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A Theoretical Study of Heterojunction and Graded Band Gap Type Solar Cells

(NASA-CR-143439) A THEORETICAL STUDY OF HETEROJUNCTION AND GRADED BAND GAP TYPE SOLAR CELLS Semiannual Status Report (North Carolina State Univ.) 8 p HC $3.25 CSCL 10A

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Summary of Research

The basic objective of this research is a theoretical study of heterojunction and graded band gap type solar cells. There is strong theoretical and experimental evidence to suggest that heterojunction and graded band gap solar cells can be fabricated with higher efficiencies than obtainable with conventional silicon solar cells. In this research, a computer program is being developed to account for energy band gap variations and the resulting built-in electric fields which result from heterojunctions and graded energy band gaps. This program is then to be used in studying solar cell operation under various optical irradiation conditions. This report summarizes work which has been accomplished to date on these objectives and plans for the remainder of the present grant period.

The basic equations describing heterojunctions and graded band gap solar cells can be written as

$$J_n = \mu_n n \frac{dE_{Fn}}{dx} \tag{1}$$

$$J_p = \mu_p p \frac{dE_{Fp}}{dx} \tag{2}$$

$$\frac{\partial n}{\partial t} = - U + Ge + \frac{1}{q} \frac{\partial J_n}{\partial x} \tag{3}$$

$$\frac{\partial p}{\partial t} = - U + Ge - \frac{1}{q} \frac{\partial J_p}{\partial x} \tag{4}$$

$$\frac{\partial}{\partial x} (\varepsilon \frac{\partial V}{\partial x}) = - q(p - n + N) \tag{5}$$

where E_{Fn} and E_{Fp} are the electron and hole quasi-Fermi levels. These are related to n and p as

$$n = n_{io} \exp[(qV + E_{Fn} + \theta_n)/kT], \quad (6)$$

$$p = n_{io} \exp[-(qV + E_{Fp} - \theta_p)/kT], \quad (7)$$

where θ_n and θ_p are functions of position accounting for the electron affinity, energy band gap and effective mass variations. In explicit form these are given as

$$\theta_n = x_c + kT\, \ell n(N_c/n_{io}) - qV_o, \quad (8)$$

$$\theta_p = -x_v + \frac{kT}{q} \ell n(N_v/n_{io}) + qV_o, \quad (9)$$

where x_c is the electron affinity, $x_v = x_c + E_g$ and V_o is a constant reference potential.

During the first six months of the present grant an existing semiconductor device analysis program has been modified to solve the above set of device equations as well as to accept the modified geometry of desired heterojunction solar cells. A block diagram of the solar cell analysis program indicating the parts which have been modified is shown in Figure 1.

The incorporation of the graded bandgap and heterojunction equations into the analysis program has been somewhat more involved and has taken longer than originally anticipated. This has been due in part to the fact that the cells to be analyzed, which are $Ga_xAl_{1-x}As$ cells, have both a direct and an indirect minimum in the energy band structure. This means there are really two classes of electrons with different mobilities and different diffusion constants. However, we have been able to demonstrate theoretically that the basic set of equations as described above still applies to the total density of electrons if appropriate averages of mobility, effective mass and θ_n values are used. Presently a paper is being prepared on this phase of the work and will be submitted for journal publication.

