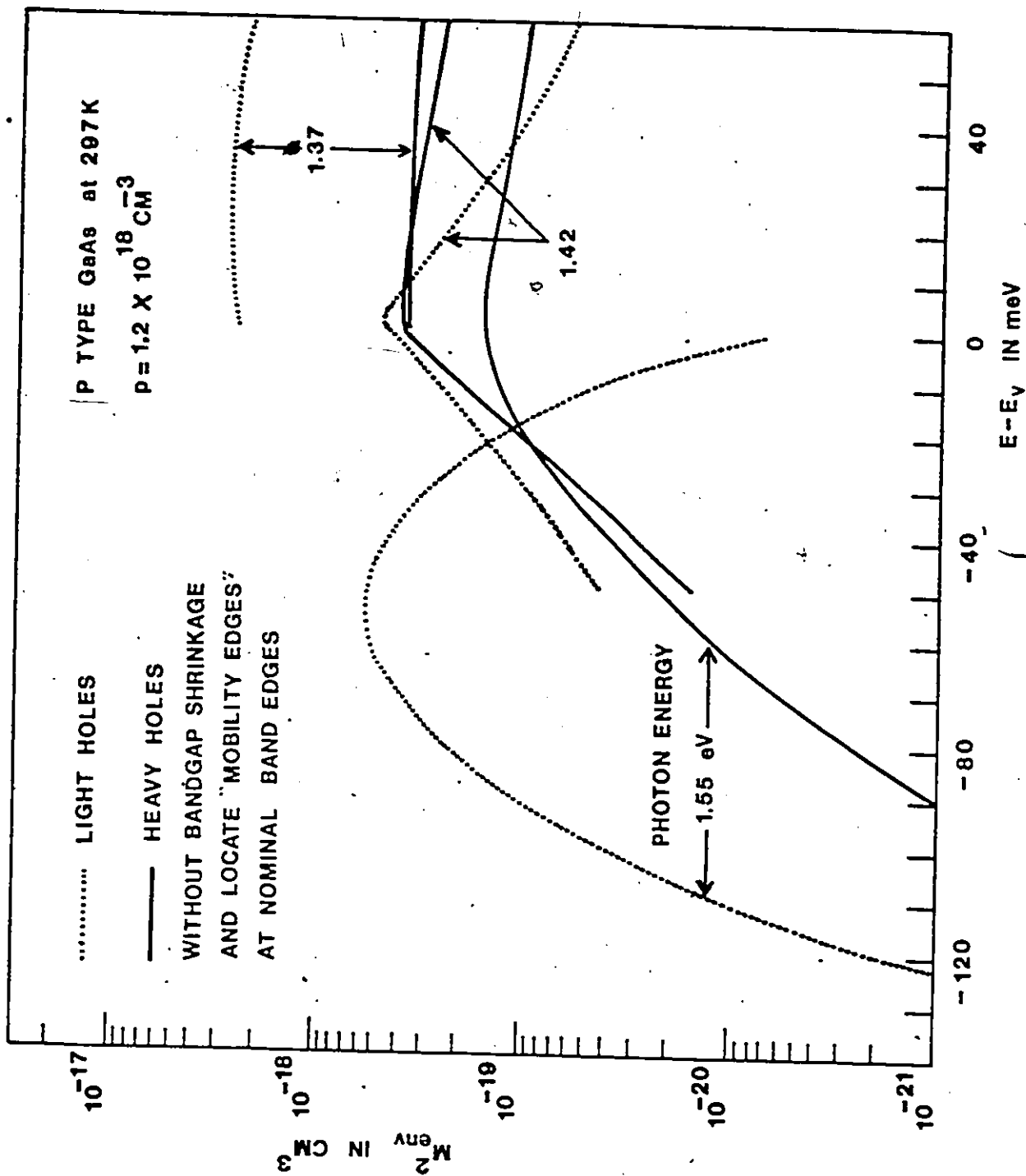


FIGURE 6.1

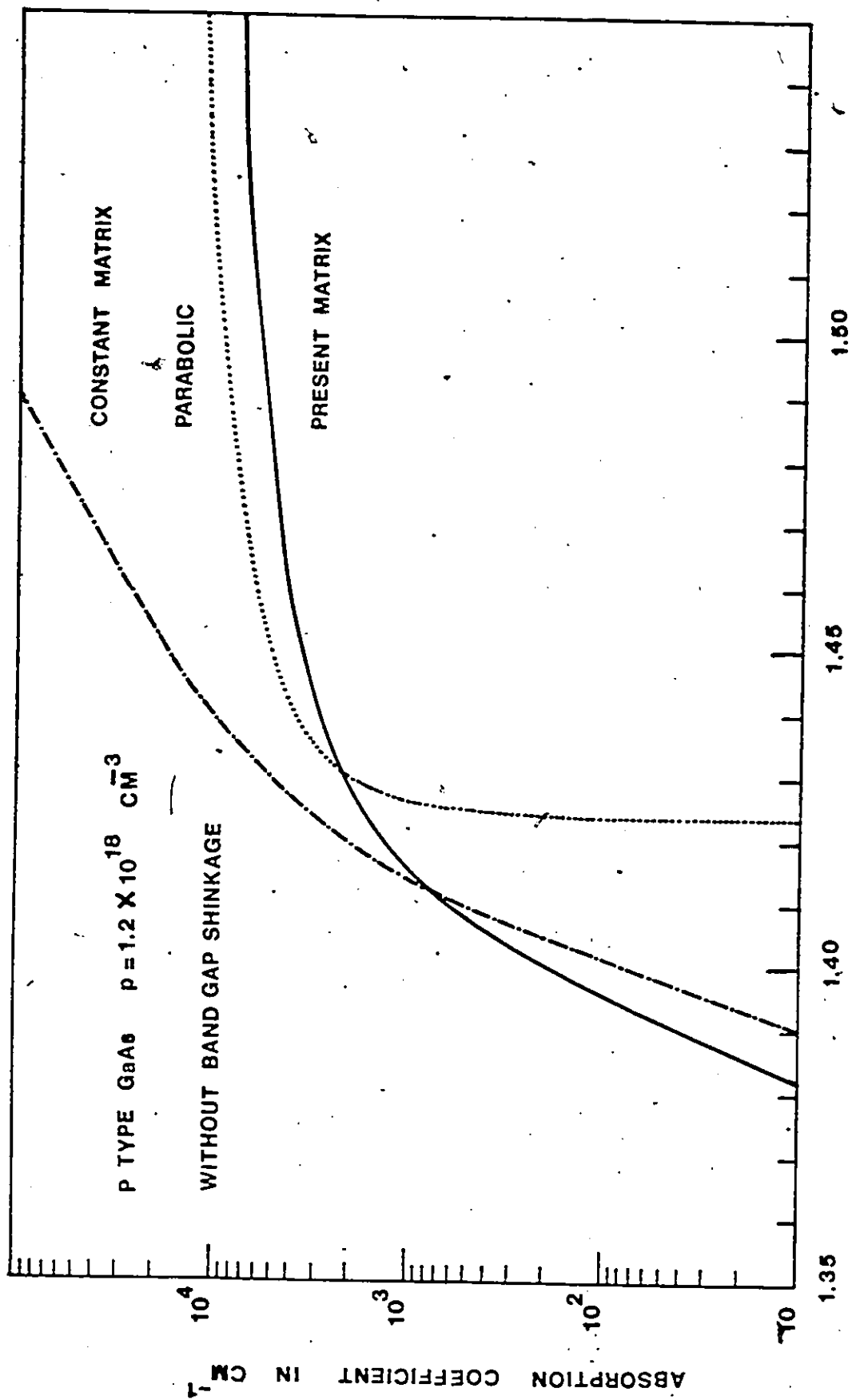


FIGURE 6.2

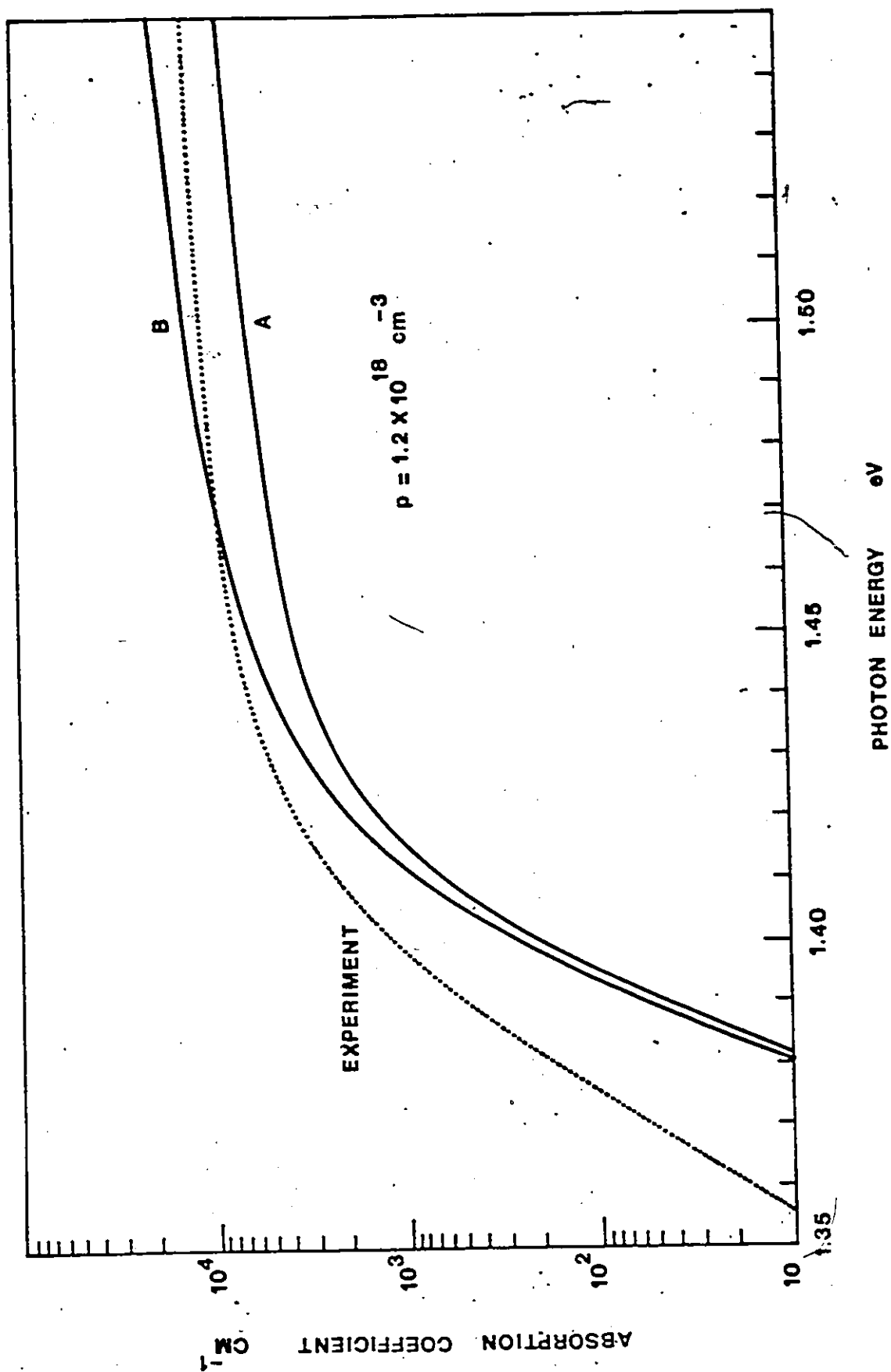


FIGURE 6.3

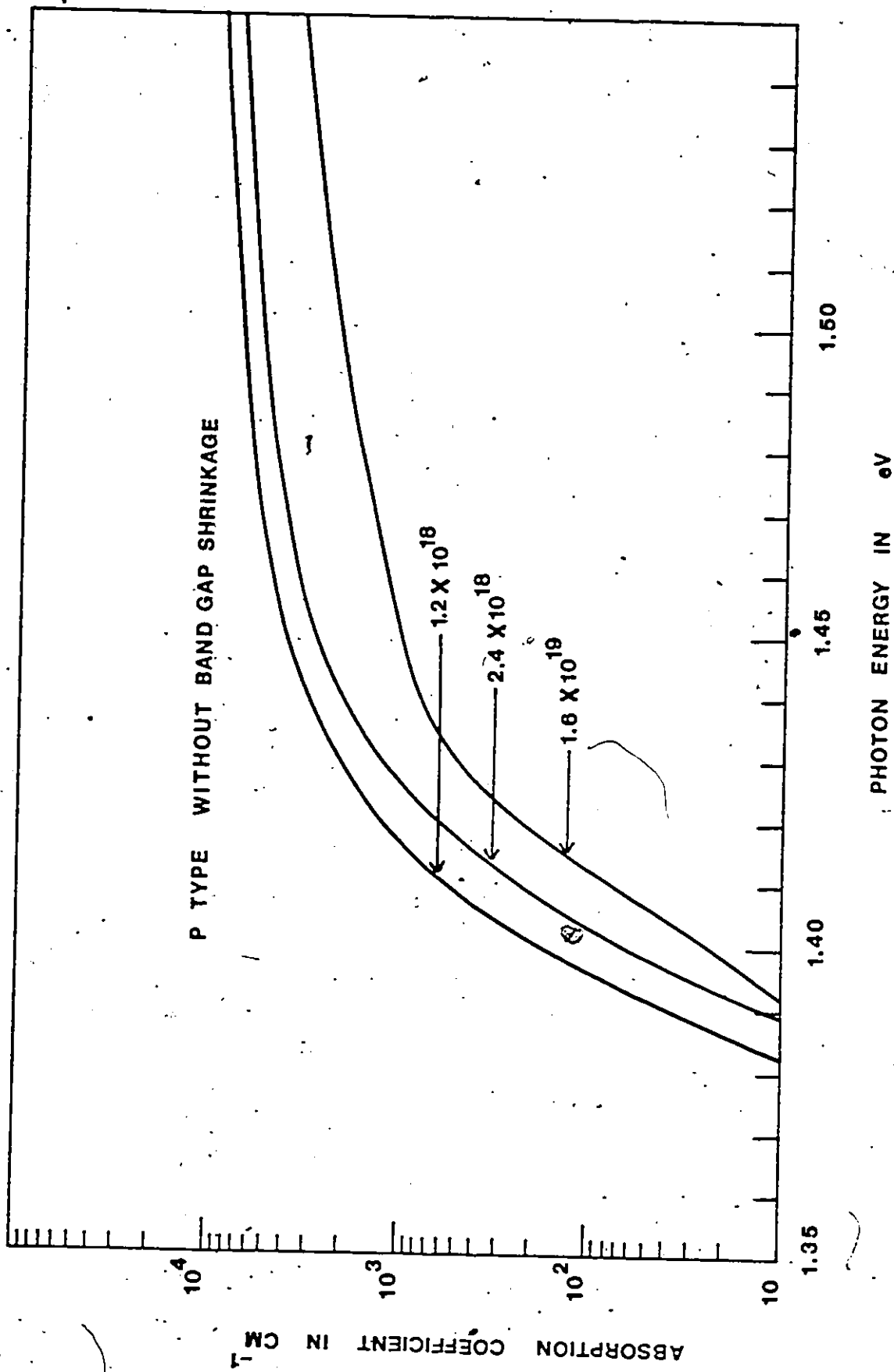


FIGURE 6.4

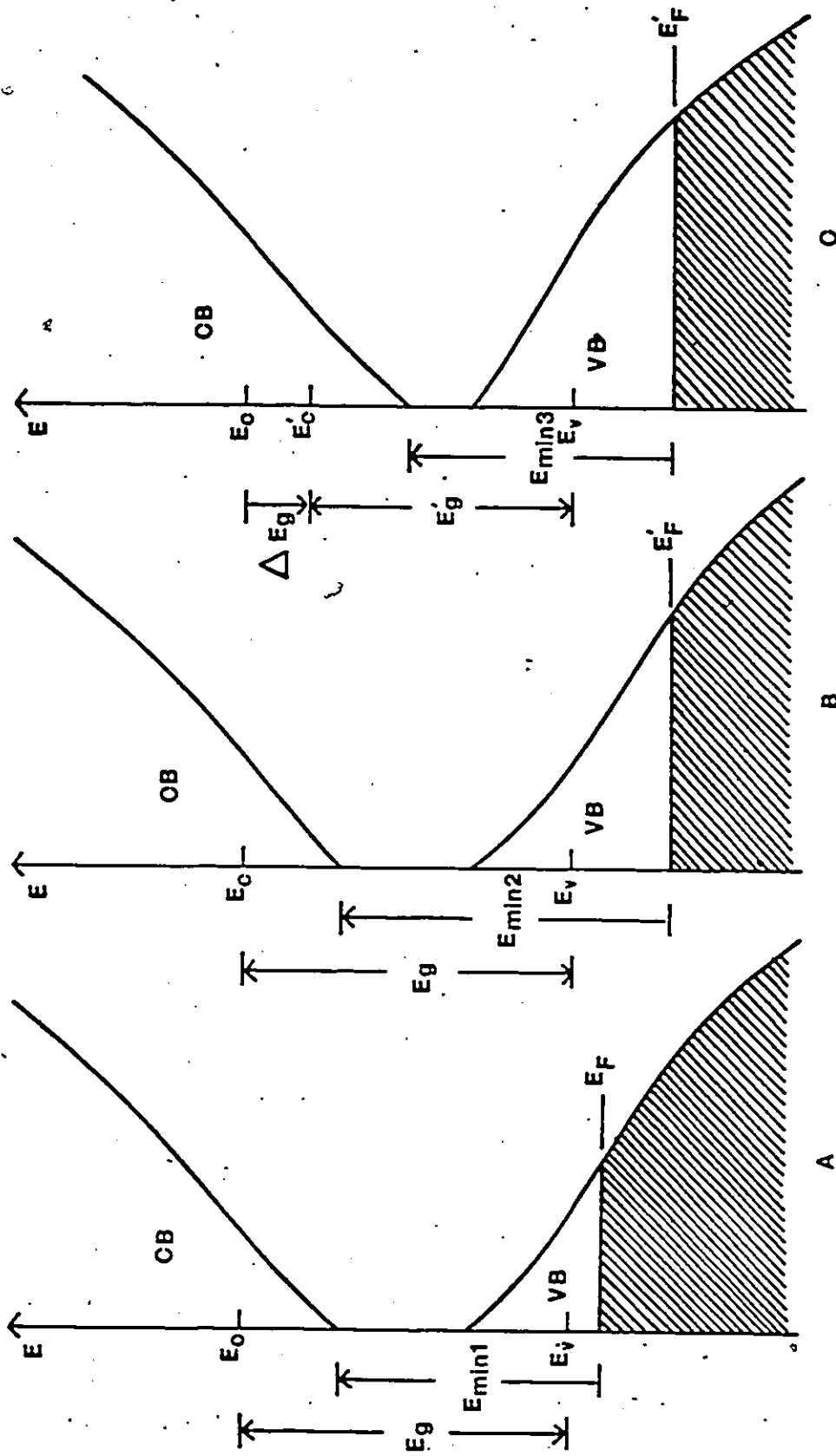


