

crystal taken at two different temperatures T and T' related by Eq. (7b). Using the relation (7c) for two different alkali iodides, e.g., NaI and KI, one can eliminate the fictitious iodine crystal and obtain the following relation between specific heats of two different alkali iodides at three different temperatures:

$$C_v^{\text{NaI}}(T) + C_v^{\text{NaI}}[T(m_{\text{K}}/m_{\text{I}})^{1/2}] \\ = C_v^{\text{KI}}(T) + C_v^{\text{KI}}[T(m_{\text{Na}}/m_{\text{I}})^{1/2}]. \quad (8)$$

The relation (8) follows only from our simple rule and the assumption of a harmonic crystal and is completely independent of the form of the normal-mode spectrum. Table I shows the agreement of experimental data⁵ with the relation (8) between temperatures of 60 to 200°K. The agreement supports the validity of our simple rule.

If a particular model is assumed for the fictitious iodine crystal, the specific heats of the alkali iodides

⁵ W. J. Berg and J. A. Morrison, Proc. Roy. Soc. (London) A242, 467 (1957).

are given as a function of temperature by Eq. (7c). If a Debye model is assumed for the fictitious iodine crystal the Debye temperature Θ_{I} can be determined by fitting the experimental data^{5,6} with Eq. (7c). The results shown in Tables II-IV indicate a good agreement with $\Theta_{\text{I}}=109^\circ\text{K}$ for $C_v^{\text{NaI}}(T)$ and $C_v^{\text{KI}}(T)$, and with $\Theta_{\text{I}}=103^\circ\text{K}$ for $C_v^{\text{RbI}}(T)$.

These results suggest that the Mössbauer f factor for iodine in the alkali iodides can be calculated from a homogeneous Debye lattice with $\Theta_{\text{I}}\cong 109^\circ\text{K}$. This gives $f\cong 0.23$ at $T=80^\circ\text{K}$, in agreement within experimental error with the results³ for all the alkali iodides.

From these examples, it seems that a good estimate for the Mössbauer f factor in a diatomic lattice is given by a Debye model for a fictitious monoatomic crystal which fits specific-heat data. The accuracy of these estimates cannot be checked until more precise experimental data are available.

⁶ K. Clusius, J. Goldman, and A. Perlick, Z. Naturforsch. 4, 424 (1949).

Luminescence and Recombination through Defects in p - n Junctions

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We have developed simple expressions for the recombination current occurring in the space-charge region of a p - n junction at high temperatures. The current passing through a defect state in the forbidden gap is shown to vary approximately exponentially with applied voltage as $I \propto \exp(eV/\beta kT)$, where $\beta = 1, 2, >2$ depending on the bias voltage relative to two "kink" voltages V_k and V_d . The energy eV_k is given approximately by twice the energy of the center as measured from midgap, while V_d is determined by the gap energy and carrier effective masses and by the ratio of the capture cross sections of the center for holes and electrons. These effects are shown to explain the kinks appearing in curves of light intensity versus voltage for electroluminescent diodes. When used to analyze emission peaks from copper-doped GaAs junctions they provide values for the cross-section ratios and identify the center producing the 0.97-eV emission as a donor lying in the upper half of the energy gap.

1. INTRODUCTION

DEFECTS are known to play an important role in recombination processes in p - n junctions. Although analyses of some of these effects appropriate for conditions of strong forward bias have appeared in the literature,¹ they are rather complex and difficult to apply. We shall present here a rather simple physical analysis, which is valid for many experimental circumstances, of the effects of deep levels on current and light output of p - n junctions.² New results are obtained

particularly for the region of low forward bias. The assumption made throughout this paper is that the electron and hole quasi-Fermi levels are constant throughout the space-charge region and are equal to the Fermi levels on the n and p sides, respectively, of the junction. Thus, the potential drops associated with the flow of current are assumed negligible within the junction. In cases where this assumption is not justified a more complex analysis, as in Ref. 1, is required and the results become less tractable.