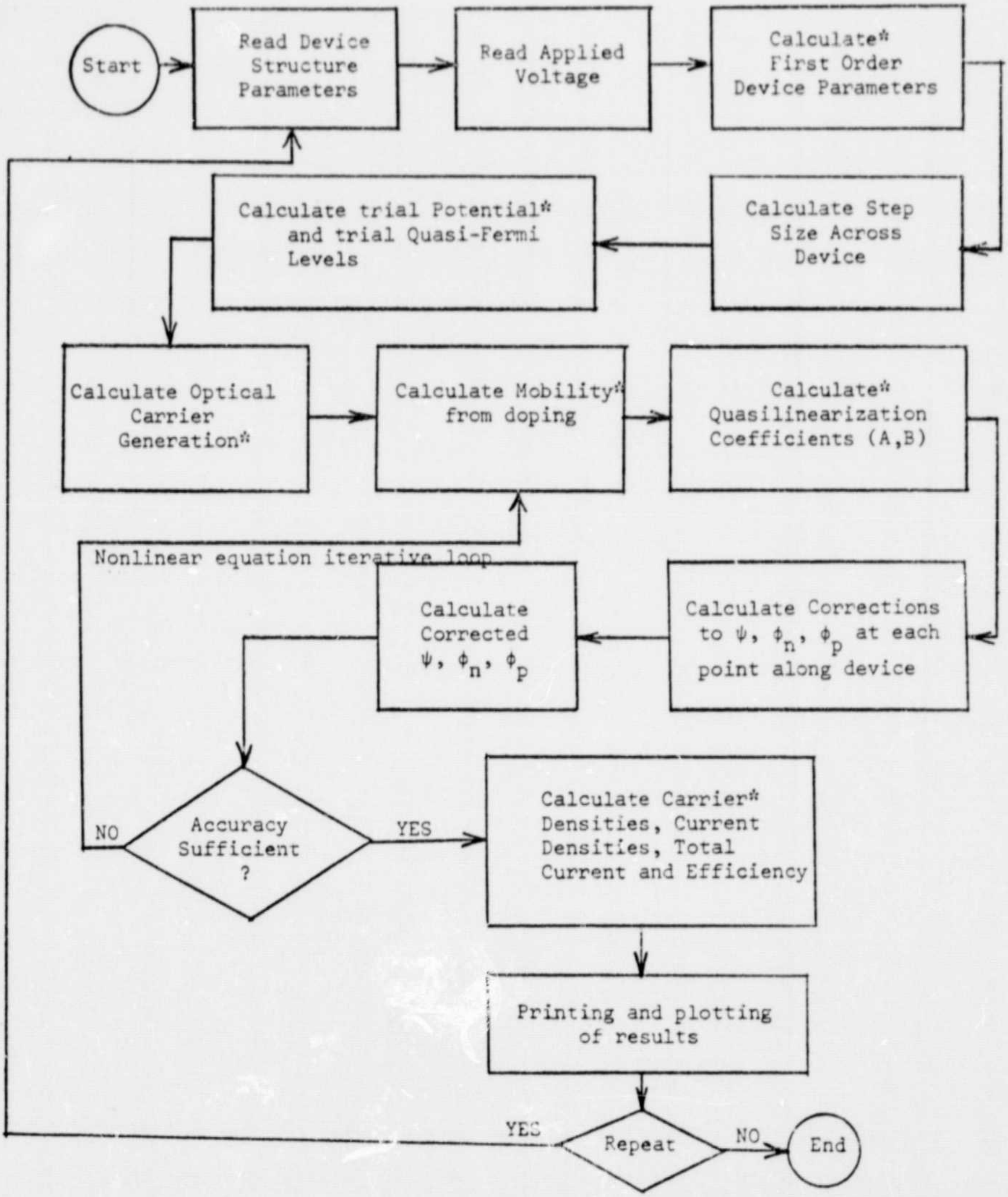


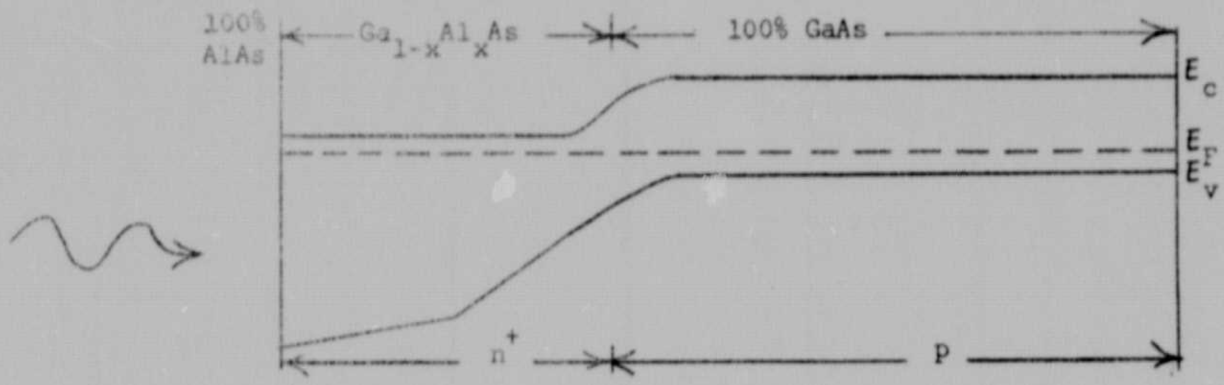
Figure 1. Flow Diagram of Solar Cell Analysis Program. *Indicates sections of program which have been modified for heterojunction and graded band gap cells.