FIGURE 6.5

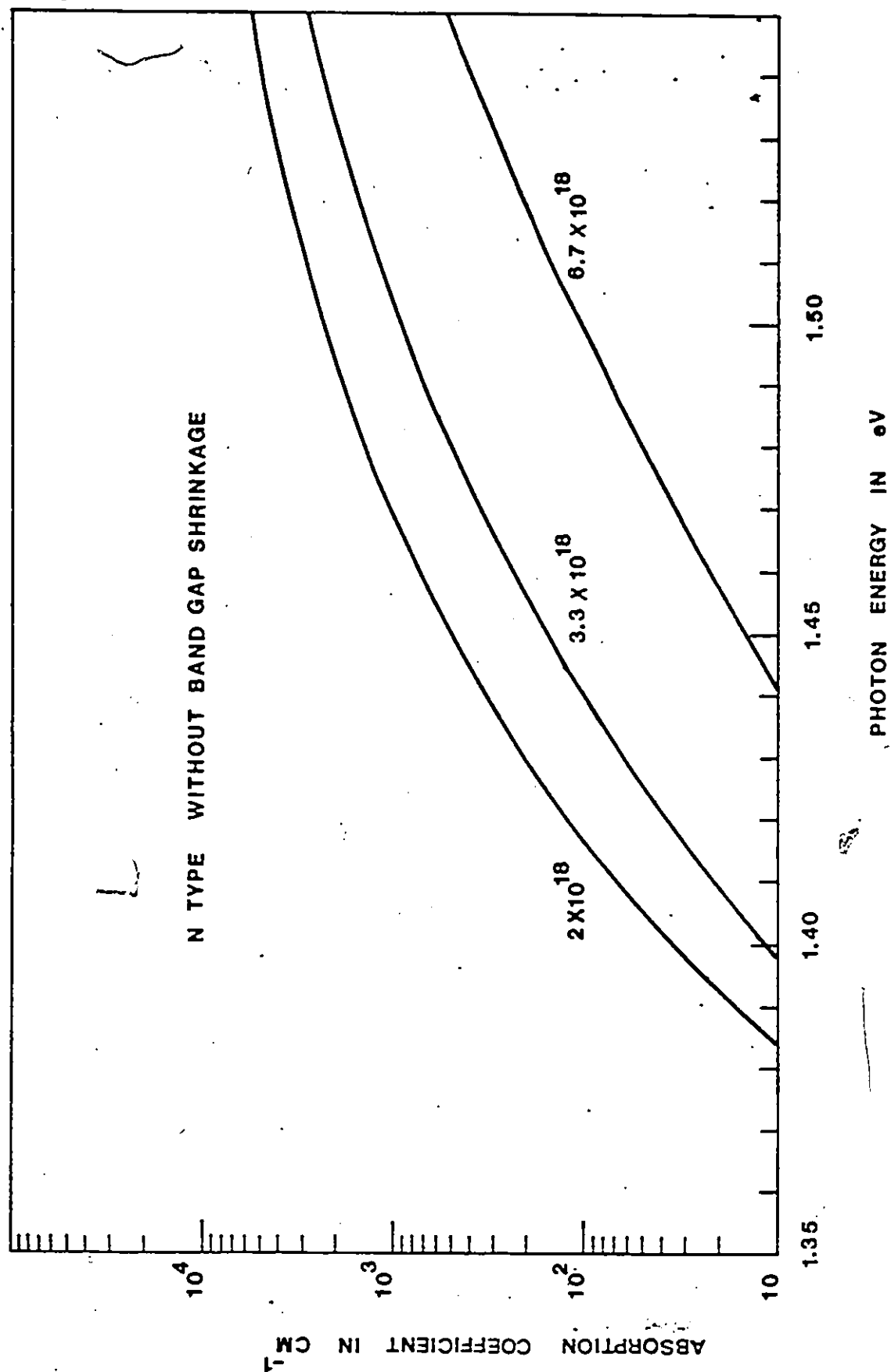


FIGURE 6.6

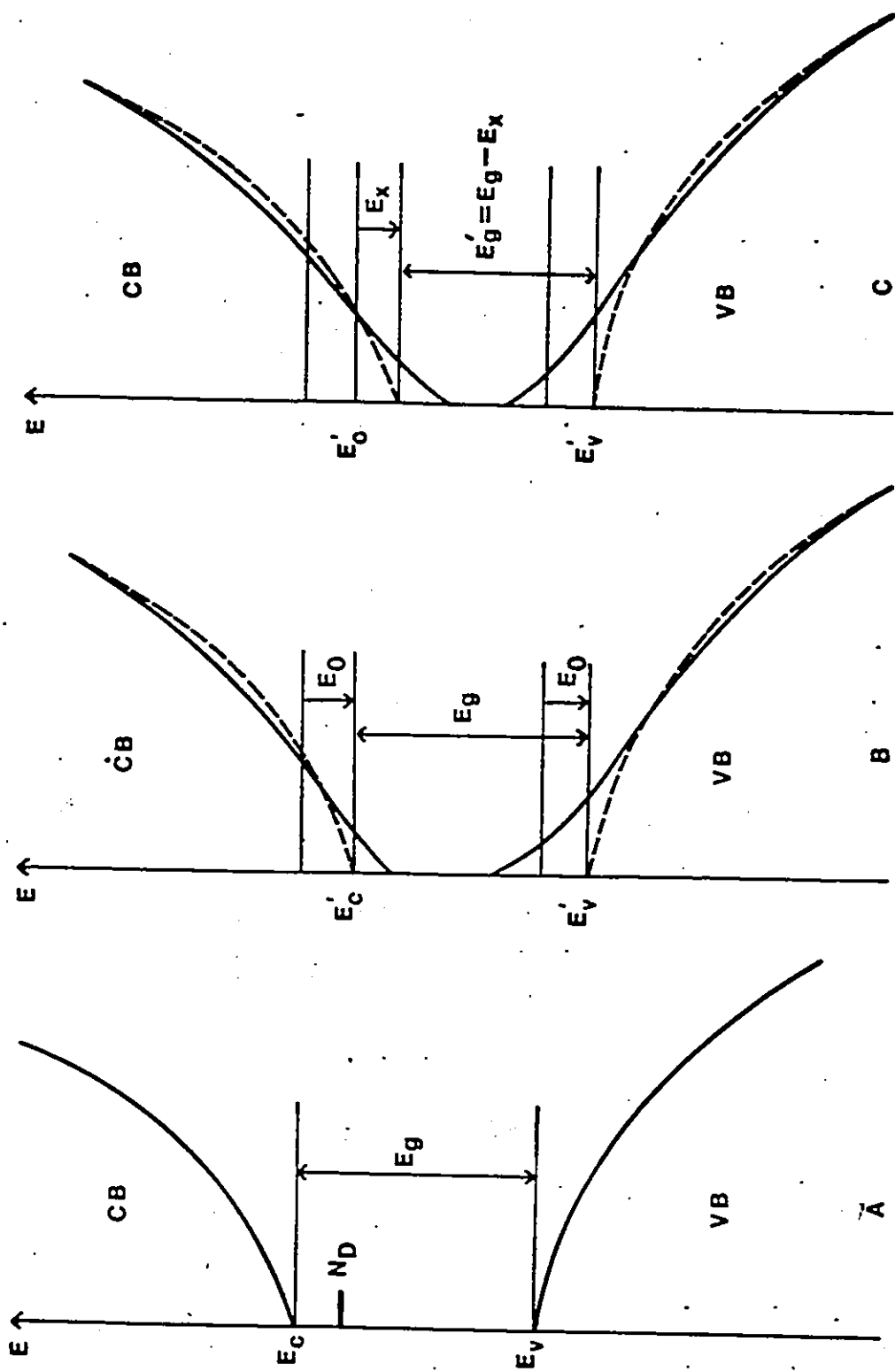


FIGURE 6.7

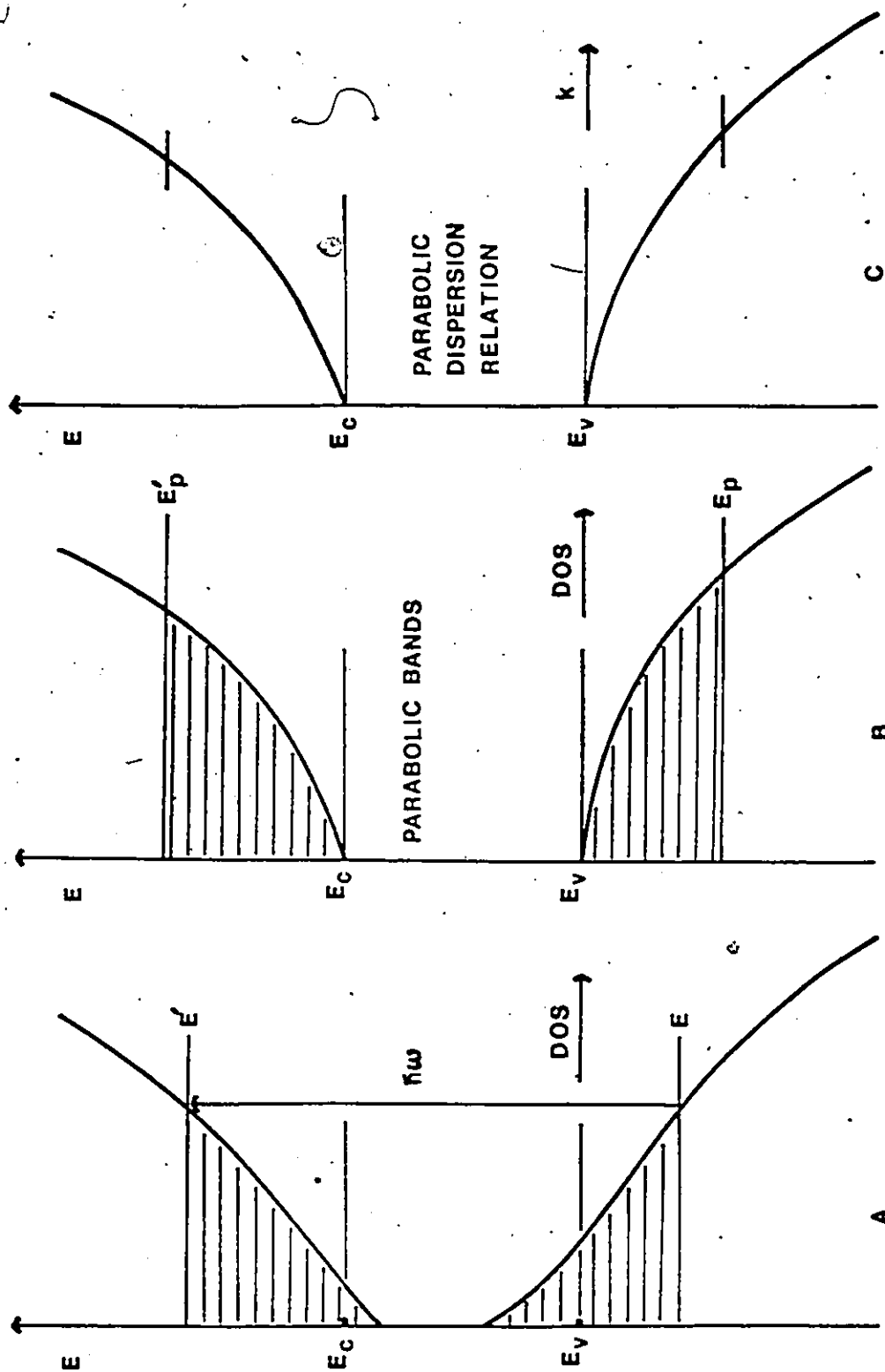


FIGURE 6.8

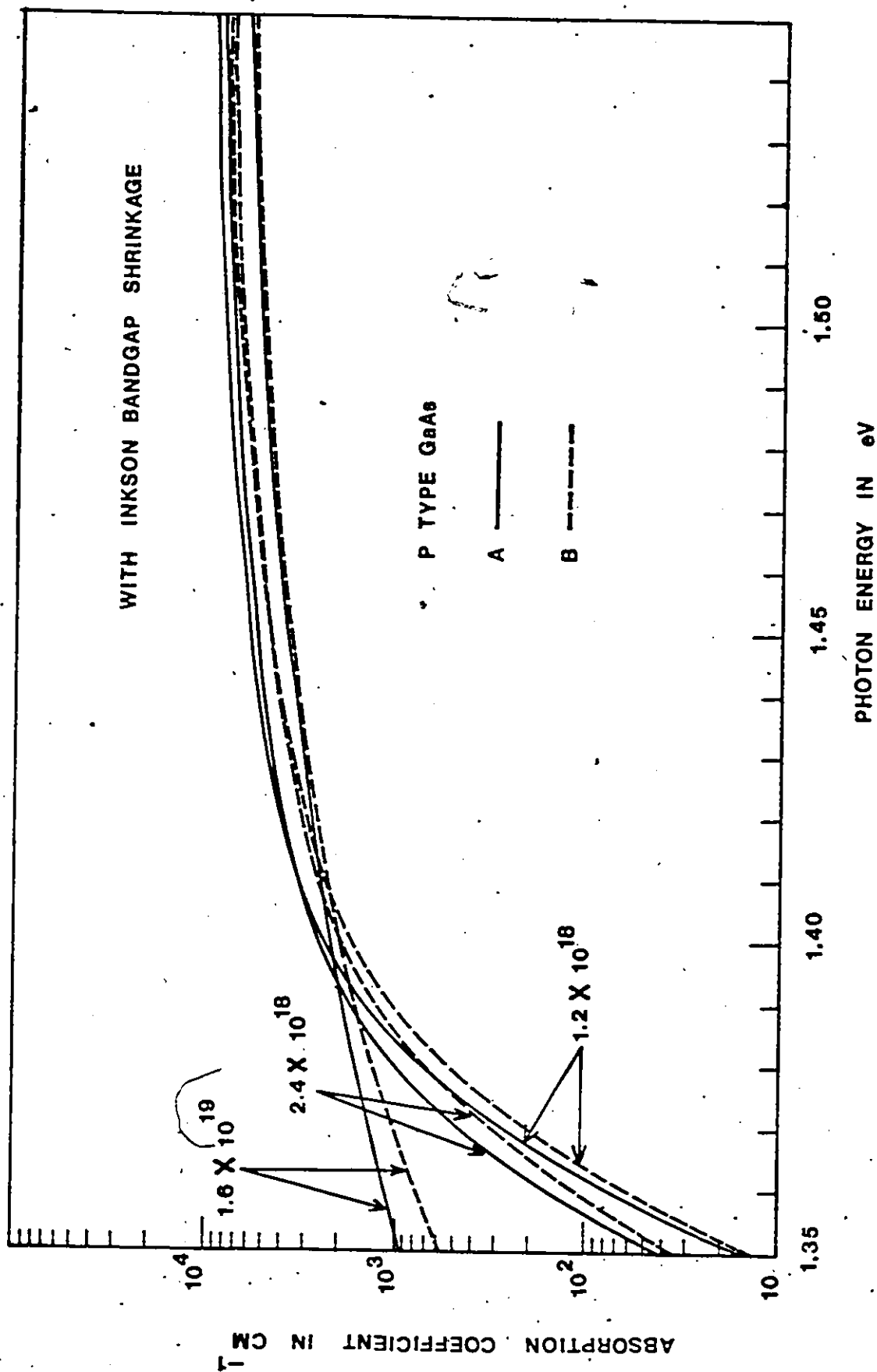


FIGURE 6.9

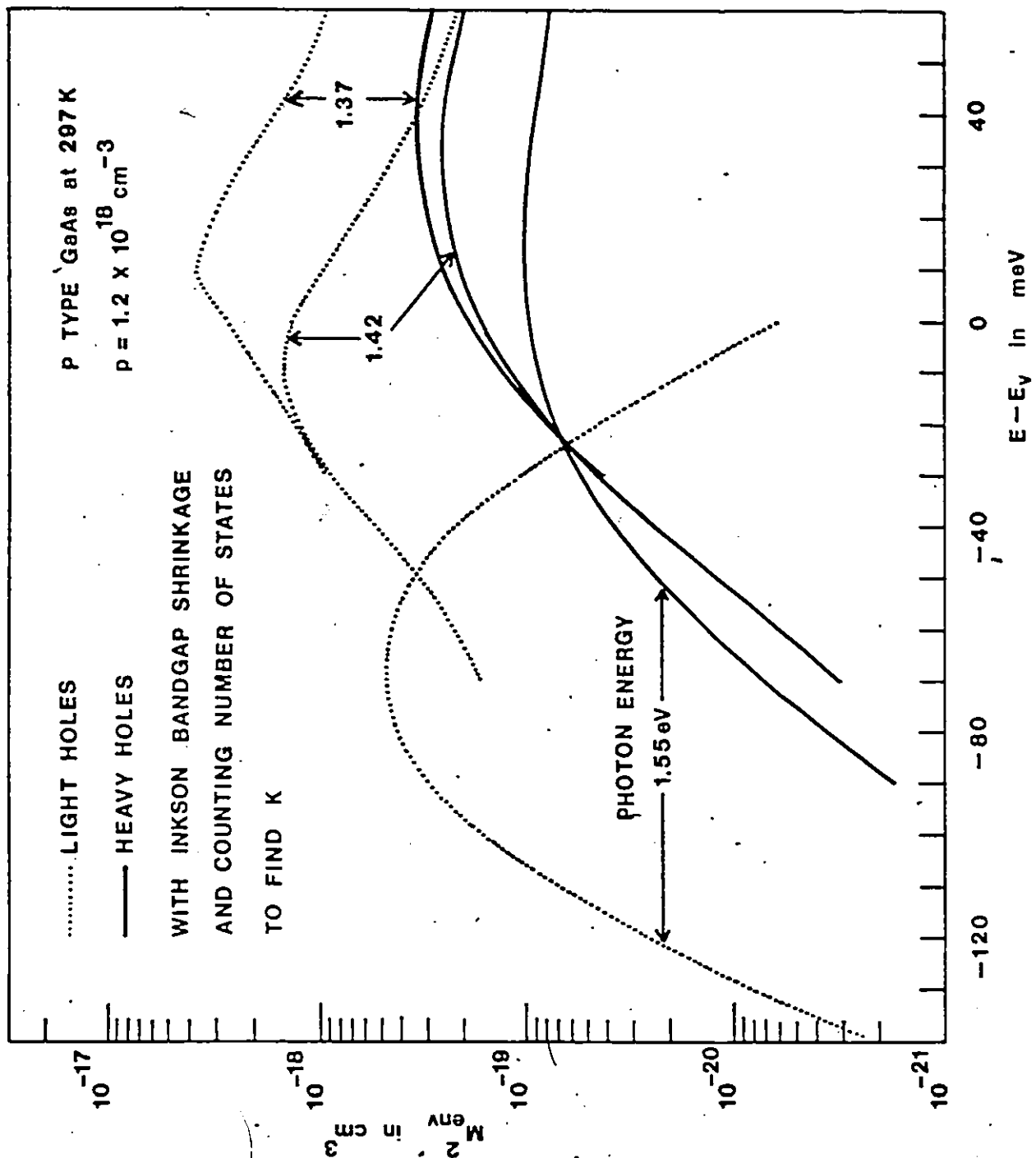