In Sec. 2 we develop the nonequilibrium statistics of deep-lying states in the space-charge region of a p - n junction, and in Sec. 3 we derive expressions from this for the rate of recombination for electrons and holes passing through these states. In Sec. 4 we use these

¹ C. T. Sah, R. N. Noyce, and W. Shockley, Proc. Inst. Radio Engrs. 45, 1228 (1957); A. Herlet, Z. Naturforsch. 11A, 498 (1956).

² Some of these conclusions have been reported briefly at the Solid State Devices Research Conference in Boulder, Colorado, July, 1964 (unpublished).

results to interpret electroluminescence spectra of copper-doped GaAs diodes.

2. STATISTICS OF DEEP CENTERS AT HIGH TEMPERATURE

In a junction in thermal equilibrium, with no external bias applied, the densities of free and trapped carriers are given by products of the appropriate densities of states and Fermi functions. When an external bias is applied, the resulting nonequilibrium situation can be described in terms of three "quasi"-Fermi levels, ϕ_n , ϕ_p , and ϕ_t , one for each type of state, with the applied bias determining the difference between the electron and hole Fermi levels, assumed to be constant within the space-charge region, $v_b = \phi_n - \phi_p$. (All potentials are expressed in units of kT/e to simplify the mathematical expressions.) Thus if the energy of the electron state associated with a center of density N_t is written $\mathcal{E}_t = kTv_t$, the density of trapped electrons is given by

$$n_t = N_t f_t(v_t - \phi_t). \quad (1)$$

The value of the Fermi function f_t for the center depends upon the Fermi level of the center ϕ_t , which is determined by the electron and hole Fermi levels, and the recombination statistics of the traps. In Appendix A we show that this Fermi level is determined by the applied bias and the value of a single parameter B , which depends exponentially upon the energy of the center as measured from midgap.³ Thus

$$B = \exp[v_g - 2(v_t - v_v) + \delta], \quad (2)$$

where v_g is the band-gap energy and $v_t - v_v$ the energy of the defect state above the valence-band edge, in units of kT , and

$$\delta = \ln(g^2 N_v c_p / N_c c_n) \quad (3)$$

depends logarithmically on the degeneracy g , the carrier densities of states, and the ratio of the capture coefficients of the center for holes and electrons. In particular, for nondegenerate electron and hole distributions at the location in the junction where the centers are half-filled, the value of ϕ_t is given quite accurately by very simple expressions. If $B > 1$, we say the center has " p character" and

$$\begin{aligned} \phi_t &= \phi_p + \epsilon, & v_b &\leq v_k, \\ \phi_t &= \phi_p + \epsilon + (v_b - v_k)/2, & v_b &\geq v_k. \end{aligned} \quad (4)$$

If $B < 1$, we say the center has " n character" and

$$\begin{aligned} \phi_t &= \phi_n - \epsilon, & v_b &\leq v_k, \\ \phi_t &= \phi_n - \epsilon - (v_b - v_k)/2, & v_b &\geq v_k, \end{aligned} \quad (5)$$

³ These expressions are related to the work of Rose, cf. *Concepts of Photoconductivity and Allied Problems* (Interscience Publishers, Inc., New York, 1963). In particular for nondegenerate materials the natural logarithm of the coefficient of $(\mu-1)$ in Eq. (A6) equals the energy difference (in units of kT) between the energy level of the center and the "demarcation level."

where $v_k = \ln[(1-B)^2/B]$ and ϵ is a small quantity which is nearly independent of bias. Unless B is of order unity (v_t near midgap),

$$v_k \approx |\ln B| = |v_g - 2(v_t - v_v) + \delta|. \quad (6)$$

Thus the value of $\ln B$ determines a critical value of applied voltage v_k below which ϕ_t follows ϕ_n or ϕ_p , according to the "character" of the center, and above which ϕ_t follows $(\phi_n + \phi_p)/2$. The transition voltage v_k corresponds to the point at which thermal excitation from the center becomes unimportant. Where the electron or hole distribution is degenerate a voltage-dependent coefficient B' replaces B —see (A7). The implications of these results are described in the following section.