At the present time the major modifications of the device analysis program have been completed. The basic diode analysis program without optical carrier generation has been tested on three basic types of heterojunction and graded band gap devices as shown in Figure 2. In case (a) the composition was varied linearly from pure AlAs at x=0 to pure GaAs at the p-n diode interface. Two types of abrupt heterojunctions have been tested as shown in (b) and (c). In all three cases the program has been found to lead to convergent solutions up to terminal voltages of 1.0 volt.

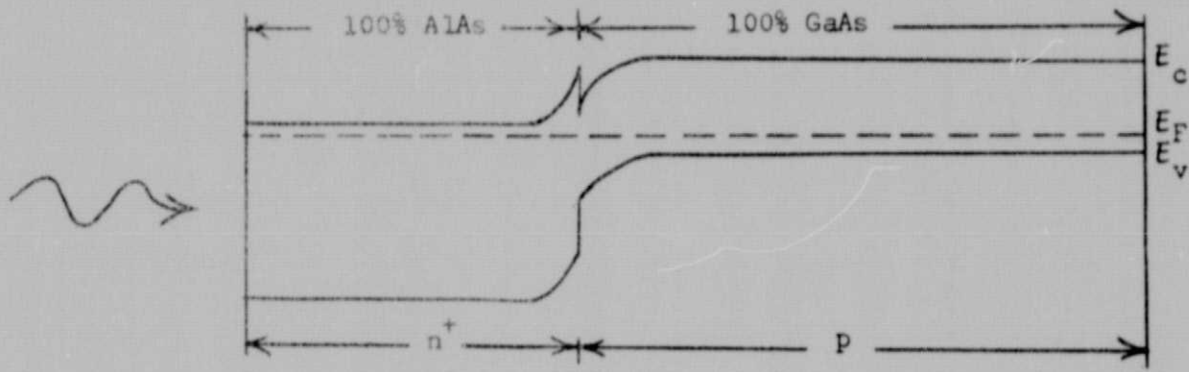
Figures 3 and 4 show calculated electron and hole densities in a device of the type shown in Figure 2(c). For this particular device, the heterojunction occurs 6 μM from the n^+ surface as seen in Figure 4 while the p-n junction occurs at 6.5 μM. As can be seen from the plots, very abrupt changes occur in n and p across the heterojunction. This is for pure AlAs on one side of the interface and pure GaAs on the other side. Since this represents the more severe case of the $Ga_xAl_{1-x}As$ system, no difficulty is expected to be encountered with less abrupt heterojunctions.

The program subroutine which calculates the spatial variation of optical generation rate has been modified for the heterojunction/graded band gap $Ga_xAl_{1-x}As$ material and has been run separate to the main device analysis program. This appears to be working satisfactorily although some minor improvements need to be made in the means of interpolating the optical absorption coefficient between GaAs and AlAs.

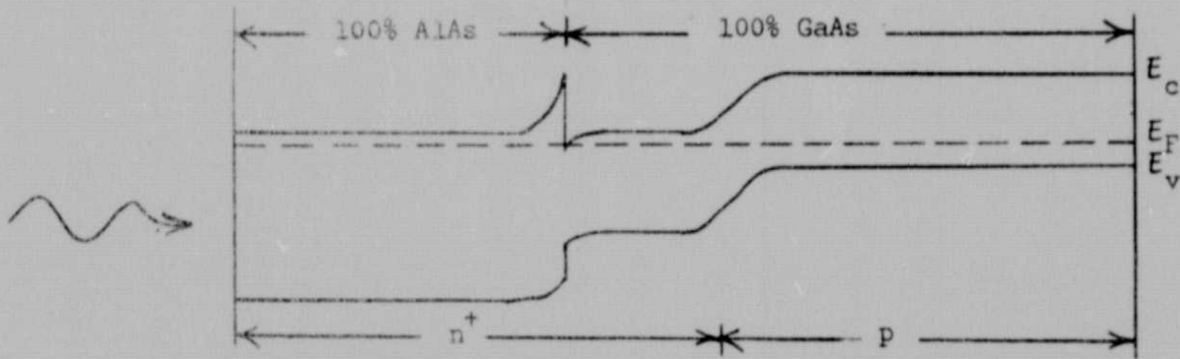
In summary, the work is progressing satisfactorily. The major parts of the programming work have been accomplished. The next step in the work is to combine the optical generation data with the analysis program to solve for the properties of heterojunction solar cells. No major problems are expected to be encountered in accomplishing this work.



