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GALLIUM ARSENIDE (GaAs) SOLAR CELL MODELING STUDIES

By

John H. Heinbockel

Final Report
For the period May 16 - August 16, 1980

Prepared for the
National Aeronautics and Space Administration
Langley Research Center
Hampton, Virginia

Under
Research Grant NAG1-64
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Old Dominion University Research Foundation
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By

John H. Heinbockel*

SUMMARY

In this report various models are constructed which will allow for the variation of system components. Computer studies are then performed using the models constructed in order to study the effects of various system changes. In particular: (1) GaAs and Si flat plate solar power arrays are studied and compared; (2) series and shunt resistance models are constructed, and (3) models for the chemical kinetics of the annealing process are prepared. For all models constructed, various parametric studies are performed.

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* Professor, Department of Mathematical Sciences, Old Dominion University, Norfolk, Virginia 23508.

INTRODUCTION

Mathematical modeling is a flexible tool for assessing and guiding research. A good mathematical model can take the abstract results of research and project future applications. Models are also useful in helping to explain the results of laboratory experiments. As a tool, mathematical modeling and computer simulation can make comparisons between different approaches to a problem. It can also be helpful for an analysis of a proposed system and an assessment of the advantages and disadvantages of one system over the other. Also, mathematical modeling provides an inexpensive, rapid means for estimating the magnitude of changes produced by each variable in a multiple variable program. This is particularly important for guiding research into productive directions. In this report, various mathematical models are constructed and then experiments are conducted with the model for the purpose of better understanding the theoretical behavior of the system. The results of this theoretical experimentation are usually expressed in terms of graphs. This report considers three different types of models: (1) GaAs and Si flat plate solar power arrays in space, (2) series and shunt resistance effects on the open-circuit voltage and short-circuit current of a GaAs solar cell, and (3) models for the chemical kinetics associated with the annealing of GaAs solar cells.

LIST OF SYMBOLS

TMC	total mission cost ($/W)
C1	total transportation costs ($)
C2	solar cell costs ($)
C3	cost of solar cell array ($)
P_S, P_G	end of mission power (W), Si and GaAs solar cell
A	solar cell area (cm^2)
TRC	transportation cost ($/g)
ρ_S, ρ_G	density of Si and GaAs (g/cm^3)
t_{sc}	thickness of Si solar cells (μm)
t_{cg}	thickness of cover glass (μm)
X	proportionality factor
C_{Si}	cost of Si solar cell ($/W)
I	solar intensity (W/cm^2)
η_{Si}	efficiency of Si
η_G	efficiency of GaAs
f_S, f_G	end of mission power fraction for Si and GaAs
TMCS, TMCG	total mission cost of Si and GaAs power arrays ($/W)
T	temperature (°C)
α^*	parameter for radiation defects not annealed
C_{sc}	cost of structural container ($/g)
t_{sc}	thickness of GaAs solar cell (μm)
I_o	Sun's intensity at I.A.U. (0.137 W/cm^2)
ε	emissivity
σ	Stephan Boltzman constant
R_1, R_2	resistances (ohms)

I_D	diode current (mA)
I_{sh}	shunt current (mA)
I_{rec}	recombination current (mA)
I_{inj}	injection current (mA)
I	solar cell current (mA)
V	solar cell voltage (V)
V_j	junction voltage (V)
R_s	series resistance (ohms)
R_{sh}	shunt resistance (ohms)
A	solar cell area (cm^2)
n_i	intrinsic carrier density (cm^{-3})
τ_p, τ_n	lifetimes (sec)
W	width of space charge region (cm)
q	electron charge (coulombs)
K	Boltzman constant (JK^{-1})
T, T_o	temperature (°K)
N_a	number of acceptors (cm^{-3})
N_d	number of donors (cm^{-3})
h	Planck constant (Js)
X_j	junction depth (cm)
H	total cell thickness (cm)
S_n, S_p	recombination velocities (cm/sec)
D_n, D_p	diffusion coefficients (cm^2/sec)
L_{no}, L_n, L_p, L_{po}	diffusion lengths (cm)
I_{sc}	short-circuit current (mA)
V_{oc}	open-circuit voltage (V)
V_o	theoretical maximum open-circuit voltage (V)

M_n^*, M_p^*	effective masses of holes and electrons (kg)
M_o	electron rest mass (kg)
E_g	band gap energy (eV)
$\varepsilon = \varepsilon_o \varepsilon_r$ =	$[8.85(10^{-14})](10.9)$ permitivity of GaAs (F/cm)
μ_{no}, μ_{po}, μ_n, μ_p	mobilities (cm^2/volt-sec)
α	$(0 \leq \alpha \leq 1)$ fraction of defects with Schottky characteristics
α_o	number of Schottky type defects per cm^2
$I_{o,pn}$	Pn model diode coefficients
$I_{o,sk}$	Schottky model diode coefficient
A_r	Richardson constant $A/(cm^2 {}^\circ K^2)$
ϕ_{bn}	barrier height (eV)
I_L	illuminated current (mA)
I_o, I_1	current coefficients
D	window thickness (cm)
I_1^*, I_2^*	currents (mA)
V_1^*, V_2^*	voltage (V)
r	distance from the Sun

MISSION COST ANALYSIS OF FLAT PLATE SOLAR POWER ARRAYS

We define the total mission cost (TMC) for a power array constructed with solar cells as

$$TMC = \frac{C1 + C2 + C3}{P} \quad (\$/W)$$

where P = power output at end of mission (EOM),

C1 = total transportation costs,

C2 = solar cell costs, and

C3 = cost of solar cell array.

For a silicon solar cell power array we have shown (ref. 1) that with no concentration (C=1) we have

$$C1 = (TRC)(A)(\rho_s \; t_{sc} + \rho_{cg} \; t_{cg})(1+X) \quad (\$)$$
$$C2 = (A)(0.137) \; \eta_{Si,25} \; C_{Si} \quad (\$)$$
$$C3 = (X)(A)(\rho_s \; t_{sc} + \rho_{sc} \; t_{cg})(C_{sc}) \quad (\$)$$

and

$$P = A \; I \; \eta_{Si} \; (T) f_{Si} \quad (W)$$
$$= A(0.137)(0.15) \; 1\text{-}0.0041(T\text{-}25) \; (0.56)$$

where

TRC = transportation costs (\$/g),

A = area of solar cell (cm^2),

ρ_S, ρ_G = density of Si and GaAs (g/cm^3),

ρ_{cg} = density of cover glass (g/cm^3),

t_{sc} = thickness of Si solar cell (μm),

t_{cg} = thickness of cover glass (μm),

X = proportionality factor, then

$$WSC = X \cdot W_S$$

WSC = weight of structural container which is proportional to:

W_S = weight of Si solar cell plus cover glass (g),

C_{Si} = Cost of Si solar cell (\$/W),

C_{sc} = cost of structural container (\$/g),

I = solar intensity (W/cm^2),

η_{Si} = efficiency of Si,

T = temperature (°C), and

f_{Si} = end of life power fraction for Si solar cells.