3. ELECTROLUMINESCENCE AND CURRENT

Recombination processes in solids can occur either nonradiatively or with the emission of radiation characteristic of the process involved. In either case the rate of recombination at any point in the crystal is proportional to the product of the density of electrons in the upper state and the density of holes in the lower state and is increased in a $p-n$ junction by the application of a forward bias. Thus the rate of recombination within a junction can be calculated from the integrals of these products over the extent of the space-charge region while the rate for injected carriers is determined by the injection current. For recombination through centers in the depletion region of a junction we may apply the results of the preceding section. With no applied bias, recombination and generation are equal. When a forward bias v_b less than v_k but satisfying $\exp(v_b) \gg 1$ is applied, thermal generation to one of the bands may be neglected. [If $\exp(v_b - v_k) \gg 1$, thermal generation may be neglected for both bands.] Thus for a center having p character the recombination current is determined by the product of the electron density n and trapped hole density $(N_t - n_t)$ integrated over the junction width,

$$J = \alpha_n \int_0^w n(N_t - n_t) dl, \quad (p \text{ character}). \quad (7)$$

For a center having n character

$$J = \alpha_p \int_0^w p n_t dl, \quad (n \text{ character}). \quad (8)$$

In Appendix B, by assuming that the field E is constant within the space-charge region (thus introducing relatively minor errors into the calculation), we show that the recombination current densities in the two voltage ranges are as follows: For $v_b < v_k$, $\exp(v_k - v_b) \gg 1$,

$$I \approx (c_n c_p)^{1/2} n_i N_t (kT/eE) (1 + v_k - v_b) \times \exp(-v_k/2) \exp(v_b), \quad (9)$$

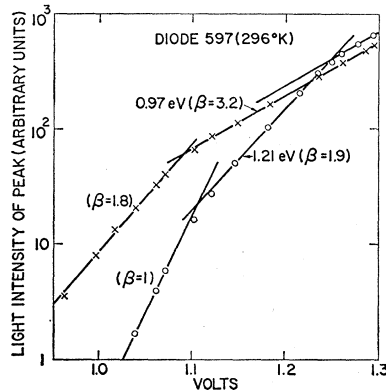


FIG. 1. Peak intensity versus voltage dependence for two emission lines of a copper-doped GaAs diode. A correction for IR drop has been included above 1.2 V. (Reprinted from Ref. 5.)

and for $v_b > v_k$, $\exp(v_b - v_k) \gg 1$,

$$I \approx \pi/2 (c_n c_p)^{1/2} n_i N_t (kT/eE) \exp(v_b/2). \quad (10)$$

These expressions are somewhat inaccurate near the critical voltage and differ by a factor of $\pi/2$ at $v_b = v_k$. Thus the slope of $\ln(I)$ versus v_b is approximately unity for $v_b < v_k$, grading to approximately one-half for $v_b > v_k$. The same voltage dependence appears in the intensity of emitted light.

If several types of centers are present and contribute to recombination, the light characteristic of the i th center will follow the expressions given above with a kink at the critical voltage v_{ki} for that center.⁴ However, as the current is the sum of the currents for all the processes, both radiative and nonradiative, its voltage dependence may be rather complex. It is for this reason that the conventional plot of light intensity versus current frequently obscures the nature of the radiative processes involved.

As the bias is increased beyond v_k , the region in the junction making the maximum contribution to the integral moves toward the edge of the space-charge region—see Eq. (B16)—and reaches it (or the edge of the degenerate part of the semiconductor) when the bias is $v_b = v_d$ with

$$v_d = v_g \pm \ln(N_v c_p / N_c c_n) \quad (11)$$

when the carrier distribution at the edge is degenerate, and

$$v_d = 2 \ln(n_0/n_i) \pm \ln(c_p/c_n) \quad (12)$$

when the carrier density at the edge is n_0 and not degenerate. The $+$ sign applies to a center of n character for which n_0 is the carrier density at the edge of the p region and the $-$ sign to p character with n_0 the electron density. If this bias is reached before the junction width goes to zero, it marks a second kink in the curve of recombination current versus voltage above which the slope $d \ln(I)/dv_b$ drops below one-half.