(a) Linearly graded device



(b) Abrupt heterojunction with p-n junction at interface



(c) Abrupt heterojunction with p-n junction below interface

Figure 2. Three test types of heterojunction/graded band gap devices.

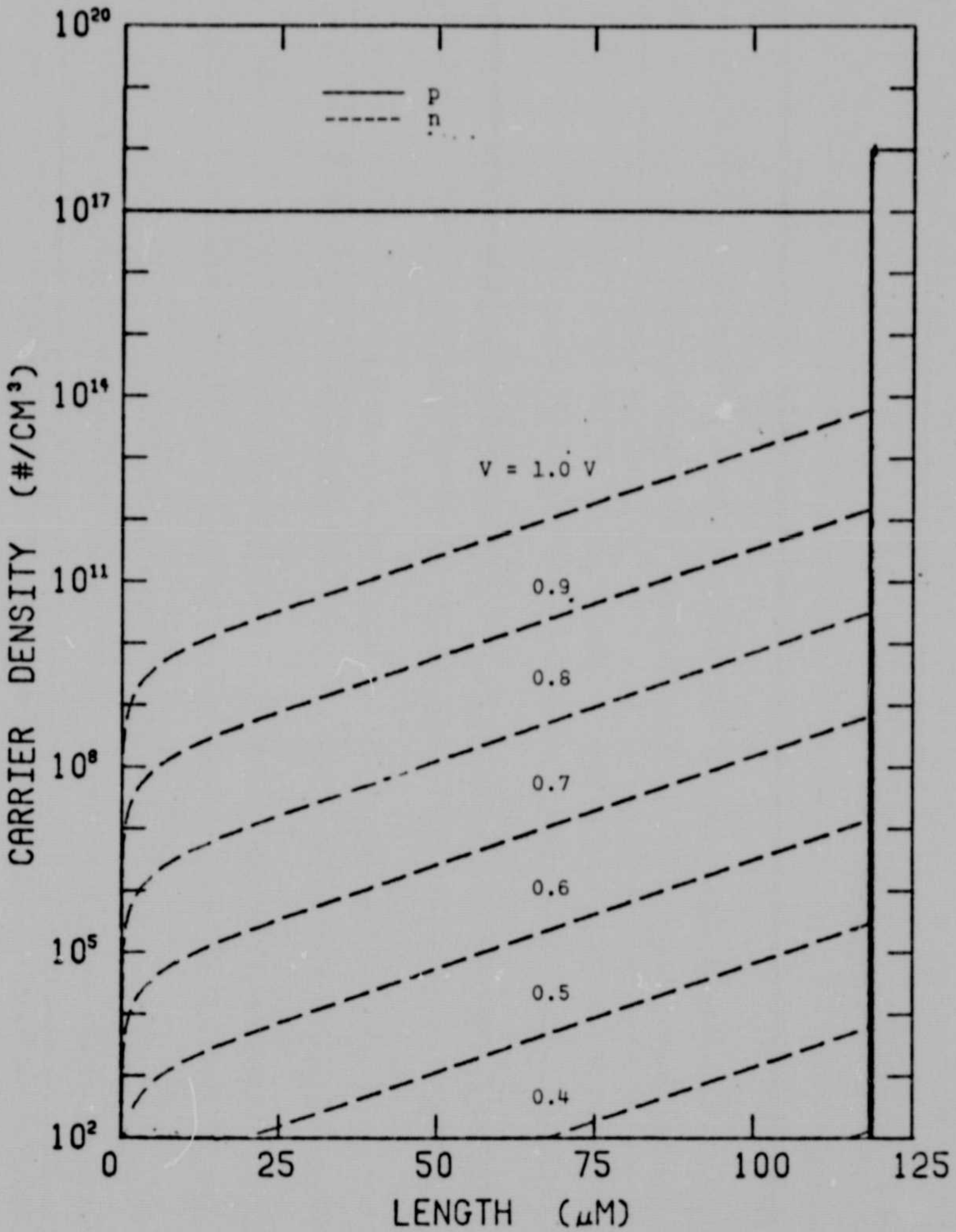


Figure 3. Electron and hole densities at various applied voltages. Surface of cell is at right at 125 μM.