FIGURE 6.10

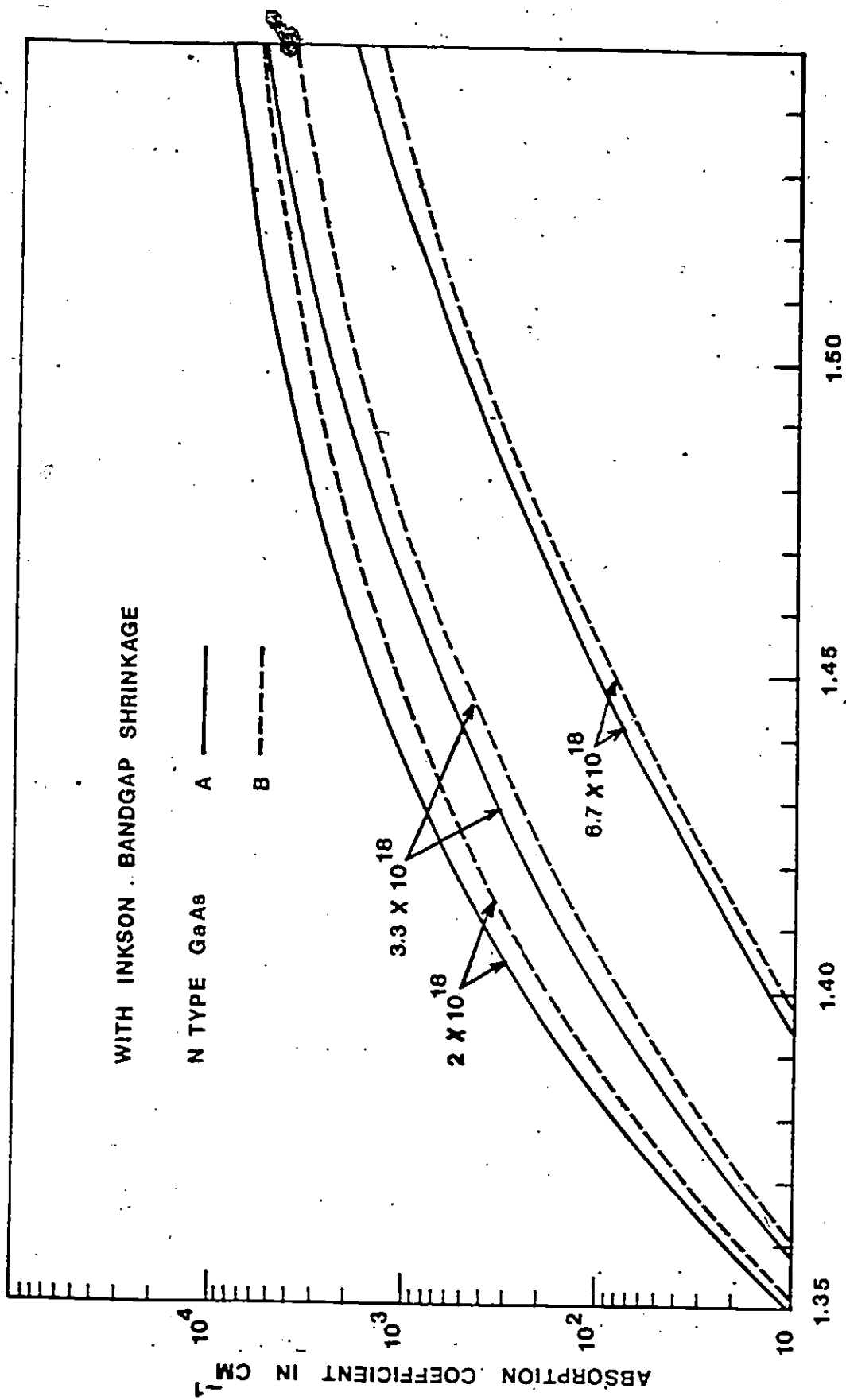


FIGURE 6.11

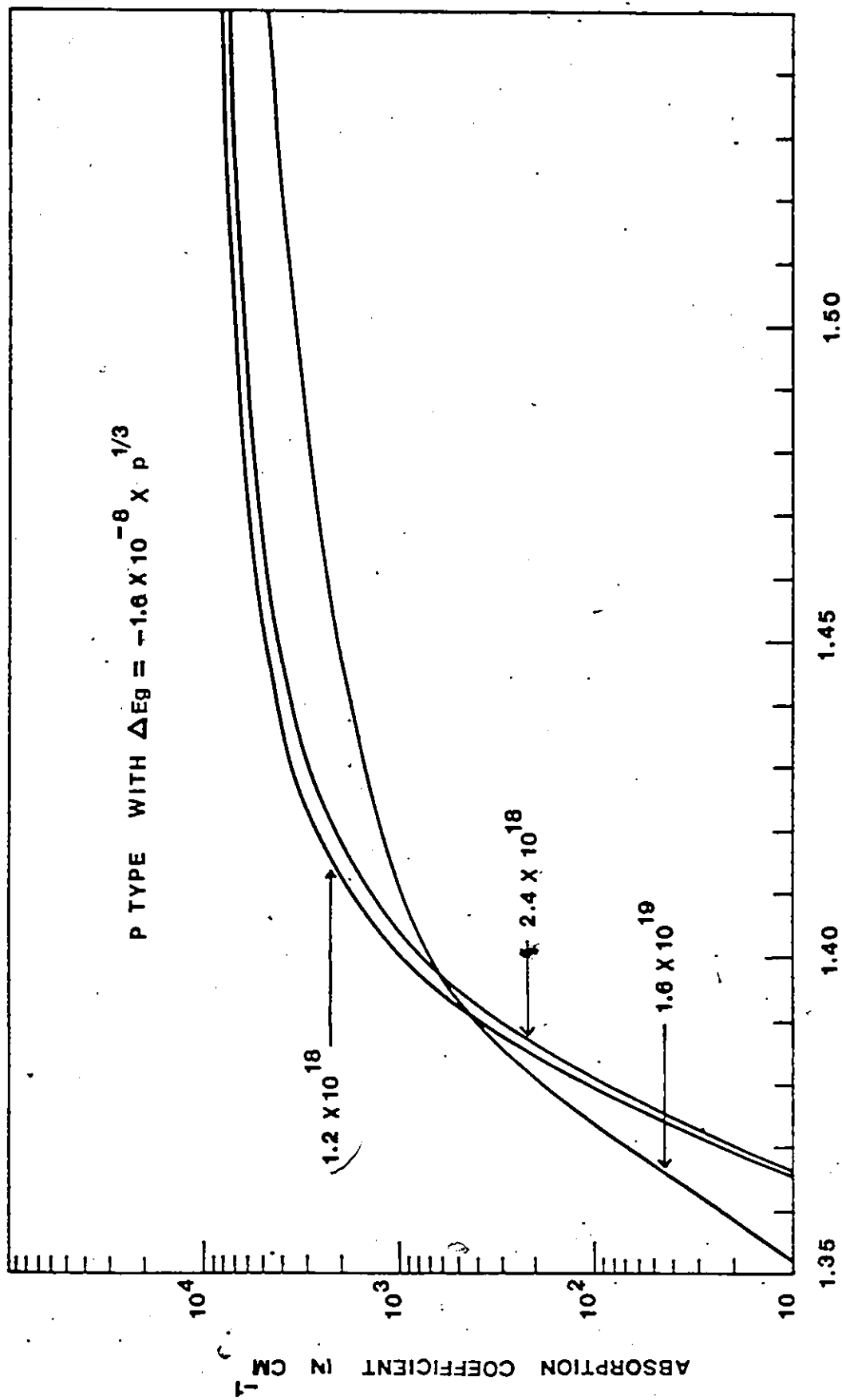


FIGURE 6.12

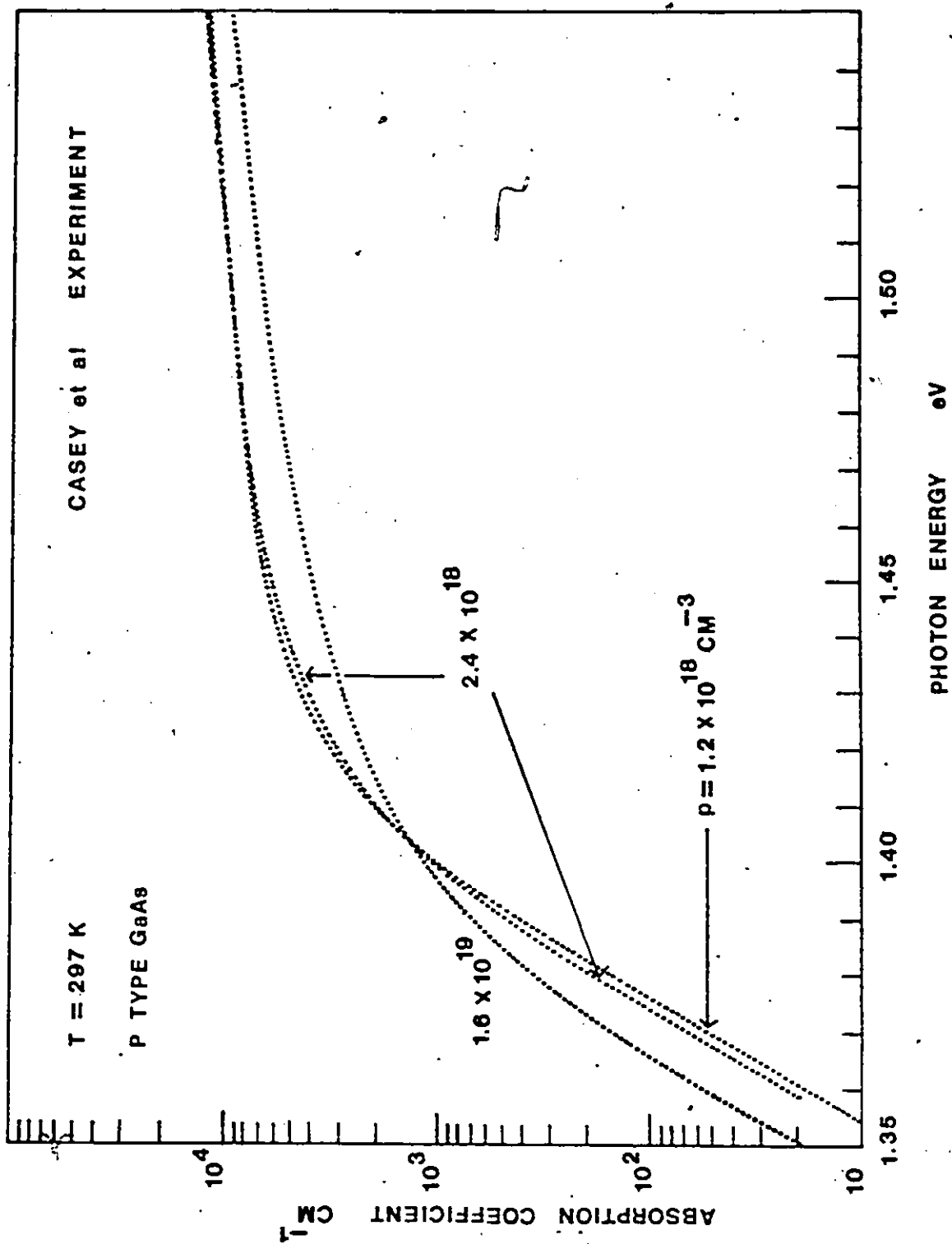


FIGURE 6.13

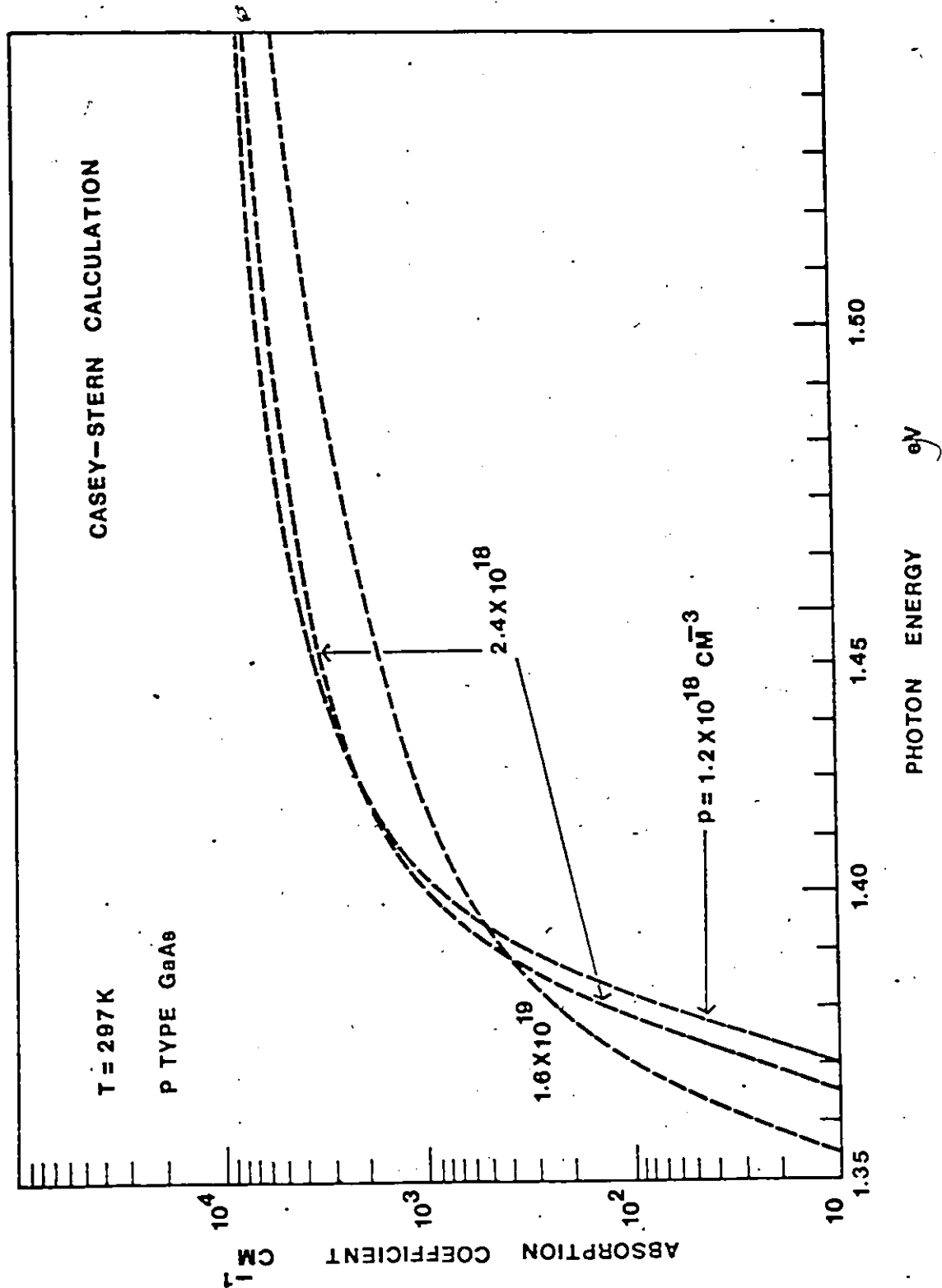


FIGURE 6.14