⁴ In applying these results to luminescence the values given by (9) and (10) must be reduced by η , the ratio of the radiative to total transition rates for the capture process being considered, $\eta = c(\text{radiative})/[c(\text{radiative}) + c(\text{nonradiative})]$.

The quantity v_d given by (11) or (12) has been determined for a constant electric field while in a real junction the field decreases rapidly near the edge. This decrease in field increases the recombination rate near the kink if all other approximations hold [cf. Eq. (10)]. An opposing decrease in recombination is caused by the rapid vanishing of the injected carrier density beyond the edge (nonconstant Fermi level), an effect which determines the slowly varying recombination rate above the kink. A detailed consideration of these two effects is needed to determine the exact location of the kink, though from the qualitative arguments given above it appears probable that the observed kink voltage will lie above the value computed from the simple theory and that the error will be larger for kinks which occur at high forward bias where the junction is narrow. The additional complications introduced by the broadening of the impurity levels^{5,6} and band edges⁷ (tailing) should be considered to improve the accuracy of the results.

At low temperature where tunneling processes replace the thermal excitation of carriers, we find the behavior to be qualitatively similar. The low-temperature results are not sufficiently complete to be included in this article.

4. EMISSION IN COPPER-DOPED GaAs DIODES

Measurements of electroluminescence from GaAs diodes doped with copper have been reported by Morgan, Pilkuhn, and Rupprecht⁵ and provide a convenient illustration of the effects considered above. Figure 1, reproduced from Ref. 5, shows the voltage dependence of the peak intensities of two lines emitted at 297°K by a zinc-diffused diode having a copper background doping. The transition producing the 1.21-eV line is identified as the capture of an electron by a neutral substitutional copper center in a state lying approximately 0.16 eV above the valence-band edge and having a degeneracy $g \approx \frac{1}{3}$, while the 0.97-eV line is associated with an unidentified level lying about 0.42 eV below the conduction-band edge at room temperature.⁵ As a consequence of the overlap of the emission bands the slopes of the lines and locations of the kinks may be slightly in error.

Three kinks are evident in Fig. 1. For the 1.21-eV line the lower kink occurs at $V_k = 1.11$ V and the upper at $V_d = 1.24$ V. For the 0.97-eV line the lower kink is not in the range of measurement $V_k < 0.96$ V and the upper is at $V_d = 1.09$ V. We do not attempt to deal with the complexities of band tails but instead employ an effective energy gap of $eV_g = 1.38$ eV, deduced from the high-current limit of the edge emission, and assume normal bands. The carriers near the edges

⁵ T. N. Morgan, M. Pilkuhn, and H. Rupprecht, Phys. Rev. **138**, A1551 (1965).

⁶ T. N. Morgan, Phys. Rev. (to be published).

⁷ E. O. Kane, Phys. Rev. **131**, 79 (1963).

of the space-charge region are taken to be nondegenerate with $n_0 = 3.7 \times 10^{17} (1.3 - v)^{1/3}$ as calculated⁵ for a graded junction of grading $a = 7 \times 10^{22} \text{ cm}^{-4}$ and built-in potential $V_0 = 1.3$. The value of $V_0 = 1.3$ is approximate though reasonable for this region of forward bias.

Turning first to the 1.21-eV line we have from Eq. (6) for a center of p character

$$V_k = kT v_k = 1.38 - 2 \times 0.16 + (kT/e) \delta.$$

To evaluate δ we use Eq. (A9) and assume that the capture coefficients c are equal to the product of the thermal carrier velocities and capture cross sections σ . Thus for $g = \frac{1}{3}$ and $m_p/m_n = 9.5$

$$\delta = \ln[g^2 (m_p \sigma_p / m_n \sigma_n)] = 0.05 + \ln(\sigma_p / \sigma_n),$$

and using $V_k = 1.11 \text{ V}$, we find

$$\sigma_p / \sigma_n = 7.$$

This value is quite reasonable for a single acceptor at room temperature and may be compared with ratios ranging from 2 to 70 for deep gold centers in silicon.⁸ Similarly from Eq. (12) with $V_d = 1.24 \text{ V}$ and $n_0 = 1.45 \times 10^{17} \text{ cm}^{-3}$

$$\sigma_p / \sigma_n = 2.3,$$

which is too small as expected from the considerations discussed at the end of Sec. 3.