Hence for a silicon solar array we have

$$\text{TMCS} = \left\{A(\text{TRC})(\rho_s \, t_{sc} + \rho_{cg} \, t_{cg})[1+X] + A(0.137)\eta_{Si,25} + XA(\rho_s \, t_{sc} + \rho_{cg} \, t_{cg})C_{sc}\right\} \div \left\{A(0.137)(0.15)[1 - 0.0041(T-25)](0.56)\right\}$$

For GaAs solar power arrays we have shown (ref. 2) that for flat plat arrays (C=1):

$$C1 = \text{TRC}(A)[\rho_g \, t^*_{sc} + \rho_{cg} \, t_{cg} + X(\rho_s \, t_{sc} + \rho_{cg} \, t_{cg})]$$

$$C2 = 300\left(\frac{t^*_{sc}}{300}\right)^{0.393} A(0.137)\eta_{G,25}$$

$$C3 = XA(\rho_s \, t_{sc} + \rho_{cg} \, t_{cg})C_{sc}$$

$$P_G = A(\bar{I})\eta_G(T)f_G$$

$$= A(0.137)(0.20)[1 - 0.00225(T-25)]f_G$$

where the end of life power fraction is

$$f_G = \frac{(1 - \alpha^*)}{1 + 0.92\exp[-0.07(T-75)]} + \alpha^*(0.5), \quad T \geq 75$$

$$= 0.5 \qquad\qquad, \quad T < 75$$

and is a function of the operating temperature.

Hence, for GaAs solar power arrays

$$\text{TMCG} = \left\{\text{TRC}(A)[\rho_G \, t^*_{sc} + \rho_{cg} \, t_{cg} + X(\rho_s \, t_{sc} + \rho_{cg} \, t_{cg})] + 300\left(\frac{t^*_{sc}}{300}\right)^{0.393} A(0.137)(0.2) + X\,A(\rho_s \, t_{sc} + \rho_{cg} \, t_{cg})C_{sc}\right\}$$

$$\div \left\{A(0.137)(0.20)[1 - 0.00225(T-25)]f_G\right\}$$

Let ΔSMC denote the change in the specific mission cost, then

$$\Delta\text{SMC} = \text{TMCG} - \text{TMCS} = \text{TRC}\;\alpha_1 + \alpha_2$$

where (with appropriate units)

$$\alpha_1 = \left\{\frac{A\left[\rho_g\, t^*_{sc} + \rho_{cg}\, t_{cg} + X\left(\rho_s\, t_{sc} + \rho_{cg}\, t_{cg}\right)\right]}{P_G}\right.$$

$$\left. - \frac{A\left(\rho_s\, t_{sc} + \rho_{cg}\, t_{cg}\right)[1 + X]}{P_S}\right\} (10^{-4})$$

$$\alpha_2 = 300\left(\frac{t^*_{sc}}{300}\right)^{0.393} \frac{A(I)(0.2)}{P_G} - \frac{(I)(A)(0.15)C_{Si}}{P_S}$$

$$+ 10^{-4}\left\{XA\left(\rho_S\, t_{sc} + \rho_{cg}\, t_{cg}\right)C_{sc}\left(\frac{1}{P_G} - \frac{1}{P_S}\right)\right\}$$

Here ΔSMC is a linear function of the transportation cost ($/g). In the case where the intensity of the Sun is inversely proportional to the distance r from the Sun in astronautical units (A.U.), then

$$I = \frac{Io}{r^2} = \frac{0.137}{r^2}$$

and the temperature of the flat array is approximately

$$2\varepsilon\, \sigma\, T^4 = I = \frac{0.137}{r^2}$$

or

$$T = \left(\frac{331.5}{\sqrt{r}} - 273\right) (°C)$$

Figures 1 through 4 illustrate how the specific mission cost difference ΔSMC changes with respect to various parameters of the system. Note that when ΔSMC is negative the Si array costs are higher than GaAs array costs. These figures illustrate that flat plate GaAs solar power arrays will be more economical in those operating regimes which require a high temperature (near Sun missions) and those missions which have a high transportation cost. In these figures we have used the nominal values given in Table 1.

Table 1. Nominal values for flat plate arrays.

$C_{Si} = 0$, $\rho_G = 5.32$, $\rho_{cg} = 2.5$, $t_{cg} = 100$
$X = 4$, $\rho_s = 2.33$, $A = 4$, $C_{sc} = 10$, $t_{sc} = 50$

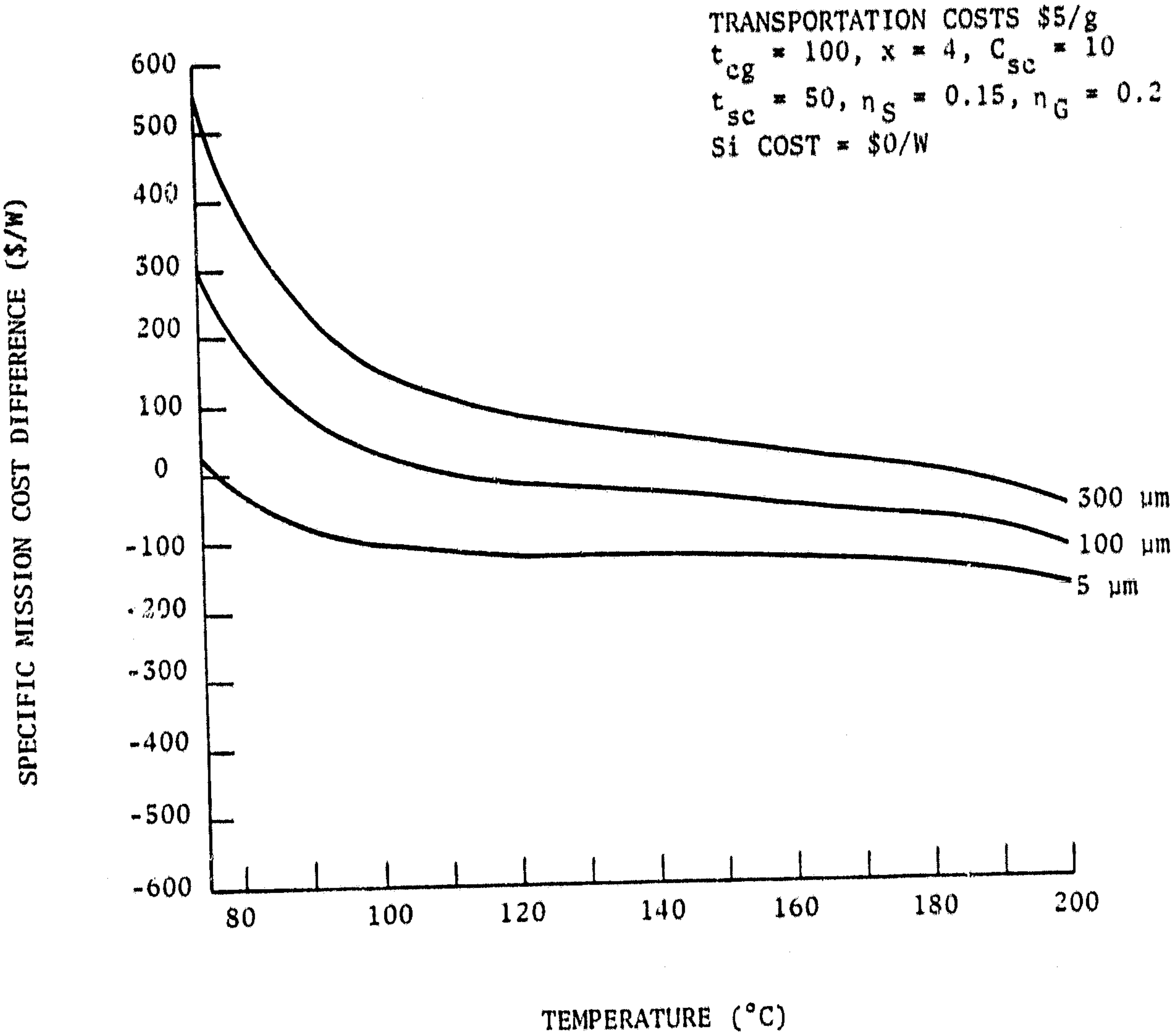

Figure 1. Specific mission cost difference vs. operating temperature.

