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**Numerical Studies of Low Temperature
Gallium Arsenide Buffer Layers and
Their Influence on Device Operation**

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13. ABSTRACT (Maximum 200 words) This report summarizes recent work on the development and application of an algorithm for studying charge transport in low temperature gallium arsenide (LT GaAs) buffer layers and their influence on device operation. During this reporting period the drift and diffusion equations were modified to include the transient dependence of electrons and holes for gallium arsenide. Calculations were performed for two-terminal, one and two-dimensional structures. Studies with the one-dimensional structures focussed on the trap kinetics. The two-dimensional studies represent a first attempt to examine the effects of clusters on transport through the LT GaAs. The one-dimensional studies are very briefly summarized, as the results were presented at the recent MRS symposium on LT materials, and will appear in the conference proceedings. A copy of the paper accompanies this report. The newer clustering results are also included. We note that these latter results are very preliminary and are included to indicate the future direction of our LT studies.				
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Numerical Studies of Low Temperature Gallium Arsenide Buffer Layers and Their Influence on Device Operation Annual Report

Introduction


The focus of the program is the development and application of an algorithm for studying charge transport in low temperature gallium arsenide (LT GaAs) buffer layers and the influence of such layers on device operation. During this reporting period the drift and diffusion equations were modified to include the transient trap dependence of electrons and holes for gallium arsenide. Calculations were performed for *two terminal, one and two dimensional structures*. Studies with the one dimensional structures focussed on the trap kinetic. The two dimensional studies represent a first attempt to examine the effects of clusters on transport through the LT GaAs.

The one dimensional studies are very briefly summarized, as the results were presented at the recent MRS symposium on LT materials, and will appear in the conference proceedings. A copy of the paper accompanies this report. The newer clustering results are also included. We note that these results are very preliminary and are included to indicate the future direction of our LT studies.

One Dimensional, Two-Terminal Studies

The device studied was a three micron $N^+(LT)N^+$ structure with N^+ regions characterized by shallow donors at $10^{17}/cm^3$. The LT region was characterized by a single level of acceptor traps of density P_a , located 0.3 eV above the valence band, and a single level of donor traps N_d located at 0.83 eV below the conduction band. The results were placed in two categories: (a) *Highly resistive LT regions* ($> 10^6$ ohm - cm) with very low current levels and sudden breakdown, and (b) higher current levels with gradual breakdown.

The *high resistivity* results generally occurred for donor concentrations in excess of acceptor concentrations, with the ionized donor and acceptor traps sustaining approximate compensation. The presence of acceptor traps in the LT region and at the boundary of the LT/N^+ cladding regions, results in the presence of PN junction-type behavior, and a local high value of electric field. Breakdown originates at this interface. The details of these results are contained in the attached paper.

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Two Dimensional, Two-Terminal Studies

The device studied was a three micron $N^+(LT)N^+$ structure with N^+ regions characterized by shallow donors at $10^{18}/\text{cm}^3$. The N^+ regions were heavily doped to provide highly conductive contacts to the LT region. The LT region was made up of clusters of traps. *Experimental* estimates of the cluster radius are 3nm, with a cluster density of $10^{17}/\text{cm}^3$.

The initial simulations did not attempt to simulate the experimental size of the actual cluster configuration. Rather, an attempt was made to determine whether clusters could be studied, and what their properties were. If success could be achieved with simulating the presence of cluster, the structure and the mesh would be modified to simulate realistic structure configuration. Thus the simulated cluster dominated structure was *scaled up* to a radius of 50nm, which is an order of magnitude larger than the experimental estimates of cluster radius.

Simulations were carried out for bias levels of 1.0, 5.0 and 20.0 volts. The 5.0 volt results are displayed below. It was determined that at low bias levels electrons are injected into the LT region where they are captured by the deep acceptor traps. As the acceptor traps become ionized, the current level, which was very small, shows a further reduction as the ionized acceptor clusters show local spherical Schottky-type behavior. That is, local regions of charge depletion surround the clusters and tend to prevent the passage of charge transport and current to flow. Once the traps within the clusters were ionized the LT region became highly insulating.