For the 0.97-eV line the value $V_d = 1.09 \text{ V}$ and $n_0 = 2.2 \times 10^{17} \text{ cm}^{-3}$ in (12) yields the result (for n character)

$$\sigma_n / \sigma_p = 200,$$

which is reasonable if the center acts as a donor $\sigma_n > \sigma_p$. Substitution of this result in (6) locates the first kink (with $g = 1$) at $V_k = 0.46$, well below the voltage range of the measurements. The low value of V_d identifies the center as a donor as long as it is known to have n character. The character depends on the location of the energy level above midgap which has been deduced from the line shapes discussed in Ref. 5. If this evidence were lacking, the center might be considered to have p character (energy below midgap) for which the same value of V_d gives $\sigma_p / \sigma_n = 2000$, an improbably high value. Thus this analysis provides supporting evidence for the assignment made in Ref. 5 of the energy level to the upper half of the forbidden gap.

ACKNOWLEDGMENT

The author wishes to thank F. Stern for helpful discussions.

⁸ Room-temperature values given for gold in silicon by G. Bemski, Phys. Rev. **111**, 1515 (1958) are, for acceptors lying just above midgap, $\sigma_p / \sigma_n = 2$, and for donors below midgap, $\sigma_n / \sigma_p \geq 35$. Recent results reported for the same two centers by J. M. Fairfield and B. V. Gokhale [Abstr. Electrochem. Soc. **13**, 120 (1964) No. 164 and to be published] are: $\sigma_p / \sigma_n = 70$ and $\sigma_n / \sigma_p = 2.6$, respectively.

APPENDIX A: NONEQUILIBRIUM TRAP DISTRIBUTION

Let the density of centers be N_t and the density of occupied centers having energy $kT v_t$ be⁹

$$n_t = N_t f_t(v_t - \phi_t),$$

where

$$f_t(v) = [(1/g) \exp(v) + 1]^{-1},$$

the degeneracy ratio is $g (g = w/w_p$ of Ref. 9), and ϕ_t is the quasi-Fermi level for the center. (All energies are measured in units of kT .) In equilibrium, $\phi_n = \phi_p = \phi_t = \phi$ and the rate equations for transfer of electrons between a given energy $x = \mathcal{E}/kT$ in the conduction or valence band and the centers may be written

$$\dot{n}(x) = 0 = N_n(x) \{ -f_0(x - \phi) c_n(x) (N_t - n_t) + e_n(x) n_t [1 - f_0(x - \phi)] \}, \quad (\text{A1})$$

and

$$\dot{p}(x) = 0 = N_p(x) \{ -f_0(\phi - x) c_p(x) n_t + e_p(x) (N_t - n_t) [1 - f_0(\phi - x)] \}, \quad (\text{A2})$$

where $N_n(x)$ and $N_p(x)$ are the densities of states in the conduction and valence bands, $c_n(x)$ and $c_p(x)$ are coefficients of carrier capture, and $e_n(x)$ and $e_p(x)$ are thermal ionization coefficients for release of carriers from the centers to an energy x in the conduction or valence band.