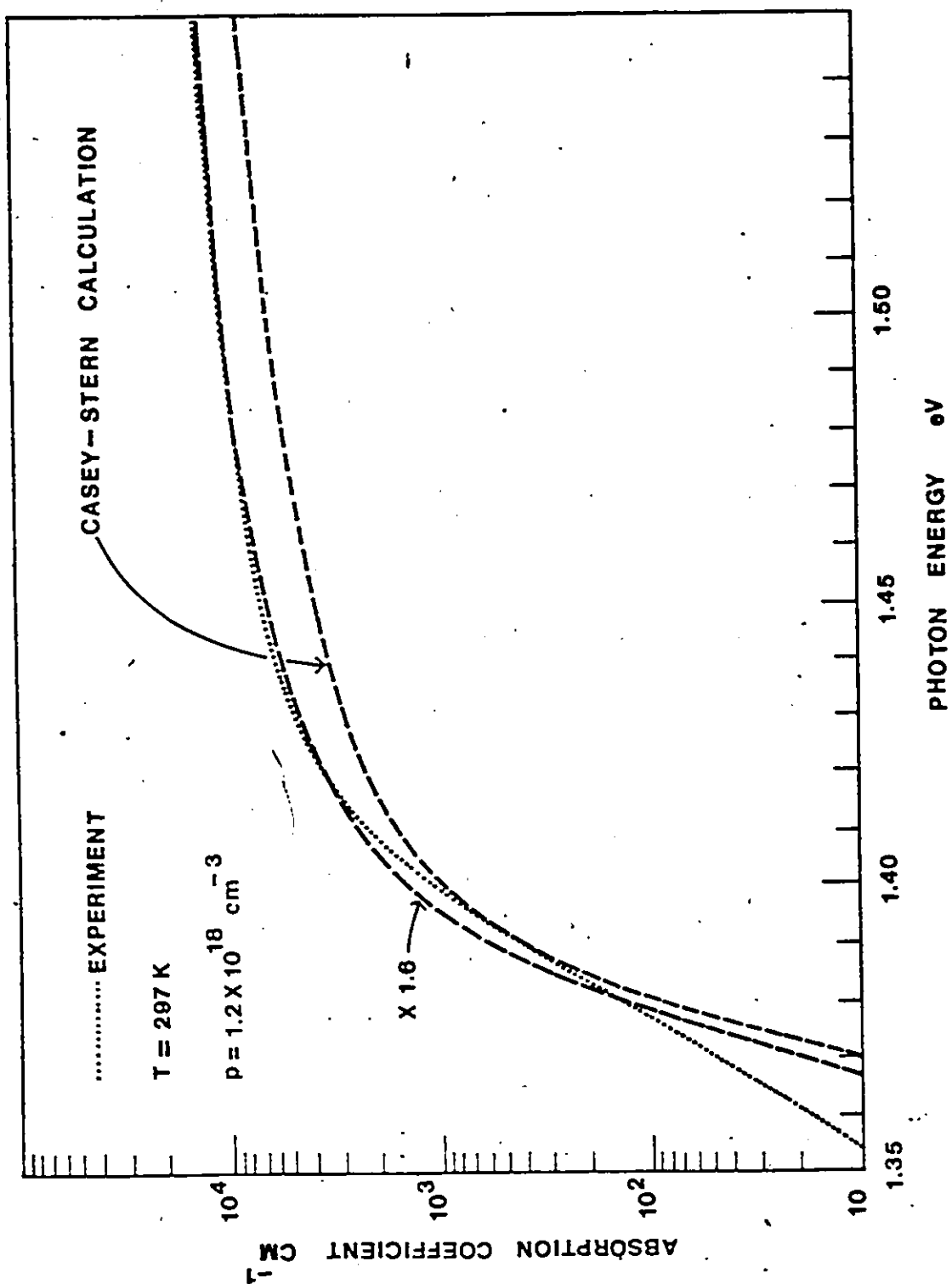


FIGURE 6.15

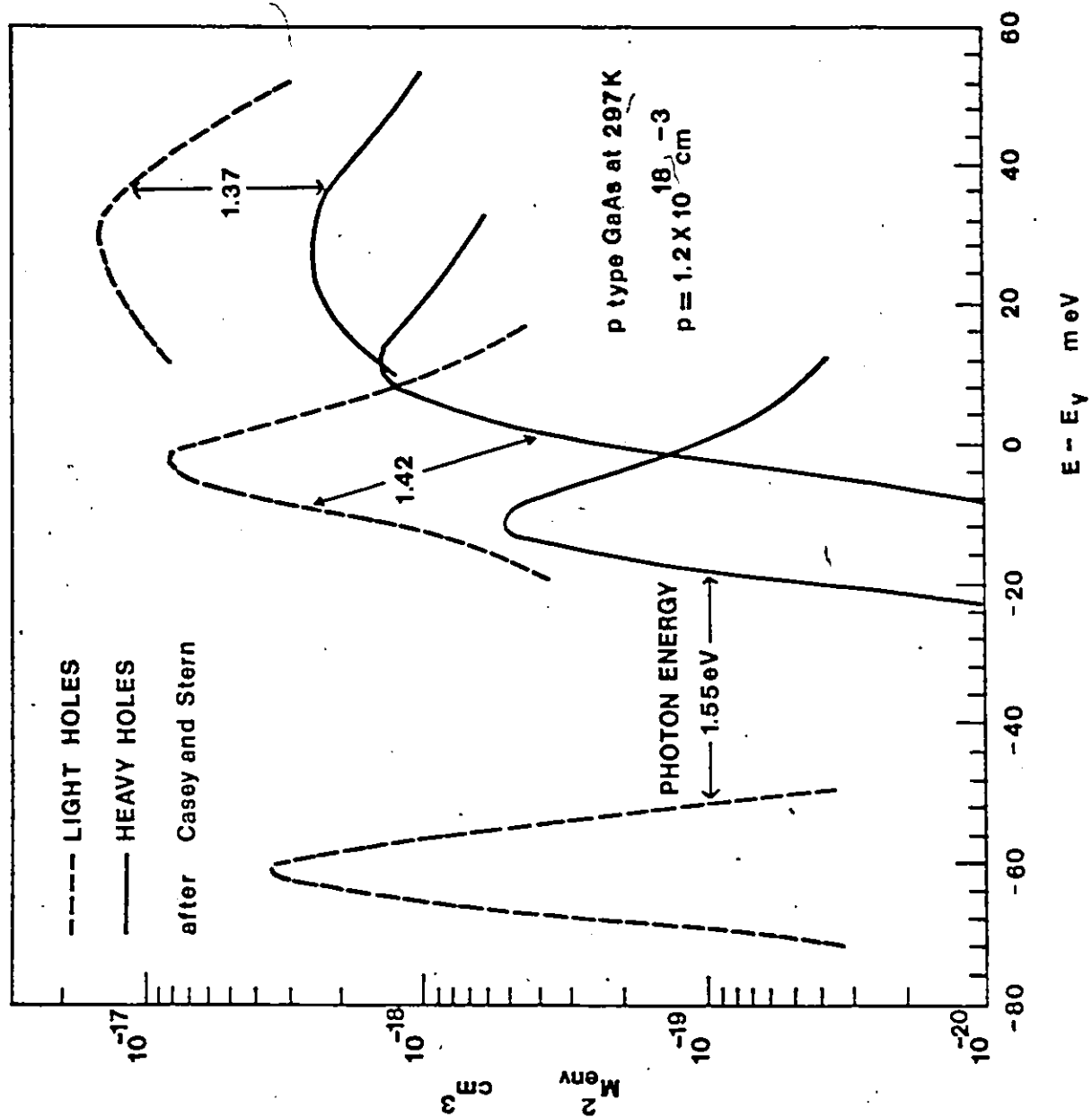


FIGURE 6.16

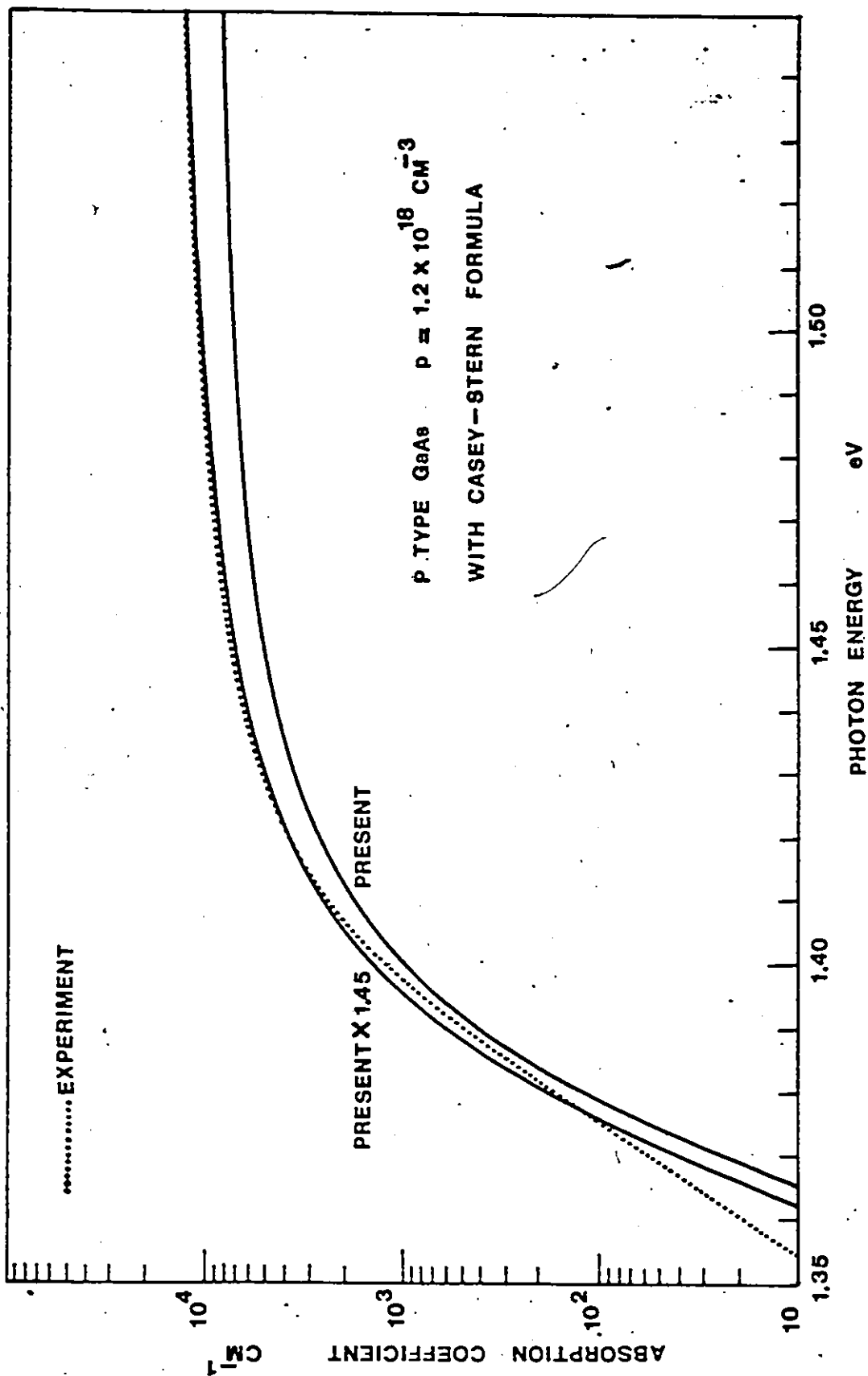


FIGURE 6.17

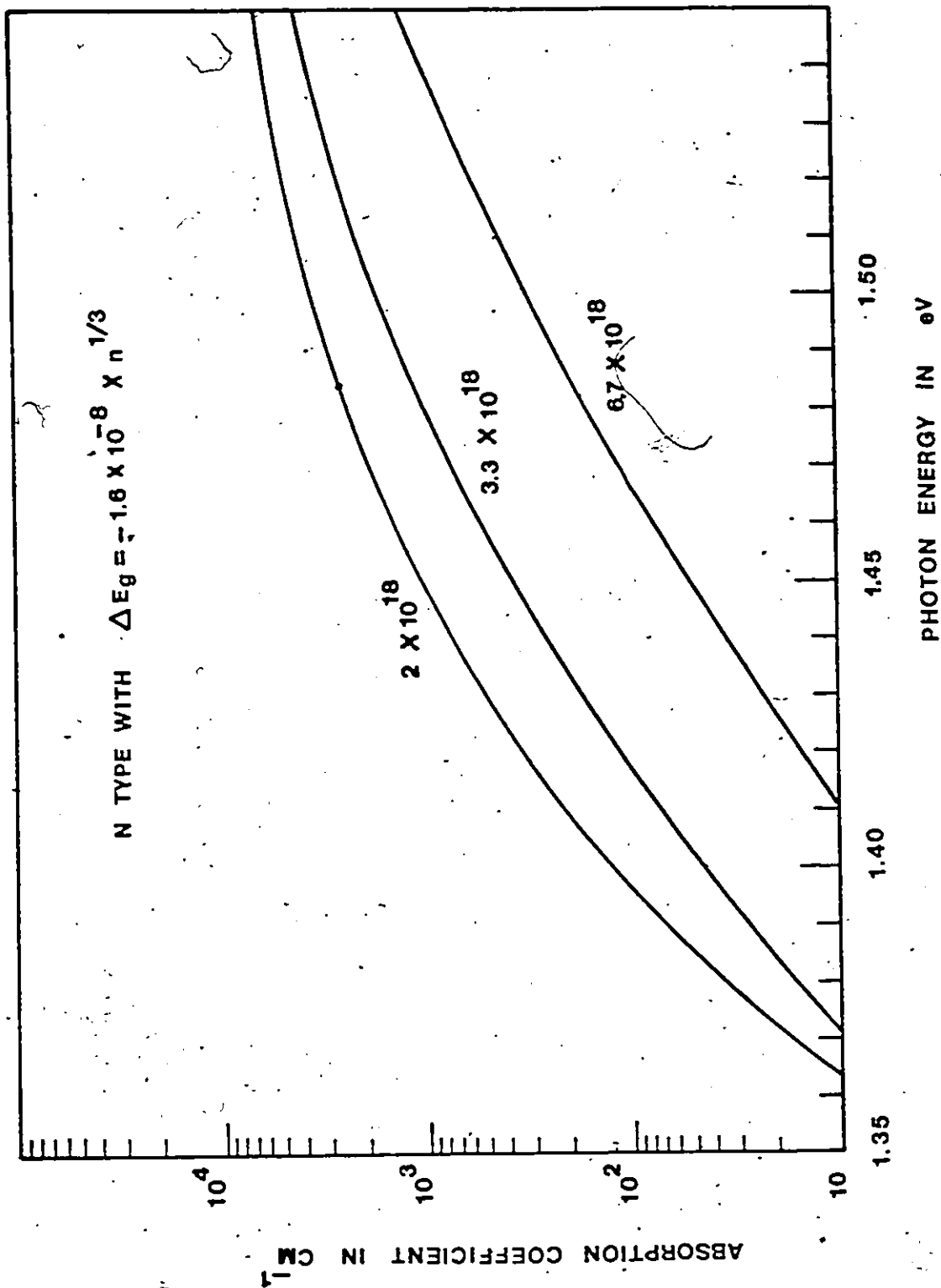


FIGURE 6.18

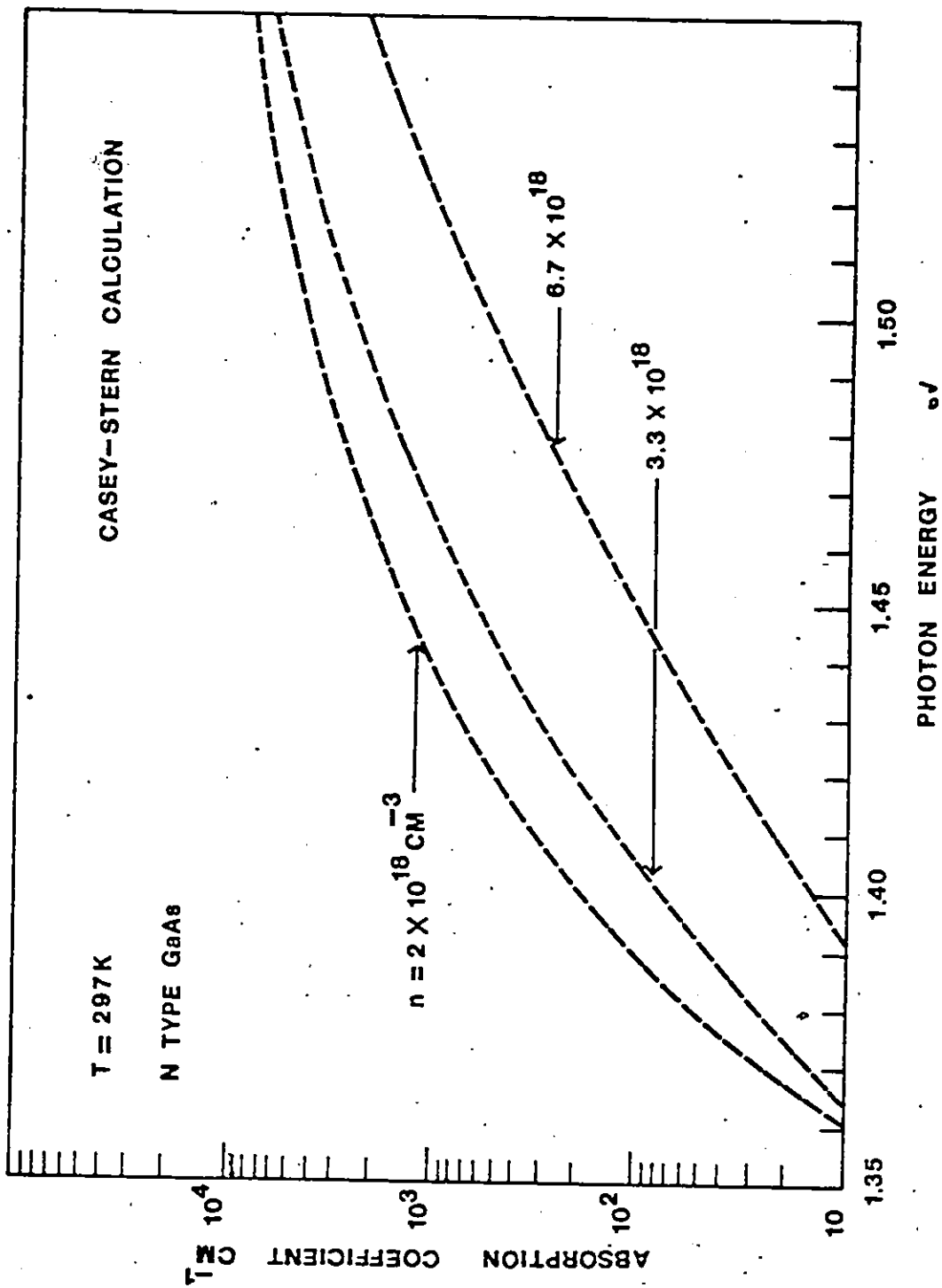