Avalanche breakdown effects were not included in the present simulations. However, previous experience with the one dimensional LT structures indicates that if the bias is sufficiently high the device will breakdown. We cannot predict, at this point whether breakdown in the presence of clusters will occur at higher or lower bias levels.

Figure 1 displays the distribution of ionized acceptors in the N^+LTN^+ structure at a bias of 5 volts. The clusters closest to the cathode were the first to be ionized. Note that the ionization is greatest at the center of the cluster.

Figure 2 displays the distribution of electrons at this same bias level. The electrons are locally absent from the cluster regions.

Figure 3 displays the potential contours in the structure. While the choice of contour values does not reflect the presence of the depletion regions surrounding the centers of the clusters, the two dimensional nature of the potential distribution is apparent from the 'potential dimple' in the vicinity of the anode.

Figure 4 displays current streamlines in the structure. The circuitous path of current flow is one signature of clustering. In particular, notice the cathode region, where the current path is effectively blocked by the two cathode region clusters. Similarly, the anode region also displays an area that is effectively devoid of

current flow. It must be remarked at this point that the presence of such an unusual structure for current flow implies that resistance measurements may not provide a true estimate of the resistivity of the structure, as local regions of low resistance may be surrounded by other regions of high resistance. The mean current density at this bias level was less than $160\text{A}/\text{cm}^2$.

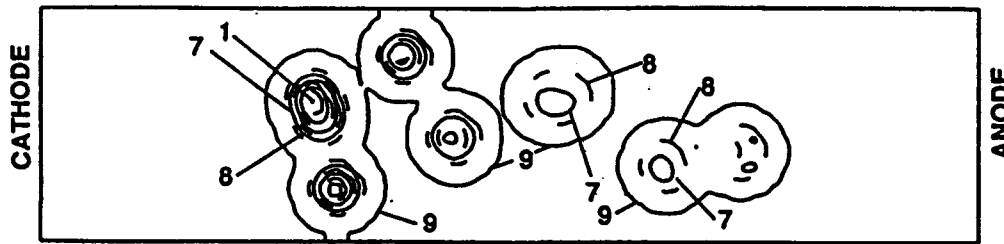


Figure 1. Distribution of ionized acceptors in the structure at a five volt bias. Contour values are evenly spaced, with '1' = $6\text{E}17$ and '9' = 0.0 .

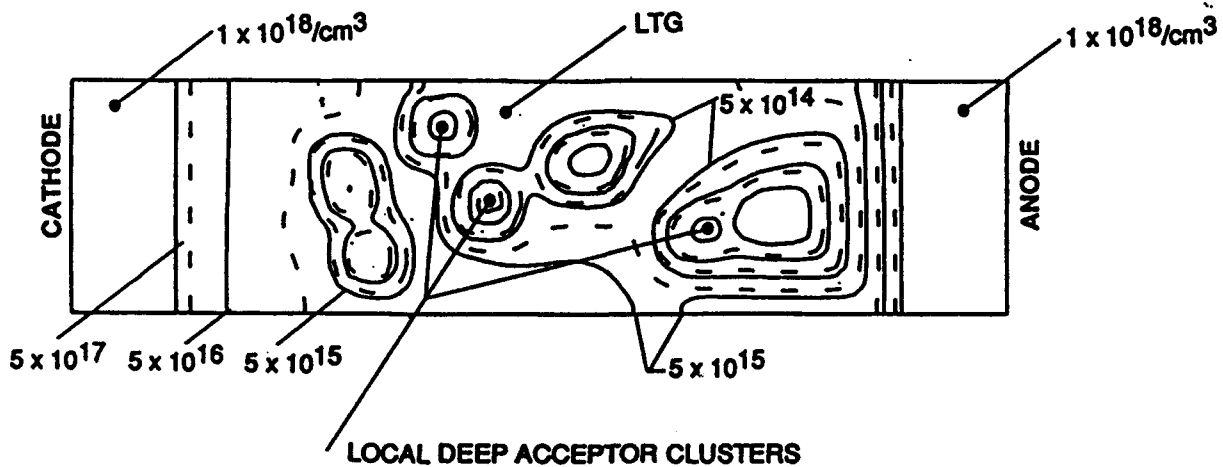


Figure 2. Distribution of electrons in the structure at a five volt bias.