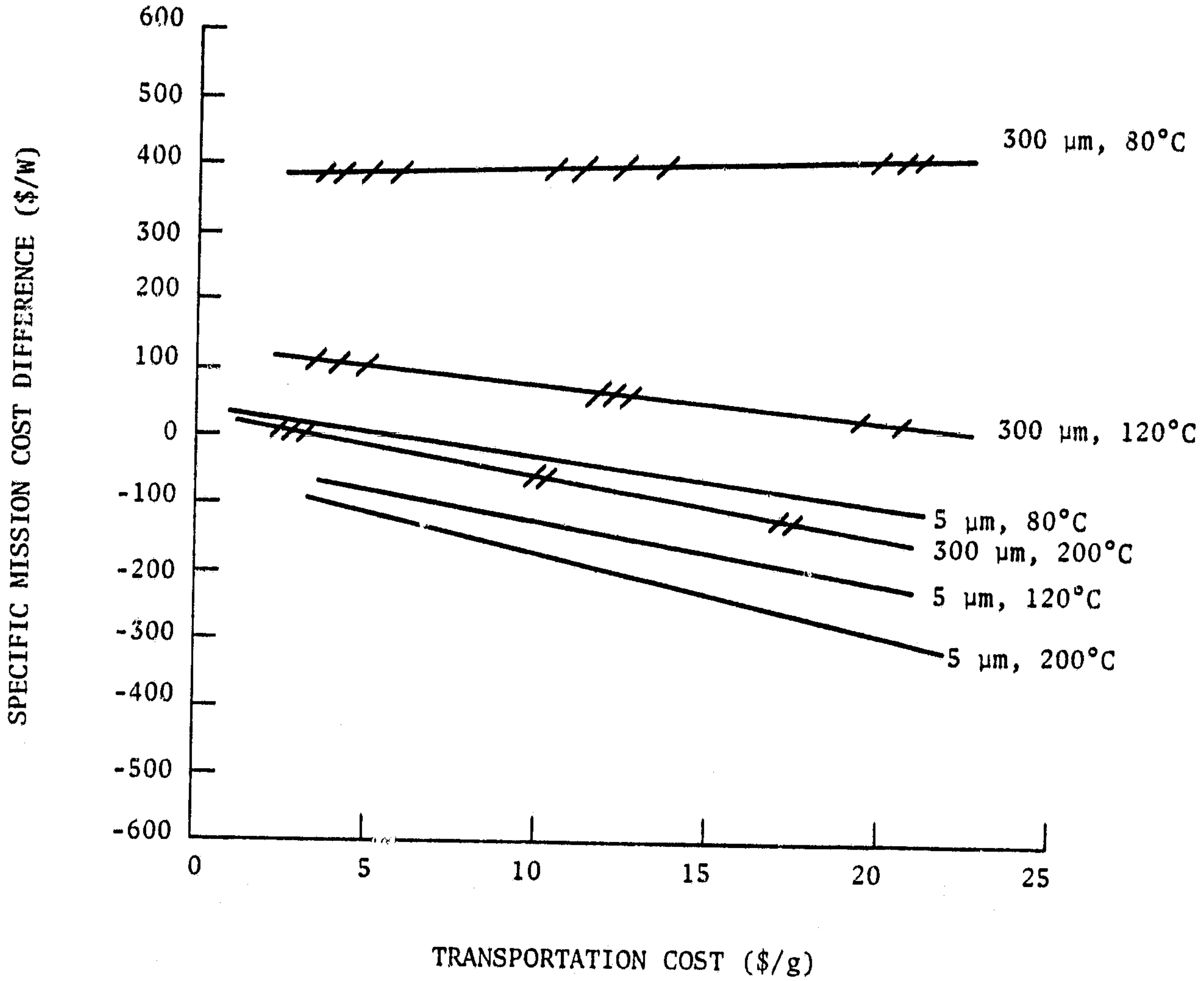

Figure 2. Specific mission cost difference vs. transportation cost for various operating conditions.

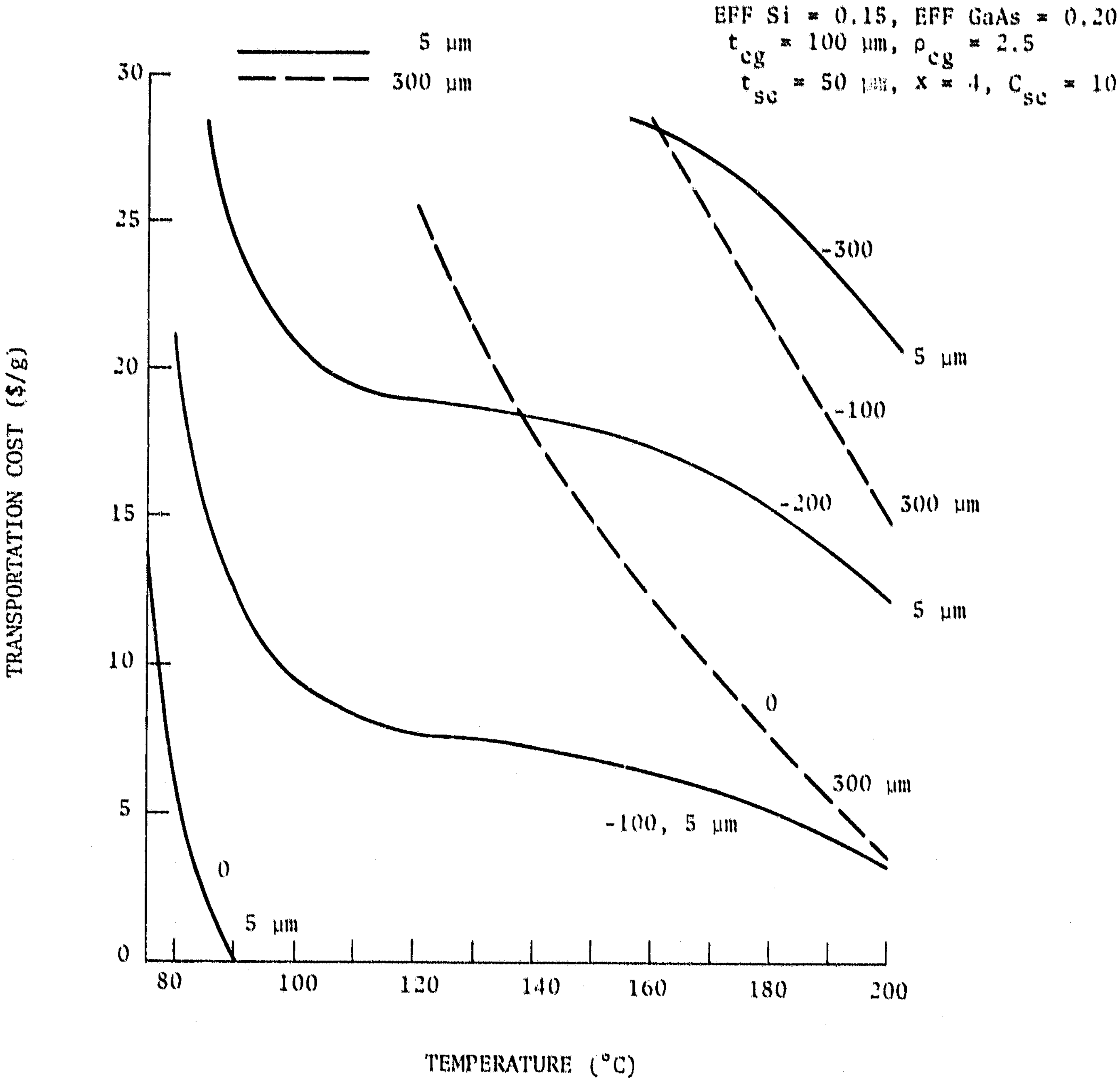

Figure 3. Level curves where ΔSMC = K is a negative constant or zero for various GaAs thicknesses.