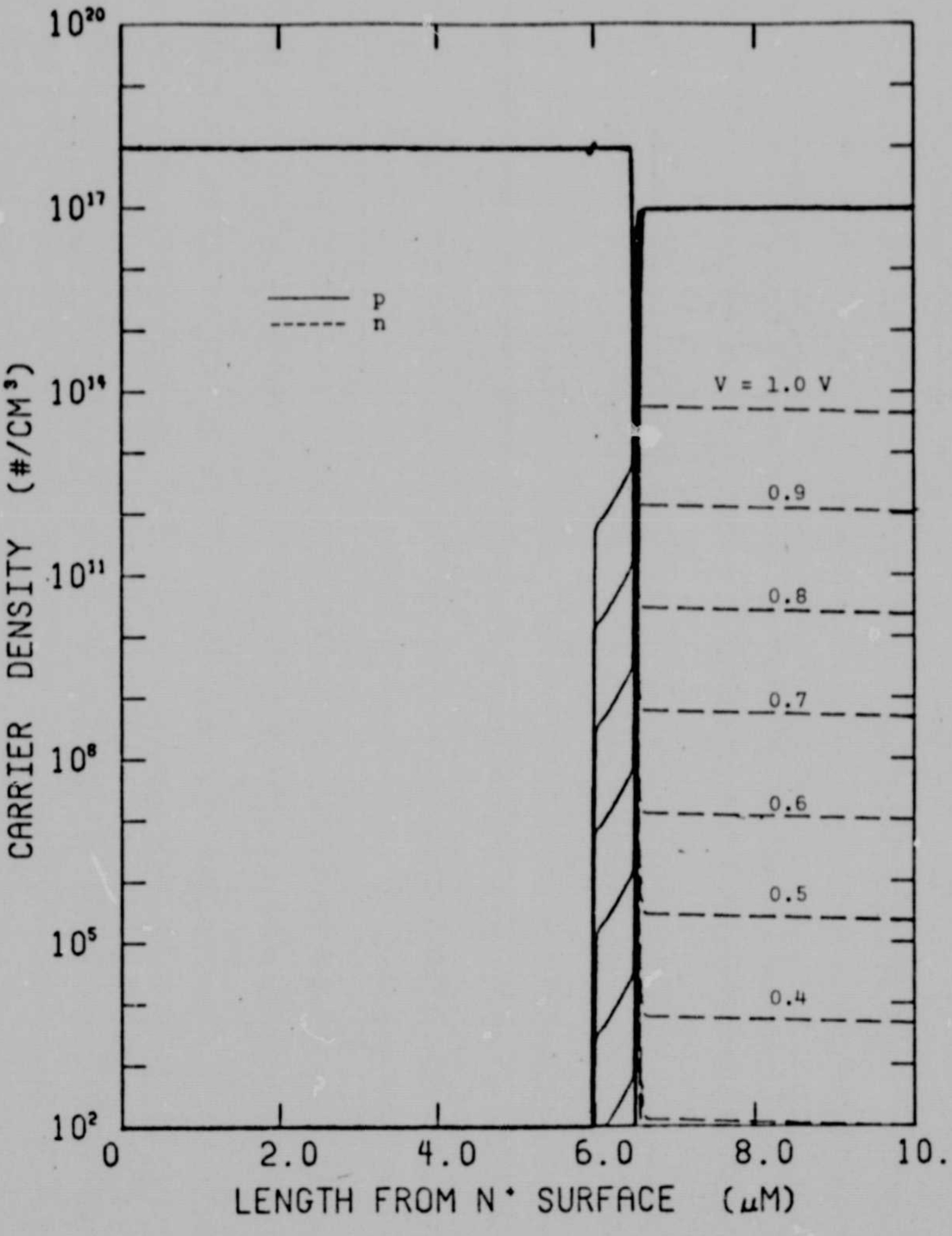


Figure 4. Expanded view of surface region. Heterojunction is at 6 μM, p-n junction at 6.5 μM.