FIGURE 6.19

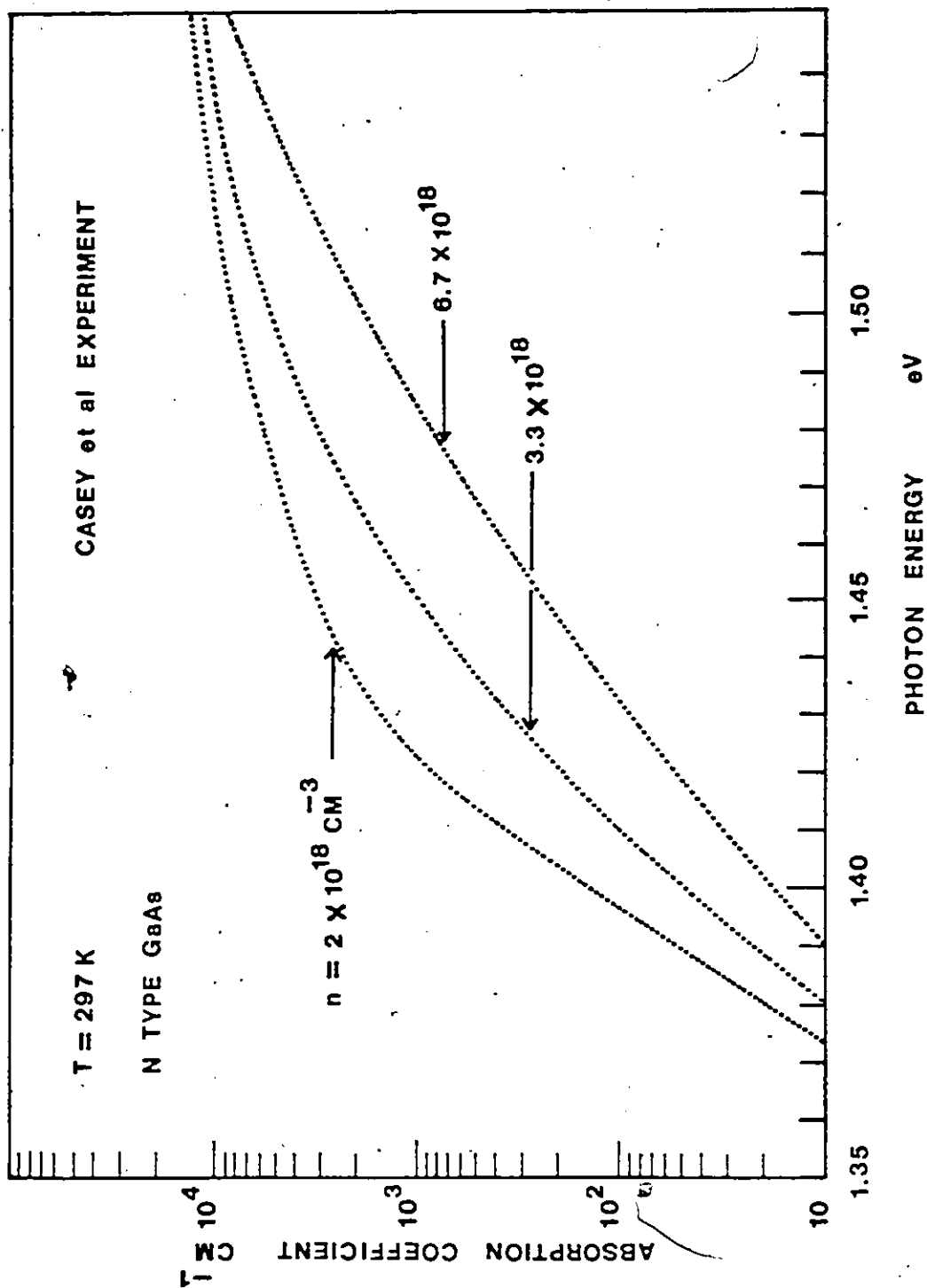


FIGURE 6.20

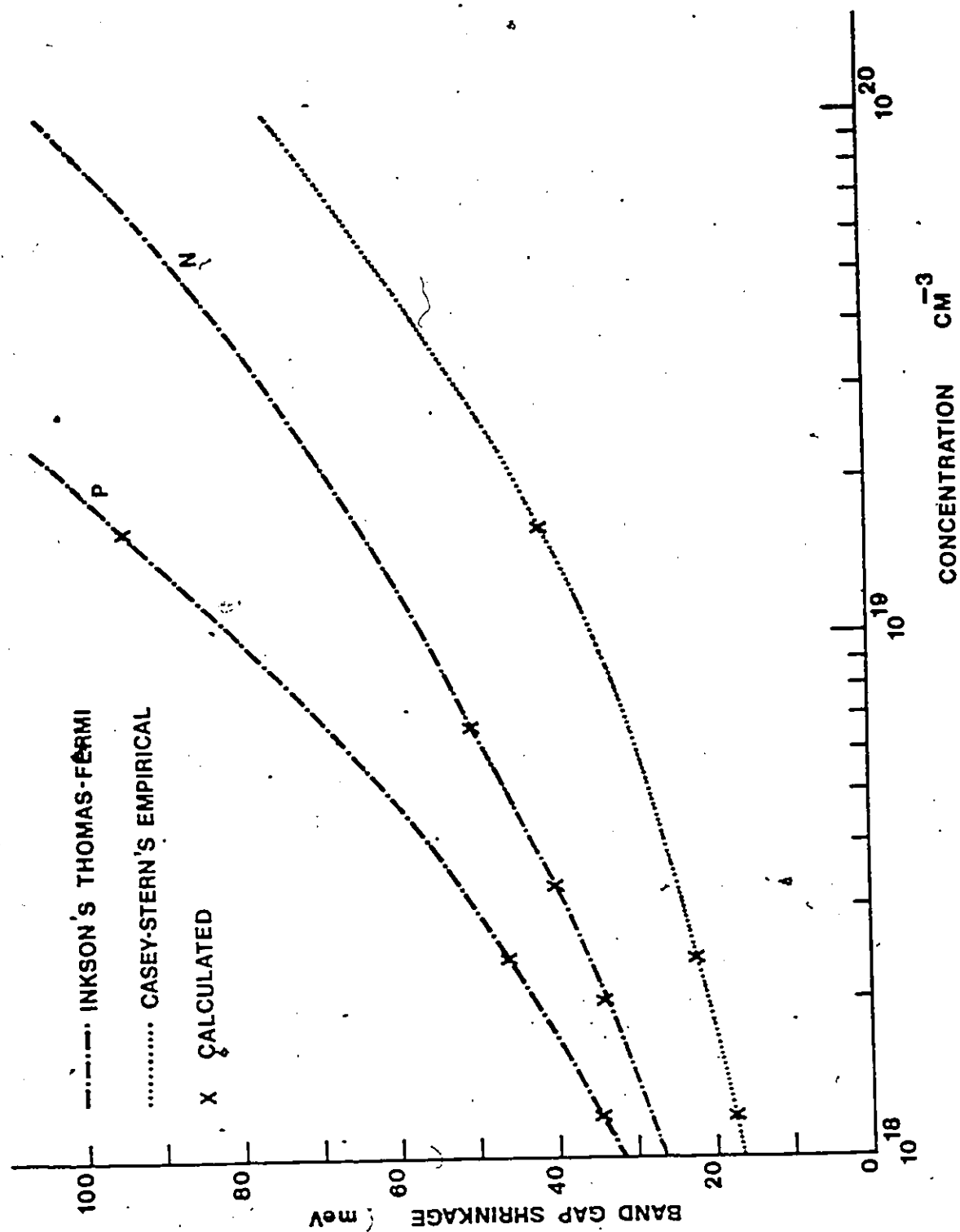


FIGURE 6.21

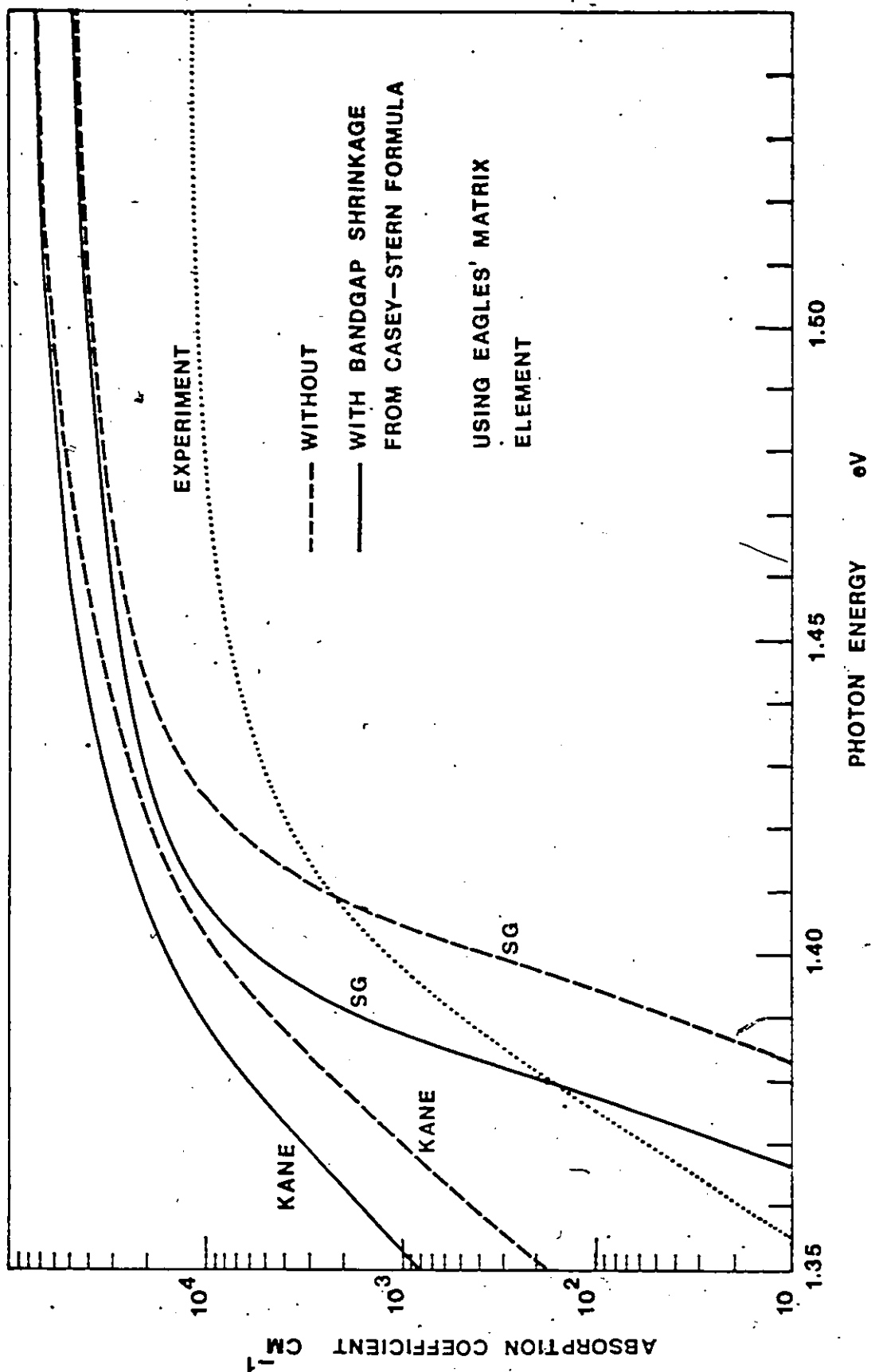


FIGURE 6.22

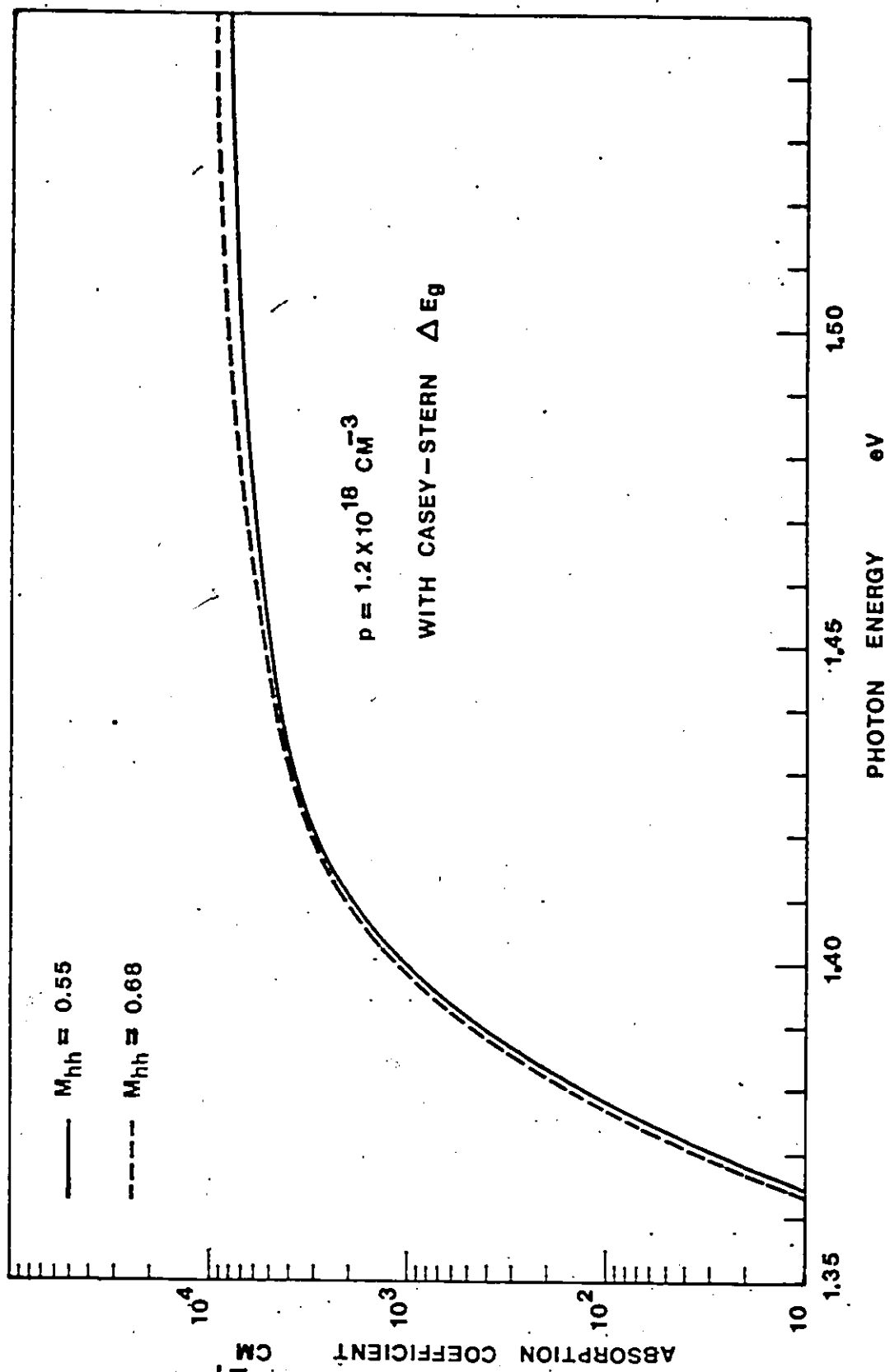


FIGURE 6.23