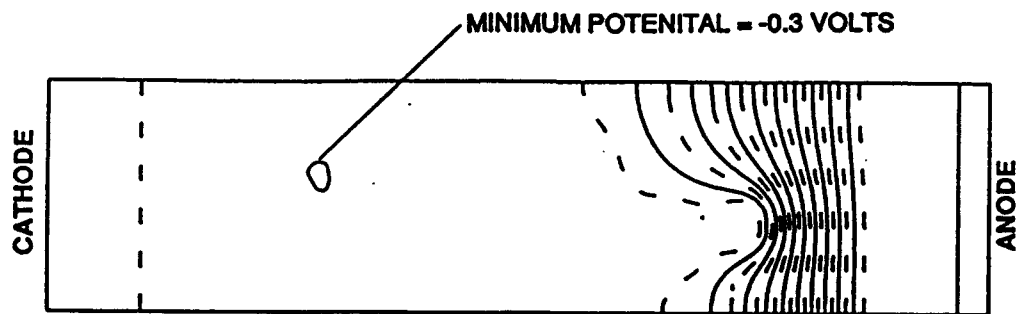


Figure 3. Potential contours in the structure at a five volt bias. Contour values are evenly spaced, with a 0.265 volt increment.



Figure 4. Distribution of current streamlines showing current paths around acceptor clusters.

Future Studies

Future studies will include a more complete analysis of the trap kinetics coupled to multiple trap levels. Detailed cluster calculations will be performed in consultation with workers at IBM. This aspect of the problem has been established. While some effort has been undertaken to examine three-terminal structures with LT layers, no results of any significance have emerged. These studies will be undertaken in earnest during the second year of the study.

INSULATING AND BREAKDOWN CHARACTERISTICS OF LOW TEMPERATURE GaAs

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ABSTRACT

The electrical characteristics of an N(LT)N structure are studied through implementation of numerical simulation techniques for the case of donor traps 0.83 eV below the conduction band and acceptor traps 0.3 eV above the valence band. The results show characteristics sensitive to the relative densities of the traps. In particular, high acceptor trap / low donor trap concentrations generally result in low breakdown voltages, whereas high acceptor / high donor concentrations result in higher breakdown voltages.

INTRODUCTION

The purpose of this discussion is to briefly summarize recent calculations of the electrical characteristics of low temperature growth GaAs (LT GaAs). The device studied was a three micron N(LT)N structure with N regions characterized by shallow donors at 10^{17} /cm³; and an LT region characterized by a single level of acceptor traps of density P_a , located 0.3 eV above the valence band [1], and a single level of donor traps of density N_d located at 0.83 eV below the conduction band.

The results are placed in two categories: Highly resistive LT regions ($> 10^6$ ohm-cm) with (a) low current levels and sudden breakdown, and (b) higher current levels with gradual breakdown. Breakdown characteristics depend upon the magnitude and distribution of the field. For high acceptor / low donor trap concentrations the fields is near zero in the LT region and approaches breakdown values at the anode (LT)N interface; for other combinations the field profile is complex. The study suggests that breakdown voltages will depend upon growth and processing temperatures of LT GaAs.

THE GOVERNING EQUATIONS

The equations include rate equations for electrons and holes, acceptor and donor traps:

$$(1) \quad \partial n / \partial t - \text{div}(j_n / e) = G + \{c_{nd}[a_d N_d^0 - n N_d^+] + c_{na}[a_a P_a^- - n P_a^0]\}$$

$$(2) \quad \partial p / \partial t + \text{div}(j_p / e) = G + \{c_{pa}[p_a P_a^0 - p P_a^-] + c_{pd}[p_d N_d^+ - p N_d^0]\}$$

$$(3) \quad \partial P_a^- / \partial t = -e_2 P_a^- + e_3 P_a^0$$

$$(4) \quad \partial N_d^+ / \partial t = -e_4 N_d^+ + e_1 N_d^0$$

Superscripts denote ionized and neutral acceptors and donors; particle currents are:

$$(5) \quad j_n = -e[nv_n - D_n \text{grad}n], \quad j_p = e[pv_p - D_p \text{grad}p]$$

and diffusivities are governed by the Einstein relation. Avalanche generation [2] is:

$$(6) \quad G = a_n [\exp(-b_n / |F|)^{m_n}] |j_n| / e + a_p [\exp(-b_p / |F|)^{m_p}] |j_p| / e$$

and the emissivity coefficients $e_1 \dots e_4$ are:

$$(7) \quad \begin{aligned} c_1 &= c_{nd}n_d + p c_{pd} & c_2 &= c_{na}n_a + p c_{pa} \\ c_3 &= c_{pa}p_a + n c_{na} & c_4 &= c_{pd}p_d + n c_{nd} \end{aligned}$$

c_{nd} , c_{na} , etc., are capture coefficients [3]; n_d , p_d , etc., are obtained at equilibrium. The above equations are coupled through Poisson's equation, which in terms of energy is:

$$(8) \quad \nabla^2 E = -[e^2/\epsilon][(n-p) - (N_d^+ - P_a^-)]$$

The energy and potential are related, $E = -e\phi$; the field in equation (6) is $F = -\nabla\phi$.

THE RESULTS

All calculations were for the figure 1 shallow doping distribution, with the results dependent upon: (i) the Fermi level, (ii) the ratios P_a/N_d , and (iii) the trap density.

Low Bias Results: Resistivities and compensation estimates were obtained at low bias levels from the density distributions within the interior of the LT region. At a bias of 1.0 volts the results are similar to those at zero bias. As seen in table 1, the resistivities exceed 10^6 ohm-cm for donor traps at 10^{18} , and acceptor traps between 10^{17} and 10^{18} . The positions of the equilibrium Fermi level (above the valence band) for $N_d = 10^{18}$, and $N_a = (10^{18}, 10^{17}, 10^{16})$ are $E_f(\text{ev}) = (0.69, 0.63, 0.45)$, respectively. For $N_d = 10^{18}$, and $N_a = 10^{16}$, $E_f = 0.63\text{ev}$. The designation 'p' identifies the region as p-type, with the mobility dominated by holes. Table 2 displays the ionization of the traps at 1.0 v. The results indicate that within the insulating LT region $P_a^- \sim N_d^+$.

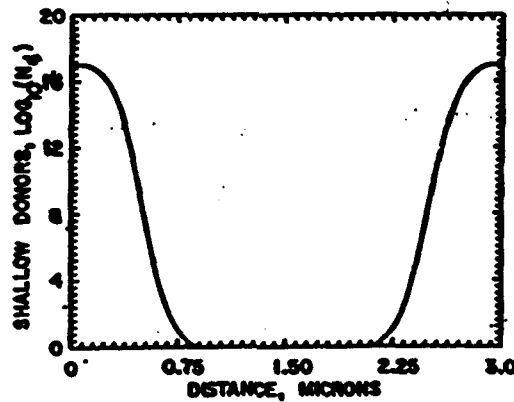


Figure 1. Shallow donor concentration of the N(LT)N structure.

$N_d^{(+)}P_a^{(-)}$	10^{18}	10^{17}	10^{16}	10^{15}
10^{18}	2.72×10^6 (p)	••	••	••
10^{17}	3.21×10^6 (p)	2.68×10^6 (p)	9.24×10^6 (n,p)	4.75×10^7 (n)
10^{16}	5.49×10^1 (p)	3.18×10^3 (p)	2.45×10^6 (p)	••
10^{15}	7.16×10^0 (p)	••	••	••

Table 1. Resistivities (ohm-cm) of the LT region at 1.0 v.

$N_d(+)/P_a(-)$	10^{18}	10^{17}	10^{16}	10^{15}
10^{18}	$P_a^- \sim P_a$ $N_d^+ \sim 0.1N_d$	••	••	••
10^{16}	$P_a^- \sim P_a$ $N_d^+ \sim N_d$	$P_a^- \sim P_a$ $N_d^+ \sim 0.1N_d$	$P_a^- \sim P_a$ $N_d^+ \sim 0.01N_d$	$P_a^- \sim P_a$ $N_d^+ < P_a$
10^{17}	$P_a^- \sim 0.1P_a$ $N_d^+ \sim N_d$	$P_a^- \sim P_a$ $N_d^+ \sim N_d$	$P_a^- \sim P_a$ $N_d^+ \sim 0.1N_d$	••
10^{16}	$P_a^- > N_d$ $N_d^+ \sim N_d$	••	••	••

Table 2. Approximate compensation conditions in LT region at 1.0 v.