These two equations determine the ratios of the capture to the ionization coefficients which are functions only of the energy and temperature,

$$e_p(x) / c_p(x) = c_n(x) / e_n(x) = g \exp(x - v_t). \quad (\text{A3})$$

If we now assume that the densities of carriers in the space-charge regions are determined by the majority carrier densities at the edges and are not affected by recombination or trapping, the electron and hole Fermi levels ϕ_n and ϕ_p extend unchanged from the n and p sides, respectively, across the junction, and when a voltage v_b is applied,

$$\phi_n - \phi_p = v_b. \quad (\text{A4})$$

Under steady-state conditions the density of trapped electrons must not change in time. The equation describing this condition [obtained by integrating the appropriate rates in (A1) and (A2) over energy] is

$$\dot{n}_t = N_t f_t(v_t - \phi_t) \{ (1/g) n c_n [\exp(v_t - \phi_t) - \exp(v_t - \phi_n)] - p c_p [1 - \exp(\phi_p - \phi_t)] \} = 0, \quad (\text{A5})$$

where use has been made of (A3) and

$$c_n = \int N_n(x) f_0(x - \phi_n) c_n(x) dx / \int N_n(x) f_0(x - \phi_n) dx$$

⁹ This development is similar to that of W. Shockley and W. T. Read, Jr., Phys. Rev. **87**, 835 (1952), though our goals and final results differ somewhat from theirs. Their notation is preserved where it is appropriate and equivalences are noted where our parameters differ from theirs.

with a similar expression for c_p . The integrations are taken over the appropriate bands.

To determine the energy of the center at the point where it crosses its Fermi level we write $\mu = \exp(\phi_t - \phi_p)$ and combine (A4) and (A5) to obtain the equation

$$\exp(v_b)/\mu - 1 = (B'/g) \exp(v_t - \phi_t)(\mu - 1), \quad (\text{A6})$$

where

$$B' = \frac{N_c \exp(\phi_n - v_c)}{n} \frac{\dot{p}}{N_v \exp(v_v - \phi_p)} B, \quad (\text{A7})$$

$$B = g^2 \frac{N_v c_p}{N_c c_n} \exp[v_g - 2(v_t - v_v)] = \frac{\langle c_p \rangle \dot{p}_1}{\langle c_n \rangle n_1}.$$

See Ref. 9 for notation of final expression. In regions where the electron and hole distributions are both nondegenerate $B' = B$ and is independent of bias.

It is useful to know the dependence of B upon the parameters of the center. By using the expression given above, we find

$$B = \exp[\delta + v_g - 2(v_t - v_v)], \quad (\text{A8})$$

with

$$\delta = \ln[g^2(N_v c_p / N_c c_n)], \quad (\text{A9a})$$

$$= \ln[g^2(m_p/m_n)(\sigma_p/\sigma_n)], \quad (\text{nondegenerate}), \quad (\text{A9b})$$

where for the last expression we have written $c = (2kT/m)^{1/2}\sigma$ in terms of the thermal velocity and capture cross section.

In the expressions below we assume nondegenerate distributions and set $B' = B$. Thus at a point where $\exp(v_t - \phi_t) = g$, the traps are half full and Eq. (A6) has the solution

$$\mu = [1 - B | (1 + 4h^2)^{1/2} - (1 - B)] / 2B, \quad (\text{A10})$$

with

$$h^2 = B \exp(v_b) / (1 - B)^2.$$

For other points in the junction B should be replaced by

$$B \exp(v_t - \phi_t) / g.$$

Fortunately, for most values of bias $\ln \mu$ is linear in v_b and can be expressed as

$$\phi_t - \phi_p = \ln \mu = \epsilon + v_b / (1 + A), \quad (\text{A11})$$

where A is a constant [obtained by differentiating (A6) or (A10) with respect to v_b] and ϵ is small and nearly independent of v_b . Thus,

$$A = B \mu^2 \exp(-v_b) \quad (\text{A12})$$

and depends upon the value of v_b relative to a critical voltage,

$$v_k = \ln[(1 - B)^2 / B] \approx |v_g - 2(v_t - v_v) + \delta|. \quad (\text{A13})$$