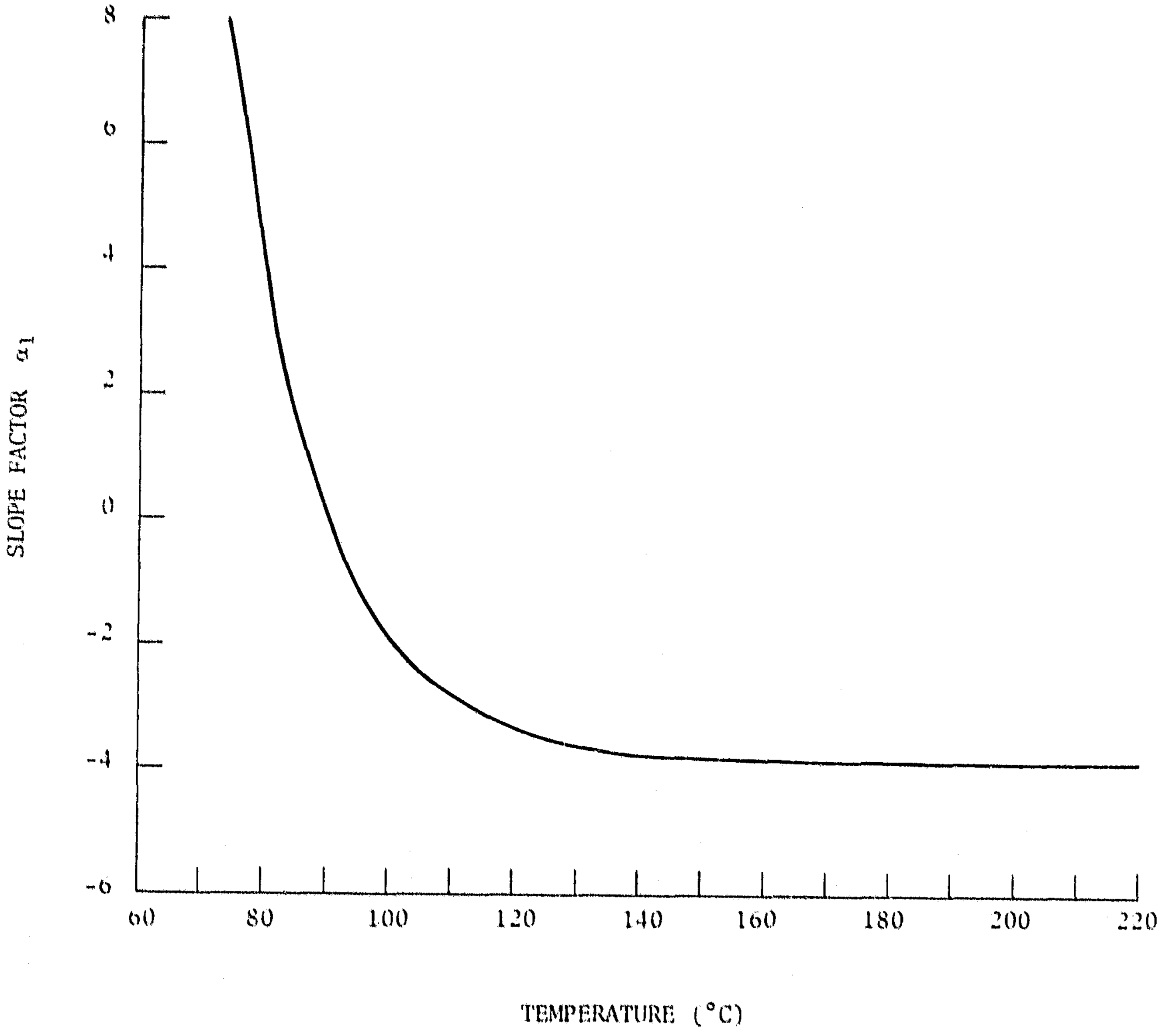

Figure 4. Slope α_1 vs. operating temperature.

SERIES AND SHUNT RESISTANCE

Various models exist for the current-voltage relationship of solar cells which include both the series and shunt resistance effects (see refs. 3 through 19). These resistance effects are of interest because they are power-dissipating factors. Figure 5 is an equivalent circuit diagram of a solar cell.

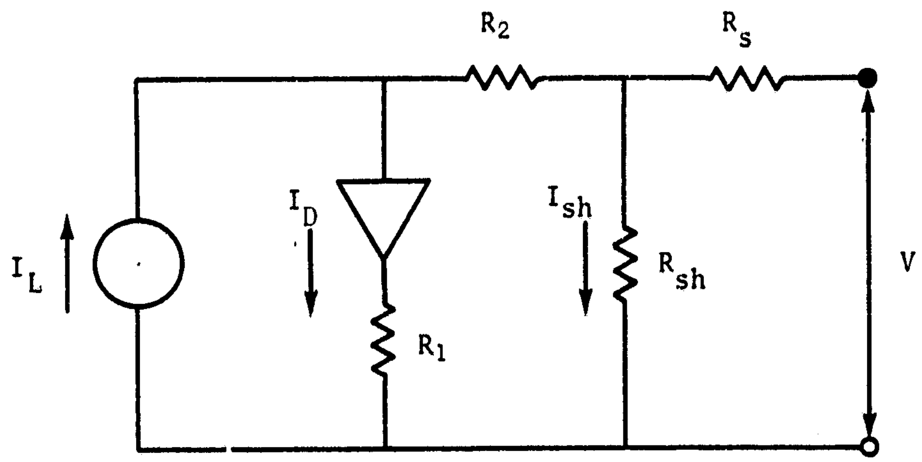

Figure 5. Equivalent circuit of solar cell.

Usually in figure 5, the resistances R_1 and R_2 are neglected, where R_1 is a lumped value for the semiconductor front layer resistance. In figure 5, R_s is the series resistance of the metal contacts and R_{sh} is the shunt resistance caused by various leakage paths. Neglecting R_1 and R_2, the current-voltage relationship for this model can be expressed as

$$I = I_L - (I_D + I_{sh}) \tag{1}$$

where I_L is the illuminated current, I_D is the diode current given by

$$I_D = I_o \left[e^{q V_j/KT} - 1\right] \tag{2}$$

I_{sh} is the shunt current given by

$$I_{sh} = \frac{V_j}{R_{sh}} \tag{3}$$

and V_j is the junction voltage

$$V_j = V + IR_s \tag{4}$$

In order to obtain a better qualitative understanding of the GaAs solar cell behavior, we will adopt the model of the equivalent circuit illustrated in figure 6.