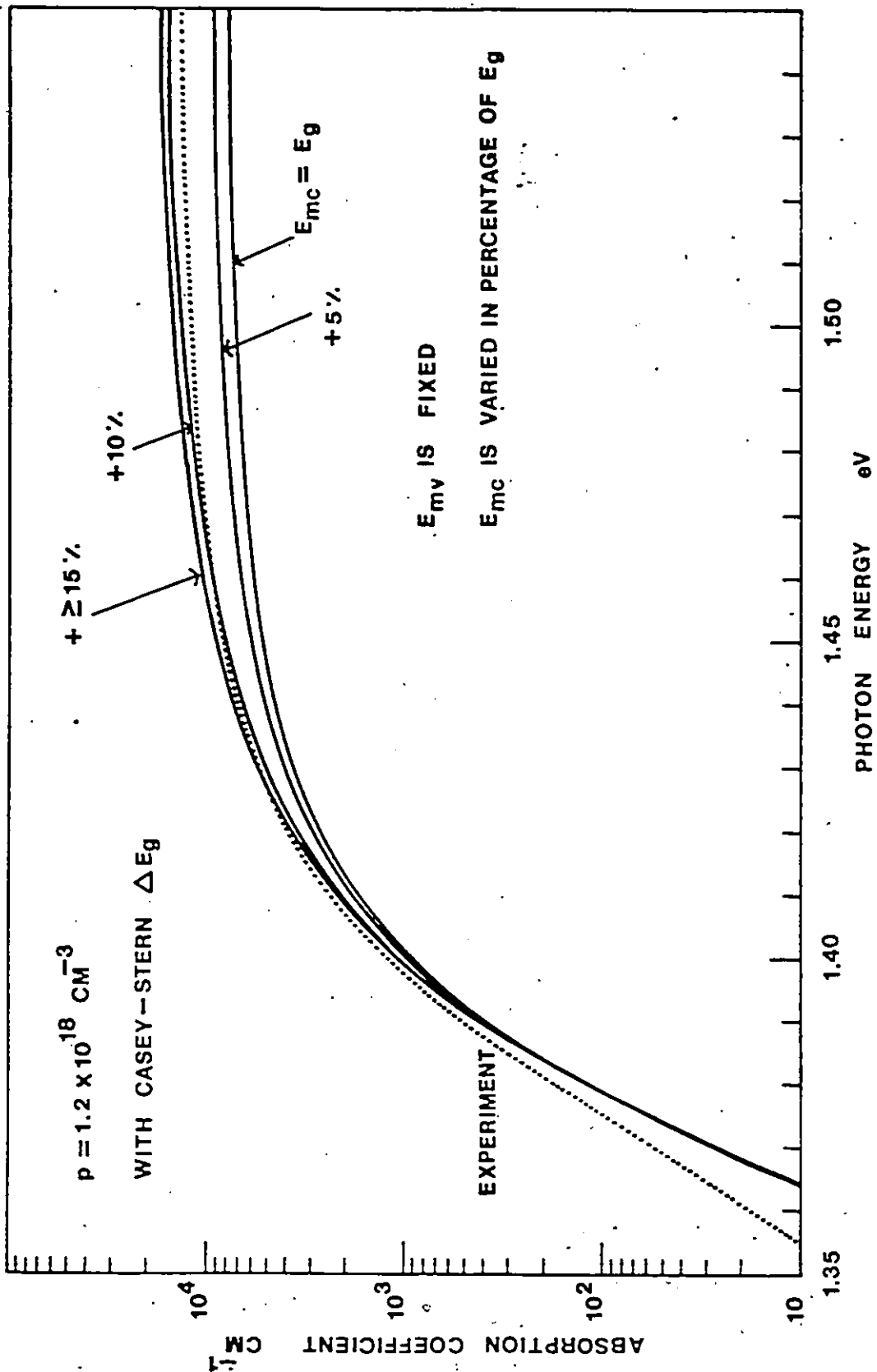


FIGURE 6.24

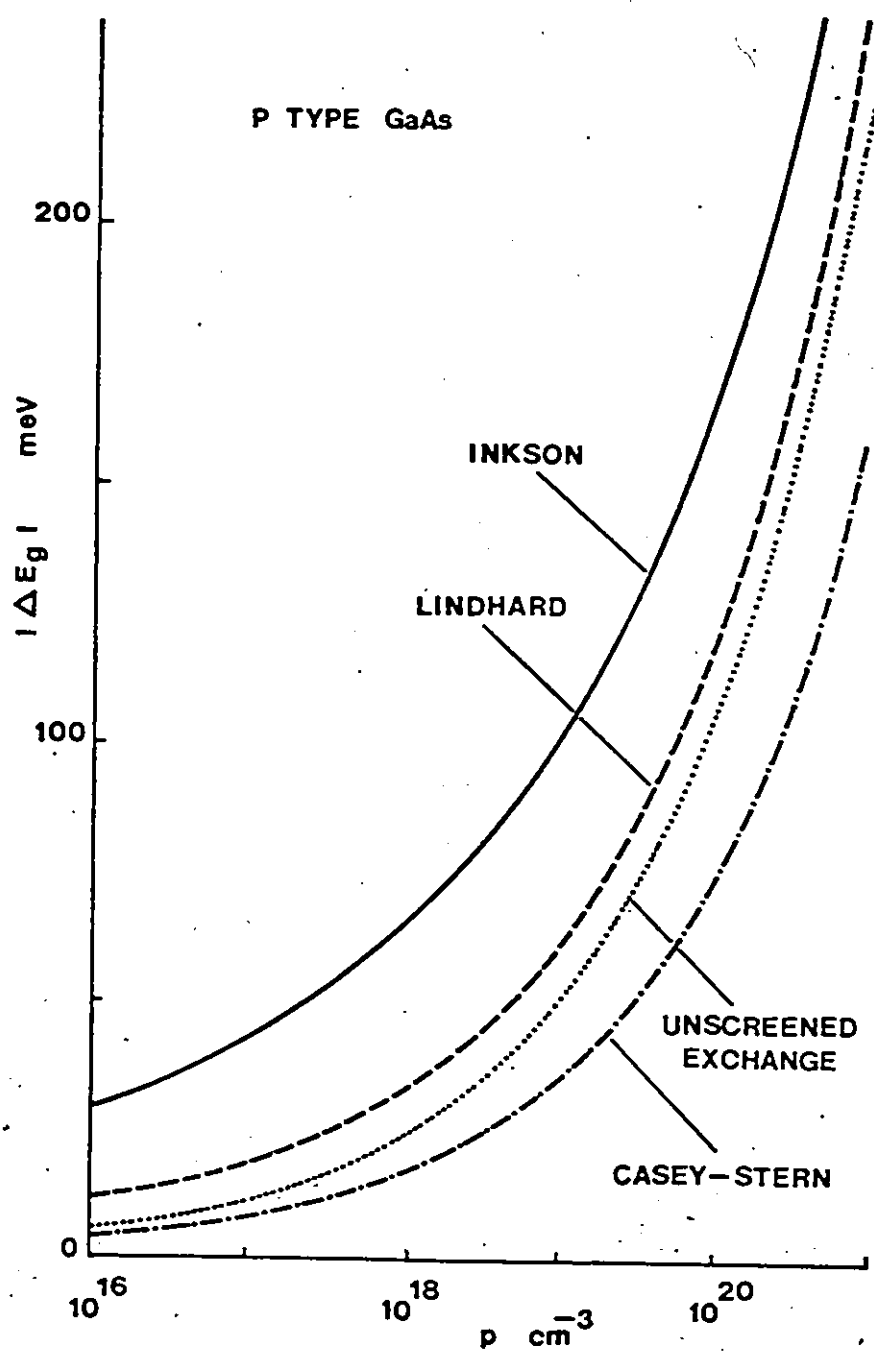


FIGURE 6.25

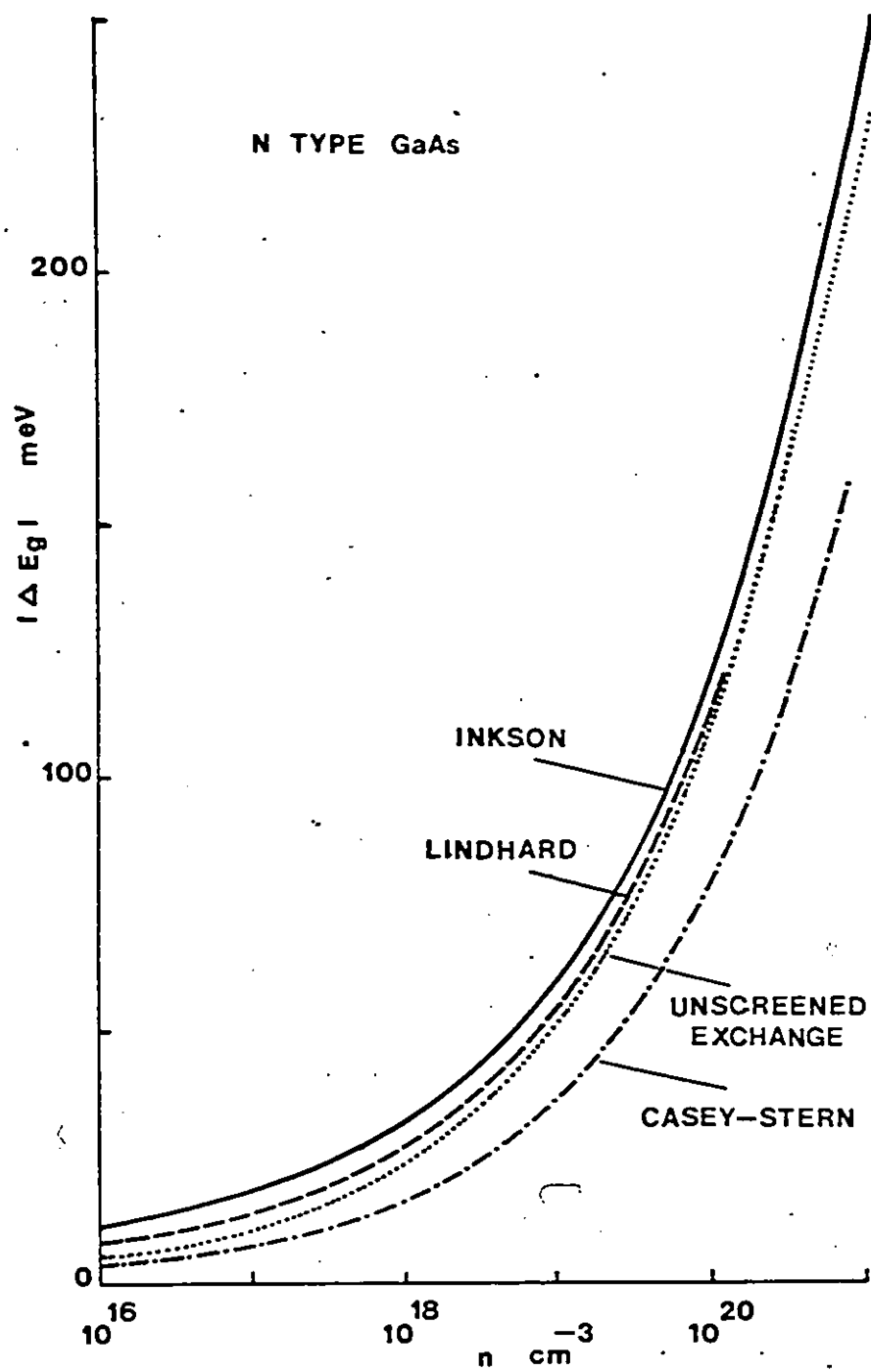


FIGURE 6.26

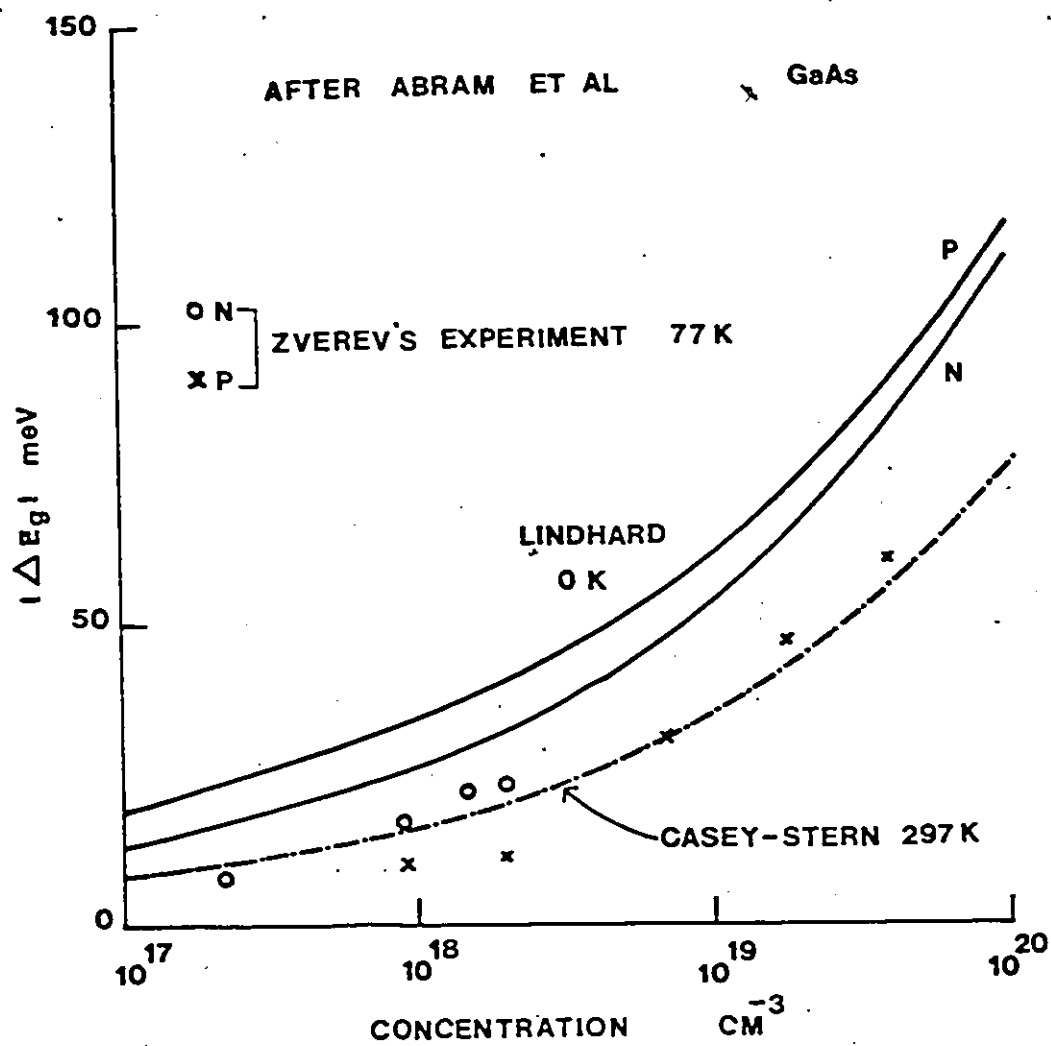


FIGURE 6.27

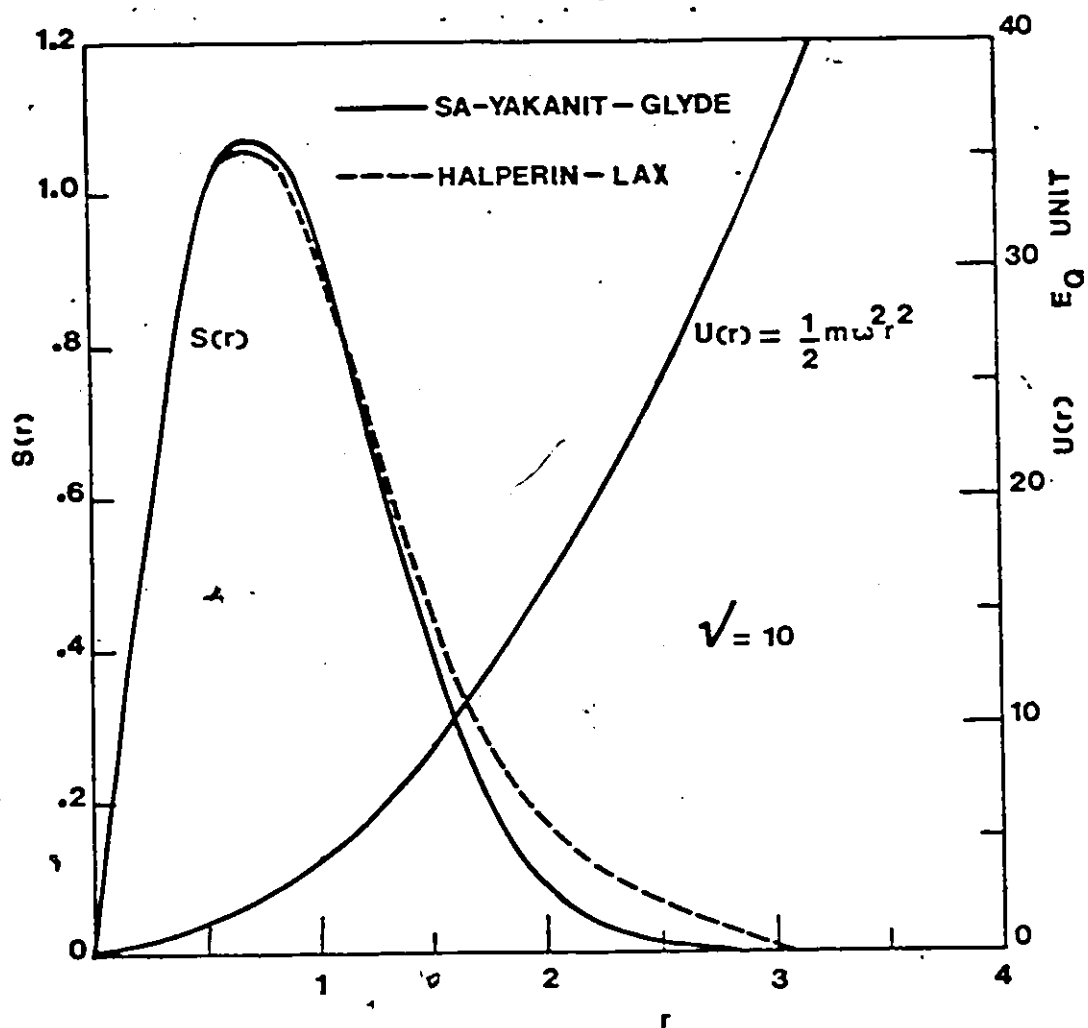


FIGURE A.1

TABLE 3.1

Self-consistent calculation of Fermi energy E_F and screening constant Q using parabolic DOS for $N_A = 9.9 \times 10^{18} \text{ cm}^{-3}$. Here, $v_F = -(E_v - E_F)/E_Q$, with $E_Q = \hbar^2 Q^2 / 2m_{hh}$ and E_v is the valence band edge.