To show that A is nearly constant we consider three special cases:

$$(1) \text{ If } v_b > v_k, h^2 = \exp(v_b - v_k) \gg 1,$$

then

$$\mu^2 = (1/B) \exp(v_b)(1 \pm 1/h + \dots),$$

$$A \approx 1, \quad (\text{A14})$$

$$\epsilon \approx -\frac{1}{2} \ln B + \frac{1}{2}(B - 1) \exp(-v_b/2) / \sqrt{B},$$

and ϕ_t follows $(\phi_n + \phi_p)/2$. This case applies to forward bias conditions as (if B is not of order unity) the condition $h^2 = 1$ is equivalent to

$$v_b = v_k \approx |v_g - 2(v_t - v_v) + \delta| \gg 1.$$

$$(2) \text{ If } h^2 \ll 1 (v_b < v_k) \text{ and if also } B < 1, \text{ then}$$

$$\mu = (1 - B)^{-1} \exp(v_b)(1 - h^2 + \dots),$$

$$A \approx h^2 \ll 1, \quad (\text{A15})$$

$$\epsilon \approx \ln(1 - B)^{-1} - h^2,$$

and ϕ_t follows ϕ_n . For this reason we say that a center for which $B < 1$ has "n character."

$$(3) \text{ If } h^2 \ll 1 \text{ and } B > 1, \text{ then,}$$

$$\mu = [(B - 1)/B](1 + h^2 + \dots),$$

$$A \approx h^{-2} \gg 1, \quad (\text{A16})$$

$$\epsilon \approx -\ln[B/(B - 1)] + h^2,$$

and ϕ_t follows ϕ_p . Such a center is said to have "p character."

The transition between case (1) and case (2) or (3) occurs for voltages within only a few kT/e of v_k because of the exponential dependence of h on v_b , though for centers having broadened energy bands of states, $kT v_k$ extends over a range of values of about twice the width of the band.

APPENDIX B: RECOMBINATION INTEGRALS

We wish to calculate the recombination current¹⁰ through deep levels in the space-charge region of a p - n junction having a uniform electric field E . As the field is assumed uniform, the energy (in units of kT) of the conduction band edge, measured from the electron Fermi level, is

$$v_c - \phi_n = (eE/kT)l = x \quad (\text{B1})$$

at a distance l from the point at which $v_c = \phi_n$. The energy of the center can be written

$$v_t = \phi_p + v_b - (v_c - v_t) + x. \quad (\text{B2})$$

We shall consider a center having p character, $B \gg 1$ (see Appendix A), and shall integrate the recombination current over that part of the junction having nondegenerate carrier distributions, $0 \leq l \leq w$, with eEw/kT

¹⁰ Similar results have been derived independently by A. L. McWhorter from the Shockley-Read formula (4.4), Ref. 9.

$=v_a-v_b$. Thus

$$J = c_n N_c N_t \int_0^w \frac{\exp(\phi_n - v_c) dl}{1 + g \exp(\phi_t - v_t)}, \quad (\text{B3})$$

though a small correction should be introduced in the limits for nondegenerate diodes. To make use of the results of Appendix A we divide the range of integration into two parts and use (A14) and (A16) with the parameter B replaced by $B \exp(v_t - \phi_t)/g$. By use of the conditions $\exp(v_k) = (B-1)^2/B \gg 1$, (A13), and $\exp(v_b) \gg 1$ it is easily shown that (A14) applies where $v_t - \phi_t - \ln(g) < v_b - v_k$, making

$$\phi_t \approx \phi_p + x_k - x,$$

or

$$\phi_t - v_t + \ln(g) \approx 2(x_k - x) + v_k - v_b, \quad x < x_k, \quad (\text{B4})$$

and that (A16) applies where $v_t - \phi_t - \ln(g) > v_b - v_k$, making

$$\phi_t \approx \phi_p,$$

or

$$\phi_t - v_t + \ln(g) \approx x_k - x + v_k - v_b, \quad x > x_k. \quad (\text{B5})$$

In these expressions the constant x_k is

$$x_k = v_c - v_t + \ln(g) - v_k = v_t - v_b - \delta + \ln(g) \quad (\text{B6})$$

and represents the energy at the point of transition between (B4) and (B5). The transition is assumed to occur abruptly.