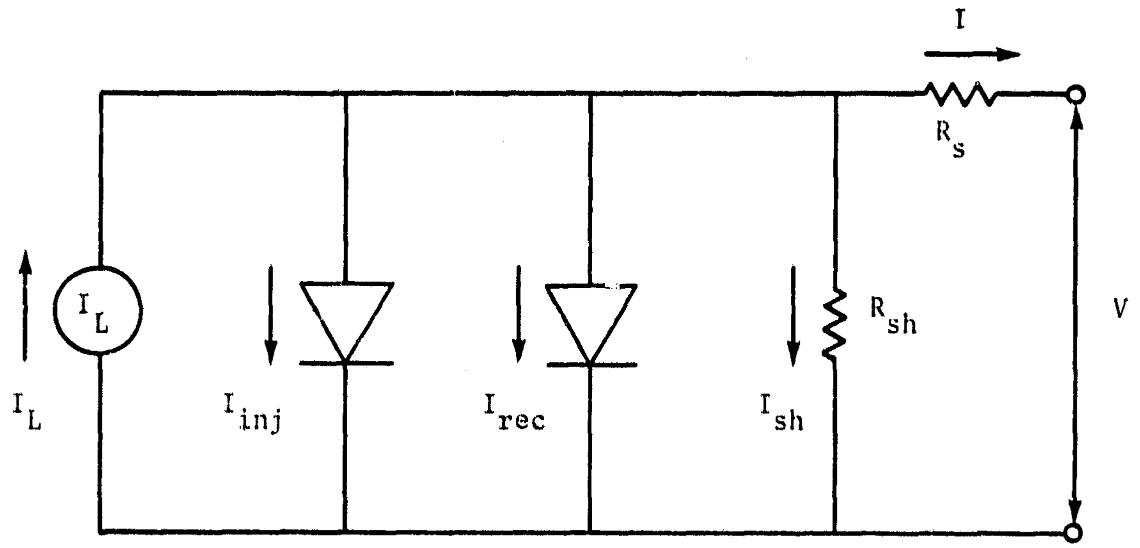

Figure 6. Another equivalent circuit of a solar cell.

In figure 6, the currents are defined as follows:

The recombination current I_{rec}:

$$I_{rec} = \frac{\pi A N_i W K T}{\sqrt{\tau_p \tau_n}} \frac{\sinh\left(\frac{qV_j}{2KT}\right)}{\left(V_o - V_j\right)} \tag{5}$$

where

$$W = \sqrt{\frac{2\varepsilon\left(V_o - V_j\right)}{q}\left(\frac{N_a + N_d}{N_a N_d}\right)} \tag{6}$$

$$V_o = \frac{KT}{q} \ln\left(\frac{N_a N_d}{N_i^2}\right) \tag{7}$$

$$N_i^2 = 4\left(\frac{2\pi K}{h^2}\right)^3 T^3 \left(M_n^* M_p^*\right)^{3/2} e^{-Eg/KT} \tag{8}$$

$$E_g = 1.522 - 5.8(10^{-4})T^2/(T + 300). \tag{9}$$

The injection current I_{inj} is defined as:

$$I_{inj} = \left[(1 - \alpha)\, I_{o,pn} + \alpha I_{o,sk}\right]\left[e^{\frac{qVj}{KT}} - 1\right] \tag{10}$$

where $I_{o,pn}$ is the coefficient for a Pn diode model, $I_{o,sk}$ is the coefficient for a Schottky barrier diode model, and α is the fraction of material having Schottky characteristics ($\alpha = 0$ for a Pn material and $\alpha = 1$ for Schottky material). It is assumed that $\alpha = \alpha_o(10^{-8})$ where $0 \le \alpha_o \le 10^8$, and α_o represents the number of defects per cm^2.

For the Pn diode model

$$I_{o,pn} = A[G(x_1,y_1,z_1) + G(x_2,y_2,z_2)] \tag{11}$$

where

$$G(\xi,\eta,\tau) = \xi\left[\frac{\sinh(\eta) + \cosh(\eta)}{\tau\sinh(\eta) + \cosh(\eta)}\right] \tag{12}$$

$$\left.\begin{array}{ll} x_1 = q\dfrac{D_n n_i^2}{L_n N_a} & x_2 = qD_p n_i^2/L_p N_d \\ y_1 = X_j/L_n & y_2 \quad [H - (D + X_j + W)]/L_p \\ z_1 = S_n L_n/D_n & z_2 = S_p L_p/D_p \end{array}\right\} \tag{13}$$

For the Schottky diode model:

$$I_{o,sk} = AA_r T^2 \exp(-\phi_{bn}/KT) \tag{14}$$

where

A_r = effective Richardson constant = 4.4 A/(cm^2°K^2),

T = temperature (°K), ϕ_{bn} = barrier height = 0.89(eV), and

A = solar cell area = 1 cm^2.

In the above models for the injection current, the diffusion lengths D_n, D_p are related to the mobilities by the Einstein relations

$$\left.\begin{array}{l} D_n = \mu_n KT \\ D_p = \mu_p KT \end{array}\right\} \tag{15}$$

where the mobilities, diffusion lengths, and lifetimes are temperature dependent and are given by

$$\left.\begin{aligned} \mu_p &= \mu_{po}\left(\frac{T_o}{T}\right)^{\frac{3}{2}}, \ \mu_n = \mu_{no}\left(\frac{T_o}{T}\right)^{\frac{3}{2}} \\ L_p &= L_{po}\left(\frac{T}{T_o}\right)^{\frac{1}{2}}, \ L_n = L_{no}\left(\frac{T}{T_o}\right)^{\frac{1}{2}} \\ \tau_p &= L_p^2/D_p, \ \tau_n = L_n^2/D_n \end{aligned}\right\} \tag{16}$$

It can be seen that the current-voltage relation for figure 6 can be expressed in the form

$$I = I_L - I_{dark} \tag{17}$$

where I = solar cell current, I_L = illuminated current, and I_{dark} is the dark current which is a function of the junction voltage $V_j = V + IR_s$. The dark current can be expressed in the functional form

$$I_{dark} = f(V + IR_s) \tag{18}$$

where R_s is the series resistance, f is a function satisfying $f(0) = 0$ and $f(x)$ is monotone increasing, and V = solar cell voltage. The function $f(V_j)$ can be expressed

$$\begin{aligned} f(V_j) &= I_{inj} + I_{rec} + I_{sh} \\ &= I_o\left[e^{qVj/KT} - 1\right] + I_1 \frac{\sinh\left(\frac{qVj}{2KT}\right)}{\sqrt{V_o - V_j}} + \frac{Vj}{R_{sh}} \end{aligned} \tag{19}$$

where I_o, I_1 are coefficients obtained from equations (10) and (5) respectively.

Equation (17) is a nonlinear current-voltage relation which can be solved using a computer. Various parameter studies were performed using the model given by equation (17). Some of the results of the parameter study are illustrated in figures 7 through 18. The various parameters occurring in the model were assigned the nominal values depicted in table 2. Figure 7 illustrates the effect of varying the shunt resistance R_{sh}. Note that the open-circuit voltage decreases and the "knee" of the current-voltage curve is greatly decreased. Figure 8 illustrates the effect of varying the series resistance R_s. These curves show that the open-circuit voltage is not affected by such changes but that the short-circuit current is affected for large values

Table 2. Nominal values used in parameter study.