Finite and High Bias, $N_d=0$: E_f is significantly below midgap. The results for: (i) P_a varying from $10^{14}/\text{cm}^3$ to $10^{16}/\text{cm}^3$, and (ii) $P_a > 10^{16}/\text{cm}^3$, are distinctly different. For P_a varying from $10^{14}/\text{cm}^3$ to $10^{16}/\text{cm}^3$, and at low voltage, charge neutrality within the LT region means $p \sim P_a^-$; and n is negligible. At elevated bias levels electrons are injected into the LT region and trapped by the acceptors. At sufficiently high bias, with the acceptor traps filled there is a significant increase in n , and a significant current increase. The electric field profile increases nearly linearly with distance. Further increases in bias result in avalanche multiplication. For larger P_a , higher bias is required to fill the acceptors, but the field profile within the structure is still linear. The relevant profiles for this calculation at a bias prior to breakdown are shown in figure 2, for $P_a = 10^{16}/\text{cm}^3$. For $P_a > 10^{16}/\text{cm}^3$, the kinetics is primarily that of holes within the valence band and the ionized deep acceptors, whose concentration is approximately two orders of magnitude below the total trap density. There is near charge neutrality within the LT region except at the downstream (LT)/N interface where a high concentration of ionized acceptor traps forms, with a reduction of mobile holes. There is also a zone depleted of electrons within the heavily doped N region. One observes the formation of a pn junction region as a result of the trap dynamics, with the generation of a local high value of electric field. As a result *avalanching occurs at lower values of voltage, than for the lower P_a study.* The high P_a study is displayed in figure 3.

The situation for $N_d \neq 0$ is qualitatively different, although there are ostensible similarities. For example with $N_d = 10^{17}/\text{cm}^3$ and $P_a = 10^{16}/\text{cm}^3$ the field profile is qualitatively similar to figure 3. The difference is that the acceptor ionization is accompanied by ionized deep donors, as seen in figure 4. The breakdown characteristics are similar to the $N_d=0$ study. The situation when $N_d = P_a = 10^{16}/\text{cm}^3$, displays characteristics that appear as a hybrid of the calculations of figures 2 and 3. At voltages up to and near 20 volts the field distribution is qualitatively similar to that of figure 3, although the peak field is approximately 60 kv/cm less. Further bias increases result in modest changes in the n and p profiles within the LT region, but an increasing share of the voltage drop across the LT region. Breakdown occurs at much higher voltage levels. *The current voltage characteristics for a select set of trap densities are displayed in figure 4. The trap density dependence of breakdown is shown in table 3.*

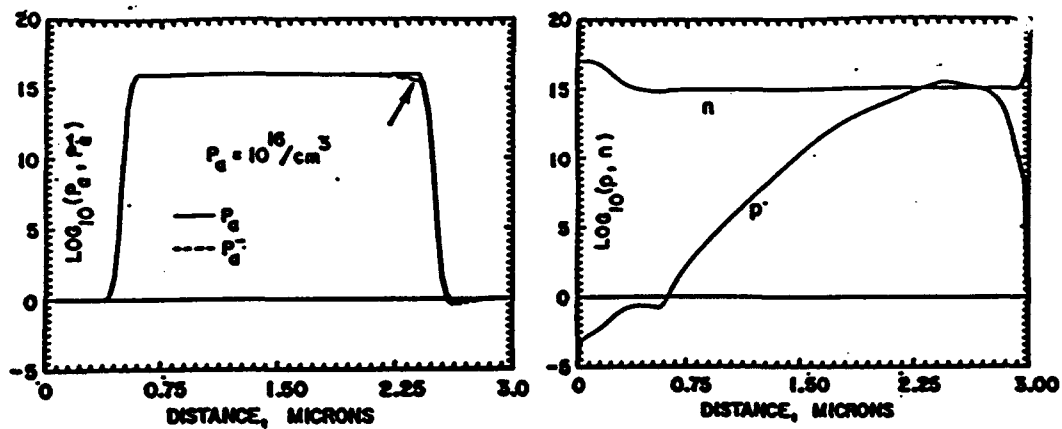


Figure 2. (a) Total and ionized trap distribution at a bias of 45 v. (2b). Distribution of electrons and holes.