T(K)	$Q(\text{cm}^{-1})$	$E_F(\text{meV})$	v_F
4.2	1.99×10^6	37.8	-1.644
297.	6.36×10^6	8.07	-0.035

TABLE 3.2

Tail DOS's in $Q^3/E_Q \xi'^2$ units for $\xi' = 50$.

ν	Halperin & Lax		Deep Tail Approx.		Full Ground State	
	z	DOS	z	DOS	z	DOS
30.	0.4922	6.80×10^{-9}	0.4377	9.03×10^{-9}	0.4378	8.97×10^{-9}
25.	0.5226	4.75×10^{-6}	0.4503	6.83×10^{-6}	0.4503	6.77×10^{-6}
20.	0.5623	1.17×10^{-3}	0.4617	1.91×10^{-3}	0.4617	1.89×10^{-3}
15.	0.6180	9.21×10^{-2}	0.4692	1.89×10^{-1}	0.4690	1.85×10^{-1}
10.	0.7059	1.90	0.4668	6.30	0.4664	6.10
5.	0.8857	6.20	0.4468	7.13×10^1	0.4456	6.73×10^1
4.	0.9528	5.51	0.4404	1.02×10^2	0.4390	9.63×10^1
3.	1.0470	3.99	0.4333	1.43×10^2	0.4316	1.32×10^2

TABLE 3.3

Tail DOS's in $Q^3/E_Q \xi'^2$ units for $\xi' = 5.0$

ν	Halperin & Lax		Deep Tail Approx.		Full Ground State	
	z	DOS	z	DOS	z	DOS
3.0	1.047	2.65×10^{-3}	0.8277	4.38×10^{-3}	0.8275	4.29×10^{-3}
2.5	1.111	1.01×10^{-2}	0.8379	1.88×10^{-2}	0.8375	1.84×10^{-2}
2.0	1.195	3.00×10^{-2}	0.8448	6.75×10^{-2}	0.8440	6.53×10^{-2}
1.5	1.313	6.59×10^{-2}	0.8463	1.99×10^{-1}	0.8450	1.91×10^{-1}
1.0	1.500	9.47×10^{-2}	0.8405	4.87×10^{-1}	0.8384	4.60×10^{-1}
0.5	1.887	6.36×10^{-2}	0.8259	9.91×10^{-1}	0.8226	9.19×10^{-1}
0.4	2.032	4.90×10^{-2}	0.8219	1.11	0.8184	1.03
0.3	2.237	3.33×10^{-2}	0.8176	1.25	0.8138	1.15

TABLE 3.4

Tail DOS's in $Q^3/E_Q \xi'^2$ units for $\xi' = 0.5$

ν	Halperin & Lax		Deep Tail Approx.		Full Ground State	
	z	DOS	z	DOS	z	DOS
.30	2.237	2.98×10^{-4}	1.653	4.69×10^{-4}	1.651	4.54×10^{-4}
.25	2.379	4.98×10^{-4}	1.676	8.60×10^{-4}	1.674	8.29×10^{-4}
.20	2.566	7.61×10^{-4}	1.697	1.50×10^{-3}	1.695	1.44×10^{-3}
.15	2.831	1.03×10^{-3}	1.716	2.49×10^{-3}	1.713	2.37×10^{-3}
.10	3.259	1.13×10^{-3}	1.731	3.89×10^{-3}	1.726	3.67×10^{-3}
.05	4.179	8.07×10^{-4}	1.738	5.74×10^{-3}	1.732	5.36×10^{-3}
.04	4.539	6.70×10^{-4}	1.739	6.16×10^{-3}	1.733	5.74×10^{-3}
.03	5.060	5.09×10^{-4}	1.740	6.59×10^{-3}	1.733	6.13×10^{-3}

TABLE 3.5

Tail DOS's in $Q^3/E_Q \xi'^2$ units for $\xi' = .05$

ν	Halperin & Lax		Deep Tail Approx.		Full Ground State	
	z	DOS	z	DOS	z	DOS
.030	5.061	4.54×10^{-7}	3.848	5.19×10^{-7}	3.847	5.08×10^{-7}
.025	5.429	8.42×10^{-7}	3.966	9.85×10^{-7}	3.964	9.60×10^{-7}
.020	5.927	1.52×10^{-6}	4.099	1.84×10^{-6}	4.096	1.79×10^{-6}
.015	6.654	2.64×10^{-6}	4.250	3.42×10^{-6}	4.426	3.31×10^{-6}
.010	7.874	4.24×10^{-6}	4.422	6.12×10^{-6}	4.415	5.98×10^{-6}
.005	10.65	5.43×10^{-6}	4.617	1.10×10^{-5}	4.606	1.05×10^{-5}
.004	11.78	5.28×10^{-6}	4.659	1.23×10^{-5}	4.688	1.03×10^{-5}
.003	13.45	4.83×10^{-6}	4.702	1.37×10^{-5}	4.688	1.31×10^{-5}

TABLE 4.1

The minimum net concentration $N_{\min} = (N_D - N_A)_{\min}$, at which the potential-fluctuation, $\xi^{1/2} = \left[\frac{2\pi e^2}{Q \epsilon_0^2} (N_D + N_A) \right]^{-1/2}$, is equal to the Fermi energy measured away from the conduction band edge, $\xi^{1/2} = E_F - E_c$ in n type GaAs.

N_A/N_D	T(K)	$N_{\min}(\text{cm}^{-3})$
0.0	20	1.0×10^{17}
	77	1.7×10^{17}
	300	7.5×10^{17}
0.2	20	1.7×10^{17}
	77	2.5×10^{17}
	300	9.2×10^{17}
0.4	20	3.7×10^{17}
	77	5.8×10^{17}
	300	1.2×10^{18}

TABLE 4.2

Self consistent results for heavily doped GaAs

T= 297 K using SG's DOS

$m_e = 0.066m_0$, $m_{hh} = 0.55m_0$, $m_{hl} = 0.085m_0$

P-type GaAs

N_D (cm^{-3})	N_A (cm^{-3})	Q (cm^{-1})	Q^{-1} (Å)	$E_V - E_F$ (meV)	$\xi^{1/2}$ (meV)	v_F
3.0×10^{17}	1.5×10^{18}	2.49×10^6	40.2	-70.2	23.3	1.96
6.0×10^{17}	3.0×10^{18}	3.45×10^6	29.0	-47.5	28.1	0.69
4.0×10^{18}	2.0×10^{19}	7.47×10^6	13.4	33.7	49.3	-0.10

N-type GaAs

N_D (cm^{-3})	N_A (cm^{-3})	Q (cm^{-1})	Q^{-1} (Å)	$E_F - E_C$ (meV)	$\xi^{1/2}$ (meV)	v_F
2.5×10^{18}	5.0×10^{17}	2.06×10^6	48.5	82.8	33.2	-3.38
4.1×10^{18}	8.0×10^{17}	2.30×10^6	43.4	121.	40.1	-3.95
8.4×10^{18}	1.7×10^{18}	2.64×10^6	37.9	198.	53.8	-4.94

N_D = donor concentration, N_A = acceptor concentration

Q = screening constant , Q^{-1} = screening length

$E_V - E_F$ = Fermi energy measured away from the valence band

$E_F - E_C$ = Fermi energy measured away from the conduction band

$\xi^{1/2}$ = potential fluctuation = $\left[\frac{2\pi e^2}{Q \epsilon_0^2} (N_D + N_A) \right]^{1/2}$

$v_F = -(E_V - E_F)/E_Q$ in p type GaAs

= $(E_C - E_F)/E_Q$ in n type GaAs

$E_Q = \hbar^2 Q^2 / 2m^*$,

m^* = effective mass of conduction or valence band

TABLE 4.3

Self consistent results for heavily doped GaAs

T= 297 K using Kane's DOS

 $m_e = 0.066m_0$, $m_{hh} = 0.55m_0$, $m_{hl} = 0.085m_0$

P-type GaAs

N_D (cm^{-3})	N_A (cm^{-3})	Q (cm^{-1})	Q^{-1} (A)	$E_v - E_F$ (meV)	$\xi^{1/2}$ (meV)	v_F
3.0×10^{17}	1.5×10^{18}	2.47×10^6	40.5	-79.9	23.5	2.27
6.0×10^{17}	3.0×10^{18}	3.40×10^6	29.4	-57.4	28.3	0.86
4.0×10^{18}	2.0×10^{19}	7.16×10^6	13.9	50.3	50.3	-0.06

N-type GaAs

N_D (cm^{-3})	N_A (cm^{-3})	Q (cm^{-1})	Q^{-1} (A)	$E_F - E_c$ (meV)	$\xi^{1/2}$ (meV)	v_F
2.5×10^{18}	5.0×10^{17}	2.03×10^6	49.2	78.3	33.4	-3.28
4.1×10^{18}	8.0×10^{17}	2.28×10^6	43.9	116.	40.3	-3.88
8.4×10^{18}	1.7×10^{18}	2.61×10^6	38.2	193.	53.9	-4.88

* see description of symbols in Table 4.2

TABLE 4.4

Self consistent results for heavily doped GaAs.

T= 297 K using parabolic DOS

$m_e = 0.066m_0$, $m_{hh} = 0.55m_0$, $m_{hl} = 0.085m_0$

P-type GaAs

N_D (cm^{-3})	N_A (cm^{-3})	Q (cm^{-1})	Q^{-1} (A)	$E_V - E_F$ (meV)	$\xi^{1/2}$ (meV)	v_F
3.0×10^{17}	1.5×10^{18}	2.49×10^6	40.1	-70.7	23.5	1.97
6.0×10^{17}	3.0×10^{18}	3.46×10^6	28.9	-46.6	28.0	0.67
4.0×10^{18}	2.0×10^{19}	7.56×10^6	13.2	30.6	48.9	-0.09

N-type GaAs

N_D (cm^{-3})	N_A (cm^{-3})	Q (cm^{-1})	Q^{-1} (A)	$E_F - E_C$ (meV)	$\xi^{1/2}$ (meV)	v_F
2.5×10^{18}	5.0×10^{17}	2.07×10^6	48.2	80.7	33.1	-3.25
4.1×10^{18}	8.0×10^{17}	2.31×10^6	43.3	118.	40.0	-3.83
8.4×10^{18}	1.7×10^{18}	2.63×10^6	37.9	194.	53.8	-4.83

* see description of symbols in Table 4.2

TABLE 4.5

Self consistent results for heavily doped GaAs

T= 297 K using SG's DOS

$m_e = 0.072m_0$, $m_{hh} = 0.68m_0$, $m_{hl} = 0.12m_0$

P-type GaAs

N_D (cm^{-3})	N_A (cm^{-3})	Q (cm^{-1})	Q^{-1} (A)	$E_V - E_F$ (meV)	$\xi^{1/2}$ (meV)	v_F
3.0×10^{17}	1.5×10^{18}	2.50×10^6	40.2	-70.2	23.3	1.96
6.0×10^{17}	3.0×10^{18}	3.45×10^6	29.0	-47.5	28.1	0.69
4.0×10^{18}	2.0×10^{19}	7.82×10^6	12.7	20.0	48.1	-0.06

N-type GaAs

N_D (cm^{-3})	N_A (cm^{-3})	Q (cm^{-1})	Q^{-1} (A)	$E_F - E_c$ (meV)	$\xi^{1/2}$ (meV)	v_F
2.5×10^{18}	5.0×10^{17}	2.06×10^6	48.5	82.8	33.2	-3.38
4.1×10^{18}	8.0×10^{17}	2.30×10^6	43.4	121.	40.1	-3.95
8.4×10^{18}	1.7×10^{18}	2.64×10^6	37.9	198.	53.8	-4.94

* see description of symbols in Table 4.2

TABLE 4.6

Self consistent results for heavily doped GaAs

T= 297 K using Kane's DOS

 $m_e = 0.072m_0$, $m_{hh} = 0.68m_0$, $m_{hl} = 0.12m_0$

P-type GaAs

N_D (cm^{-3})	N_A (cm^{-3})	Q (cm^{-1})	Q^{-1} (A)	$E_V - E_F$ (meV)	$\xi^{1/2}$ (meV)	v_F
3.0×10^{17}	1.5×10^{18}	2.47×10^6	40.5	-79.9	23.5	2.27
6.0×10^{17}	3.0×10^{18}	3.40×10^6	29.4	-57.4	28.3	0.86
4.0×10^{18}	2.0×10^{19}	7.54×10^6	13.2	1.2	49.0	0.00

N-type GaAs

N_D (cm^{-3})	N_A (cm^{-3})	Q (cm^{-1})	Q^{-1} (A)	$E_F - E_C$ (meV)	$\xi^{1/2}$ (meV)	v_F
2.5×10^{18}	5.0×10^{17}	2.03×10^6	49.2	78.3	33.4	-3.28
4.1×10^{18}	8.0×10^{17}	2.28×10^6	43.9	116.	40.3	-3.88
8.4×10^{18}	1.7×10^{18}	2.61×10^6	38.2	193.	53.9	-4.88

* see description of symbols in Table 4.2

TABLE 4.7

Self consistent results for heavily doped GaAs

T= 297 K using parabolic DOS

 $m_e = 0.072m_0$, $m_{hh} = 0.68m_0$, $m_{hl} = 0.12m_0$

P-type GaAs

N_D (cm^{-3})	N_A (cm^{-3})	Q (cm^{-1})	Q^{-1} (A)	$E_V - E_F$ (meV)	$\xi^{1/2}$ (meV)	v_F
3.0×10^{17}	1.5×10^{18}	2.49×10^6	40.1	-70.7	23.5	1.97
6.0×10^{17}	3.0×10^{18}	3.46×10^6	28.9	-46.6	28.0	0.67
4.0×10^{18}	2.0×10^{19}	7.92×10^6	13.6	18.7	47.8	-0.05

N-type GaAs

N_D (cm^{-3})	N_A (cm^{-3})	Q (cm^{-1})	Q^{-1} (A)	$E_F - E_C$ (meV)	$\xi^{1/2}$ (meV)	v_F
2.5×10^{18}	5.0×10^{17}	2.07×10^6	48.2	80.7	33.1	-3.25
4.1×10^{18}	8.0×10^{17}	2.31×10^6	43.3	118.	40.0	-3.83
8.4×10^{18}	1.7×10^{18}	2.63×10^6	37.9	194.	53.8	-4.83

* see description of symbols in Table 4.2