$T = T_o = 300\ °K$	$D = 0.4\ (10^{-4})$ cm
$A_r = 4.4\ A/(cm^2 °K^2)$	$X_j = 1.0\ (10^{-4})$ cm
$\phi_{bn} = 0.89$ eV	$S_p = 1.0\ (10^6)$ cm/sec
$N_a = 5.0\ (10^{18})\ cm^{-3}$	$S_n = 1.0\ (10^4)$ cm/sec
$N_d = 6.0\ (10^{17})\ cm^{-3}$	$H = 250\ (10^{-4})$ cm
$A = 1.0\ cm^2$	$I_L = 30$ mA
$\varepsilon = (10.9)(8.85)(10^{-14})$ F/cm	$R_s = 1.0\ \Omega$
$\mu_{po} = 2700\ cm^2$/volt-sec	$R_{sh} = 10^7\ \Omega$
$\mu_{no} = 150\ cm^2$/volt-sec	$\alpha = 0$
$L_{po} = 3.5\ (10^{-4})$ cm	

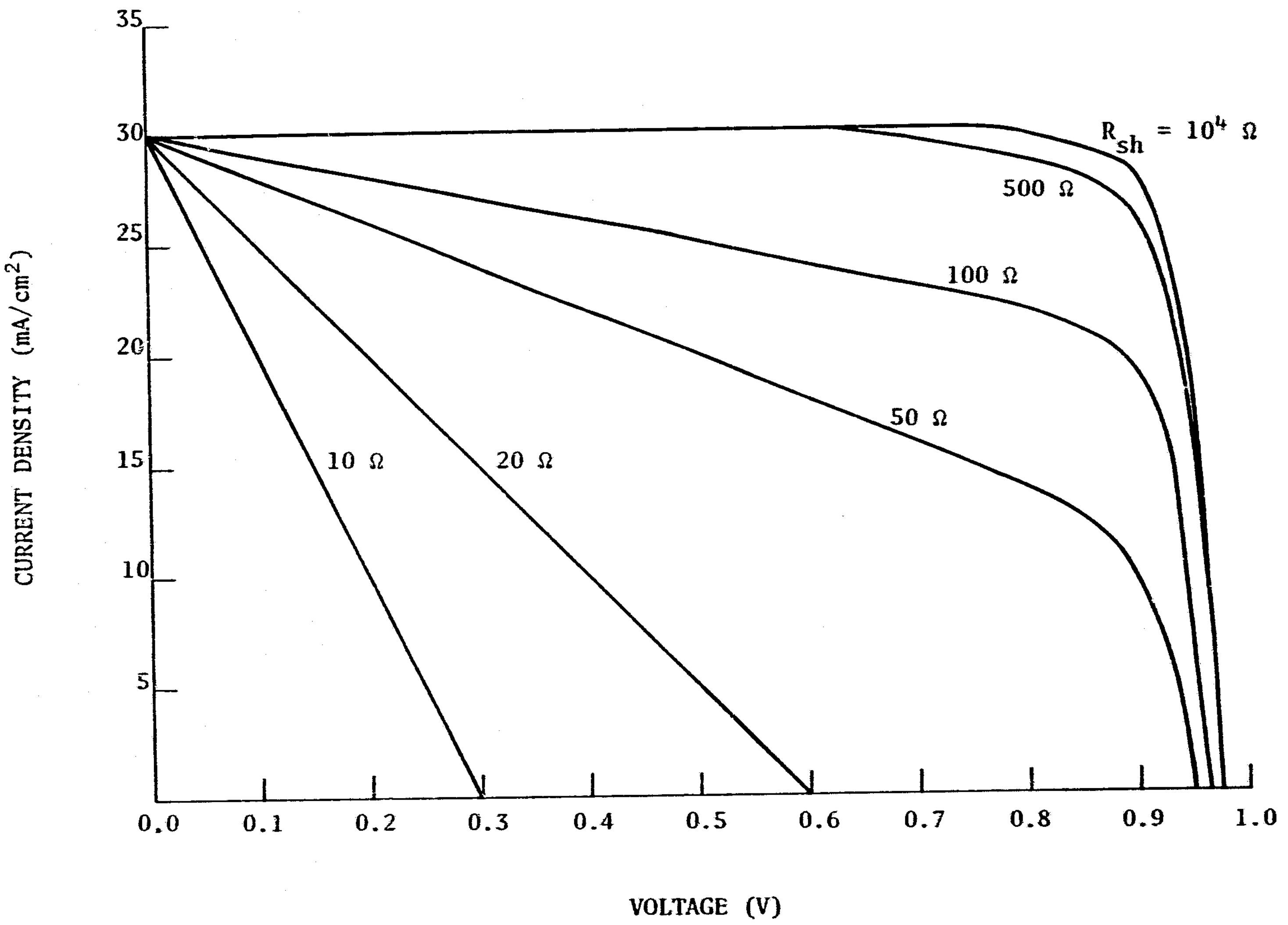

Figure 7. Pn junction current density vs. voltage for variable shunt resistance with series resistance of zero ($R_s = 0$).