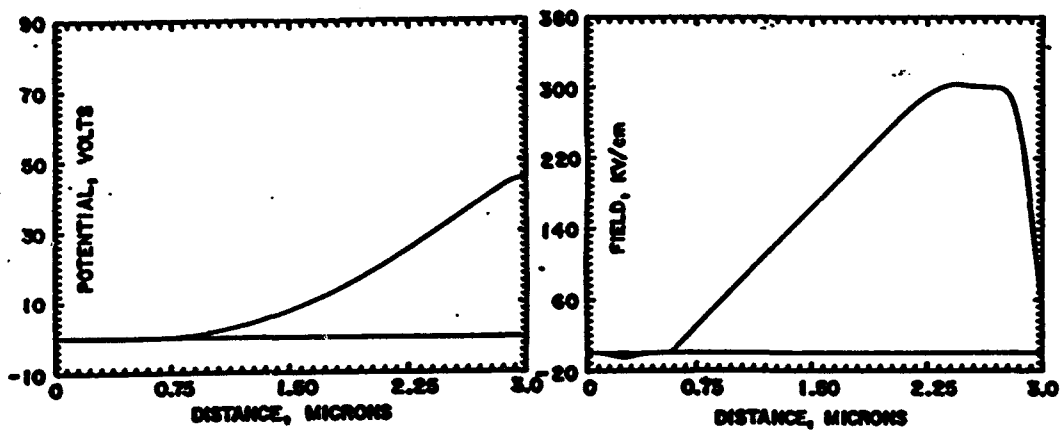


Figure 2c. Potential and electric field distribution at 45 v.

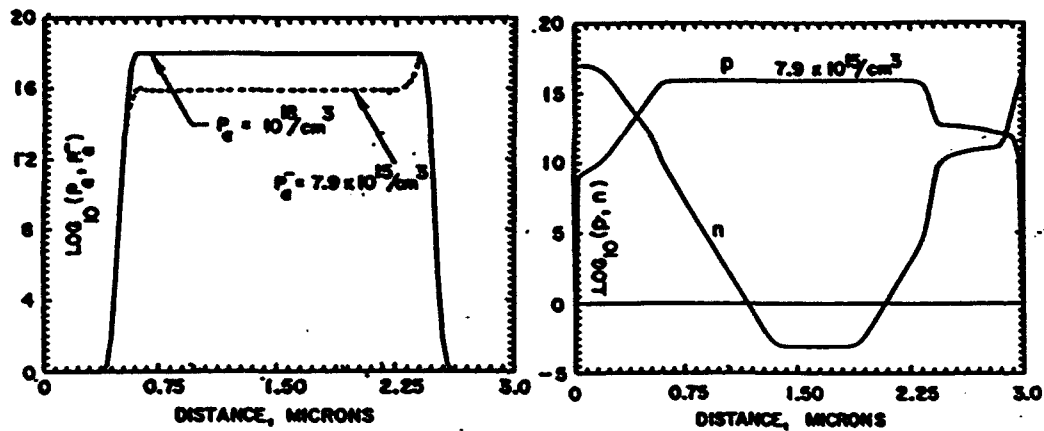


Figure 3. (a) Total and ionized trap distribution at 21v. (3b). Distribution of n and p.