Using these results we write (B3) as the sum of two integrals,

$$J = c_n N_c N_t (kT/eE) \exp(-x_k) (I_1 + I_2), \quad (\text{B7})$$

with (writing $x - x_k + y_0/2 = y$)

$$\begin{aligned} I_1 &= \exp(y_0/2) \int_{(y_0/2 - x_k)}^{y_0/2} \frac{dy}{\exp(y) + \exp(-y)} \\ &= \exp(y_0/2) \{ \tan^{-1}[\exp(y_0/2)] \\ &\quad - \tan^{-1}[\exp(y_0/2 - x_k)] \}, \quad (\text{B8}) \end{aligned}$$

and (writing $x - x_k + y_0 = y$)

$$\begin{aligned} I_2 &= \exp(y_0) \int_{y_0}^{v_a - v_k - x_k} \frac{\exp(-y) dy}{1 + \exp(-y)} \\ &= \exp(y_0) \{ \ln[1 + \exp(-y_0)] \\ &\quad - \ln[1 + \exp(x_k + v_k - v_a)] \}. \quad (\text{B9}) \end{aligned}$$

We have written $v_b - v_k = y_0$.

The result (B7) can be written in a symmetric form appropriate to centers of either p or n character by using the relation

$$\alpha_n N_c \exp(-x_k) = (\alpha_n \alpha_p)^{1/2} n_i \exp(v_k/2), \quad (\text{B10})$$

where n_i is the intrinsic carrier density. Also the last terms of (B8) and (B9) may be dropped (for most values of v_b), as $\exp(-x_k) \ll 1$ and $\exp(x_k + v_k - v_a) \ll 1$ are generally satisfied. With these simplifications the current becomes

$$J = (c_n c_p)^{1/2} n_i N_t (kT/eE) \exp(v_k/2) (I_1 + I_2) \quad (\text{B11})$$

with

$$\begin{aligned} I_1 + I_2 &= \exp[\frac{1}{2}(v_b - v_k)] \tan^{-1}[\exp[\frac{1}{2}(v_b - v_k)]] \\ &\quad + \exp(v_b - v_k) \ln[1 + \exp(v_k - v_b)], \quad (\text{B12}) \end{aligned}$$

which can be further simplified over most of the voltage range. Thus for low forward bias

$$I_1 + I_2 \approx \exp(v_b - v_k) (1 + v_k - v_b), \quad v_b - v_k \ll -1, \quad (\text{B13})$$

for critical bias

$$I_1 + I_2 \approx \pi/4 + \ln 2, \quad v_b - v_k = 0, \quad (\text{B14})$$

and for high forward bias (though with $v_b < v_a$ discussed below)

$$I_1 + I_2 \approx (\pi/2) \exp[\frac{1}{2}(v_b - v_k)], \quad v_b - v_k \gg 1. \quad (\text{B15})$$

The region of the junction making the maximum contribution to the integrals extends from $x = x_k$ to $x = x_k + v_k - v_b$ for $v_b < v_k$, but for increasing bias above v_k is at

$$x = x_{\max} = x_k - (v_b - v_k)/2 \quad (\text{B16})$$

for a center of p character and moves toward the n -type edge of the junction. The relationship between position in the junction and the value of x is given by (B1). The bias v_a at which x_{\max} vanishes for p character (or reaches $v_a - v_b$ for a center of n character) is found to be

$$v_a = v_a \pm \ln(N_v c_p / N_c c_n), \quad (\text{degenerate}) \quad (\text{B17})$$

with the lower sign for p character. This corresponds to the edge of the junction in degenerate material though in nondegenerate diodes the edge occurs where $x = \ln(N_c/n_0)$ on the n side and where

$$x = v_a - v_b - \ln(N_v/p_0)$$

on the p side. Thus

$$v_a = 2 \ln(n_0/n_i) \pm \ln(c_p/c_n), \quad (\text{nondegenerate}), \quad (\text{B18})$$

where for p character the lower sign is chosen and n_0 is the electron density at the n edge of the junction. Conversely, for n character, n_0 is the hole density at the p edge. For bias much above this value $I_2 = 0$, $I_1 = \exp(v_k)$, and capture of injected carriers by the defects outside of the space-charge region becomes the dominant recombination mechanism.