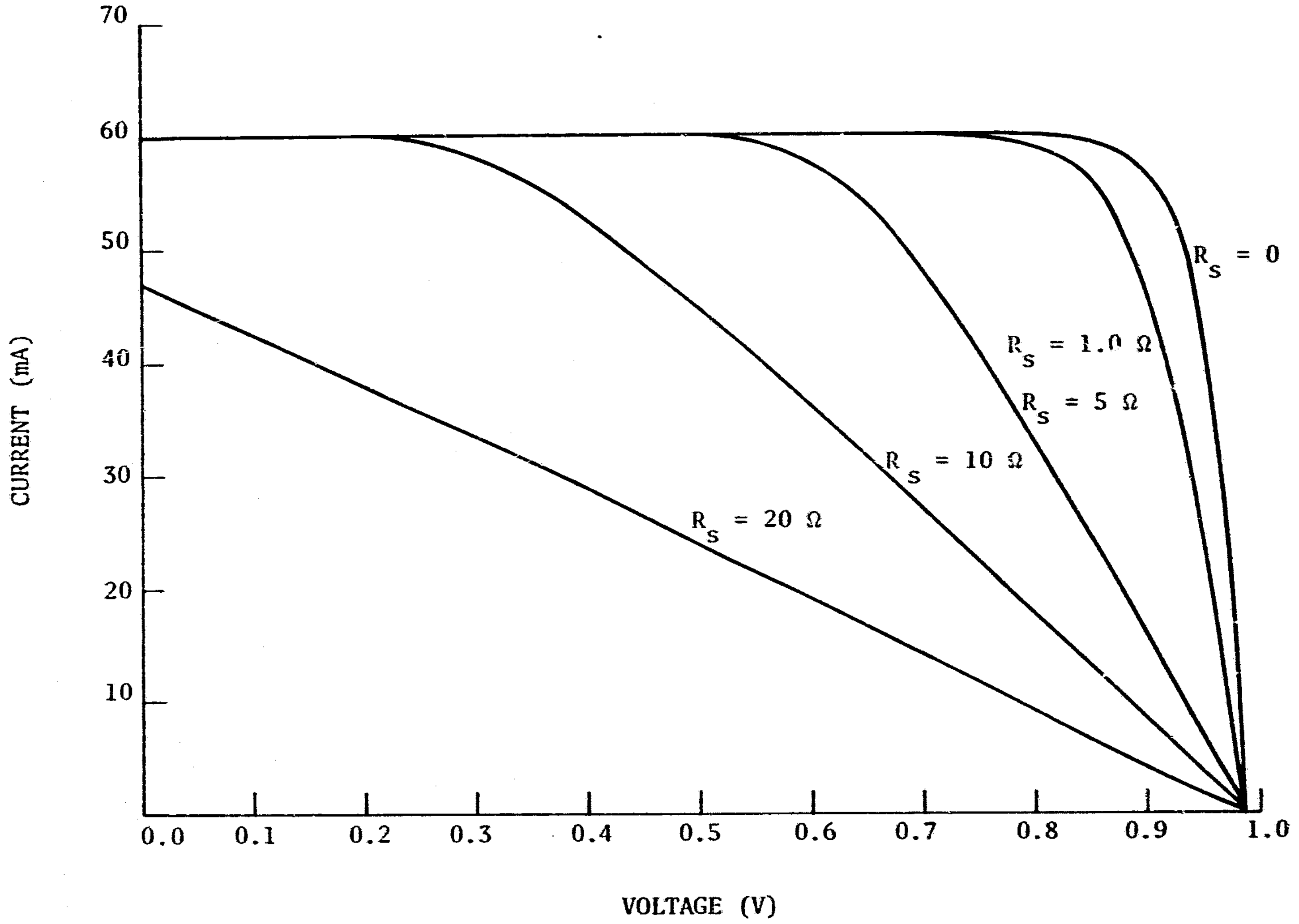

Figure 8. Pn junction current voltage curves for GaAs solar cells with variable series resistance and $R_{sh} = 10^7\ \Omega$.

of the series resistance. Figure 9 illustrates the effect of temperature changes on the Pn junction current-voltage curves. Figures 10 to 13 illustrate the effect of introducing Schottky type defects into the operation of the GaAs solar cell. These curves are for an upper and lower barrier limit of $\phi_{bn} = 0.89$ and $\phi_{bn} = 0.75$ eV. Note the decrease in the open-circuit voltage as the number of defects increases. In this study it was assumed that one defect was 10^{-8} cm^2 in surface area, and hence 10^8 is the maximum number of defects allowed. Note also the shift of the dark current curves as the solar cell changes from a Pn junction mode of operation to a Schottky barrier mode of operation.

Equation (17) for the current-voltage relation is a nonlinear equation of the form

$$I = I_L - f(V + IR_s) \tag{20}$$

where f(x) is given by equation (19). The short-circuit current I_{sc} occurs when V = 0, and hence satisfies

$$I_{sc} = I_L - f(I_{sc} R_s) \tag{21}$$

The open-circuit voltage V_{oc} occurs when I = 0, and hence satisfies

$$I_L = f(V_{oc}) \tag{22}$$

The illumination method for determining the dark current consists of changing the illumination I_L, which in turn causes changes in the I_{sc} and V_{oc} values. A plot of the I_{sc} vs. V_{oc} values obtained in this manner is called the dark current curve of the solar cell. Substituting equation (22) into equation (21), we can see that the dark current curve values obtained by this method must satisfy the relation

$$I_{sc} = f(V_{oc}) - f(I_{sc} R_s) \tag{23}$$

The dark current-voltage curves are obtained by setting $I_L = 0$ in equation (20) and changing the sign. Alternatively, one can write equation (18) in the form

$$I = f(V + IR_s) \tag{24}$$

which represents the "true" dark current-voltage relation.

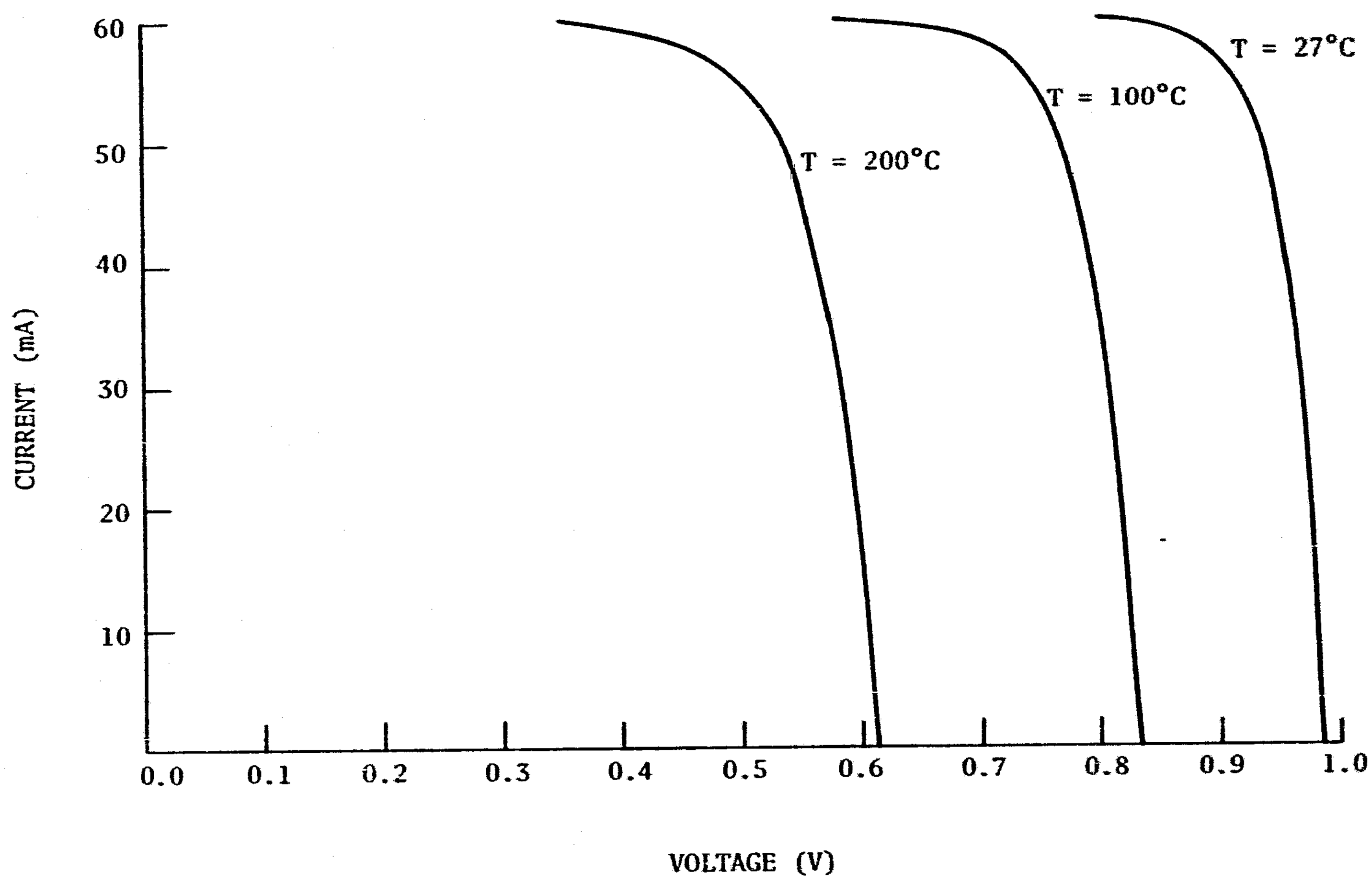

Figure 9. Effect of temperature on Pn junction current voltage curves..