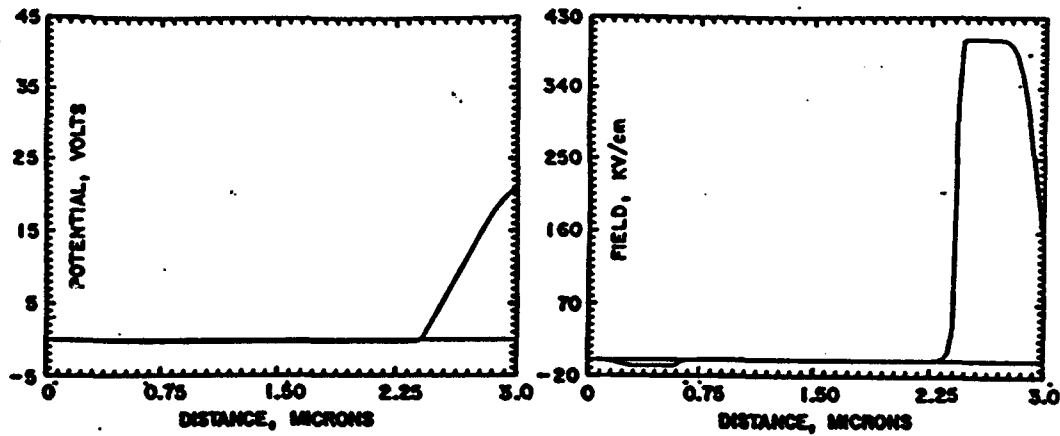


Figure 3c. Potential and electric field distribution at 21 v.

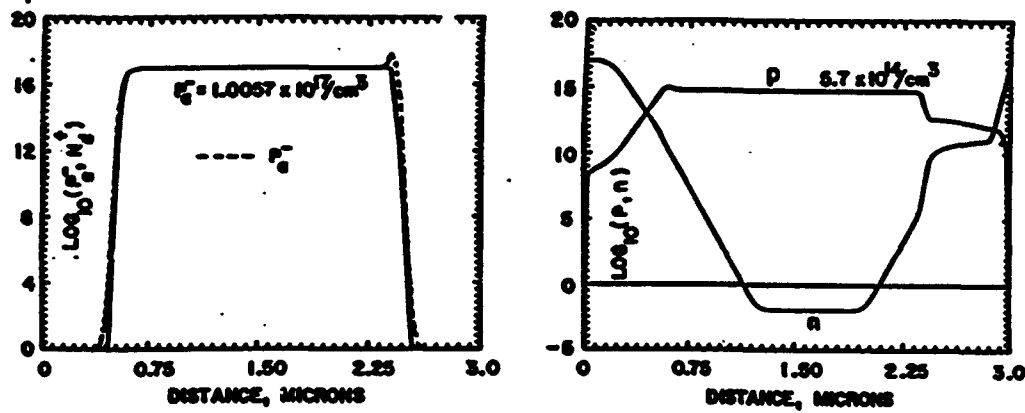


Figure 4. As in figure 3 but for $P_a = 10^{16}$, $N_d = 10^{17}$, at 20v.

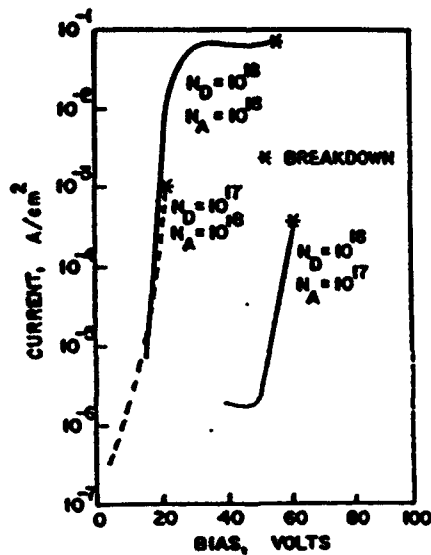


Figure 5. Current voltage characteristics to breakdown for different trap densities.

$N_d(+)/P_a(-)$	10^{18}	10^{17}	10^{16}	10^{15}	10^{14}
0	21 v	25 v	45 v	40 v	28 v
10^{16}	21 v	••	47 v	••	••
10^{17}	21 v	45 v	••	••	••
10^{18}	55 v	62 v	48 v	40 v	30 v
10^{19}	70 v	••	••	••	••

Table 3. Breakdown voltages for different densities of traps.

SUMMARY

The conclusion of this study is that the electrical characteristics of N(LT)N structures are dependent in a very sensitive way on the distribution of traps. The calculations strongly suggest that for N(LT)N structures, the low voltage and high voltage electrical characteristics may provide a signature of the relative density of donor and acceptor traps. Of particular importance is the development of pn [4] junction behavior and low breakdown voltages for acceptor trap dominated material. It is anticipated that the details of the results will depend upon the doping levels of the shallow cladding regions; preliminary studies, however, do not reveal significant qualitative dependencies.

ACKNOWLEDGEMENT

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