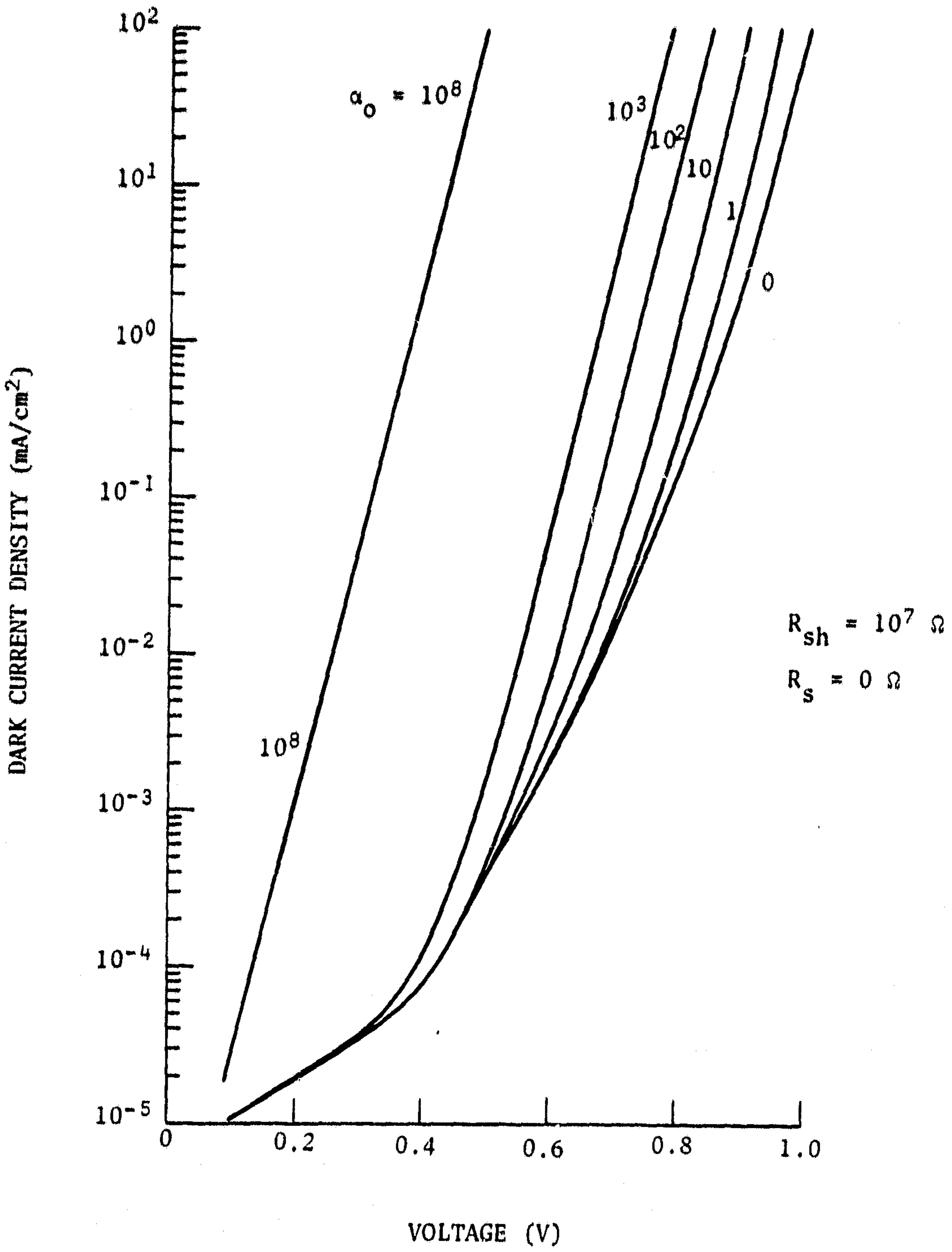

Figure 10. Dark current vs. voltage for various Shottky defects; $\phi_{bn} = 0.89$, $\alpha = \alpha_o(10^{-8})$.

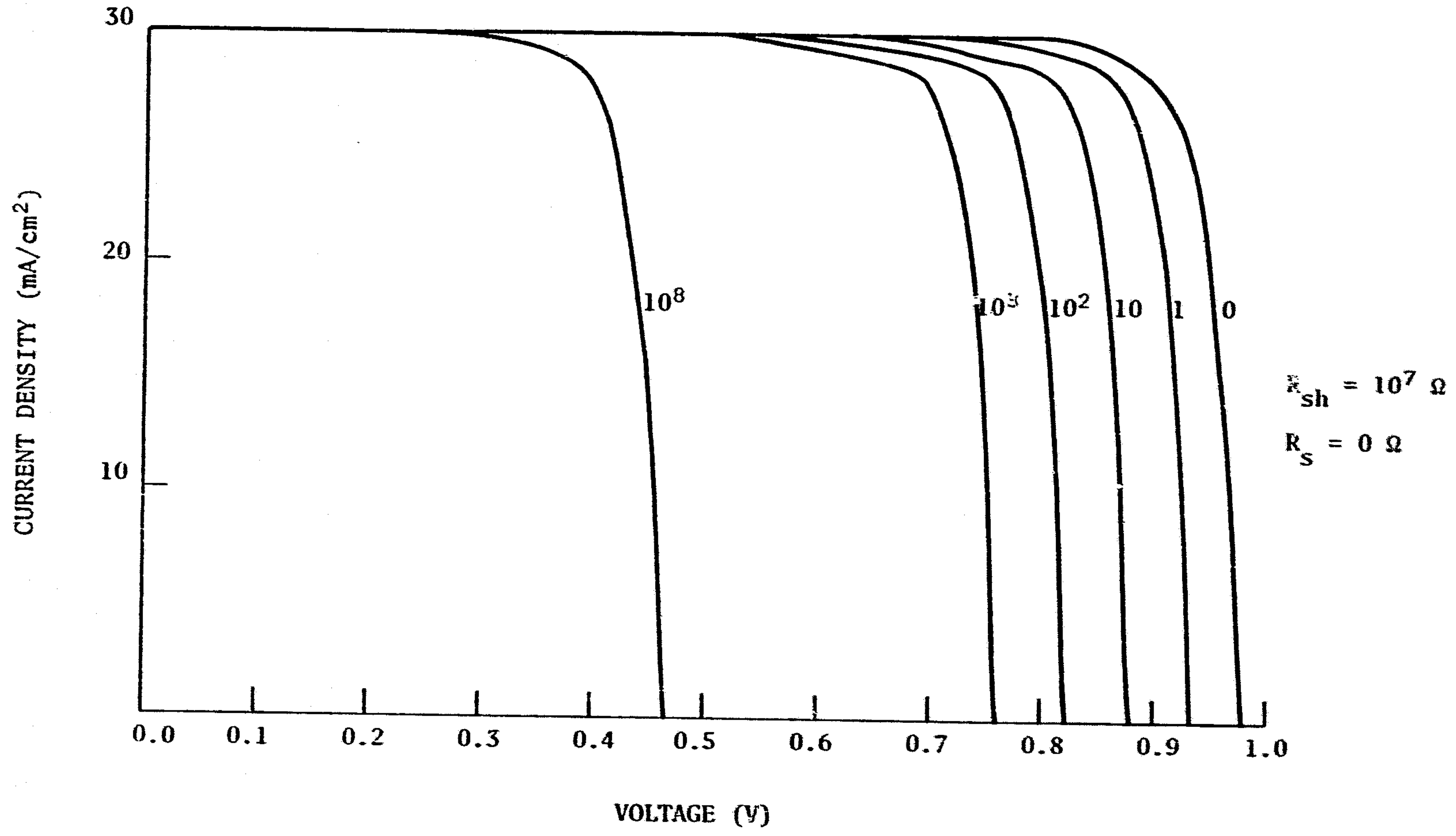

Figure 11. Illuminated current voltage curves for various values of α_o; $\phi_{bn} = 0.89$.

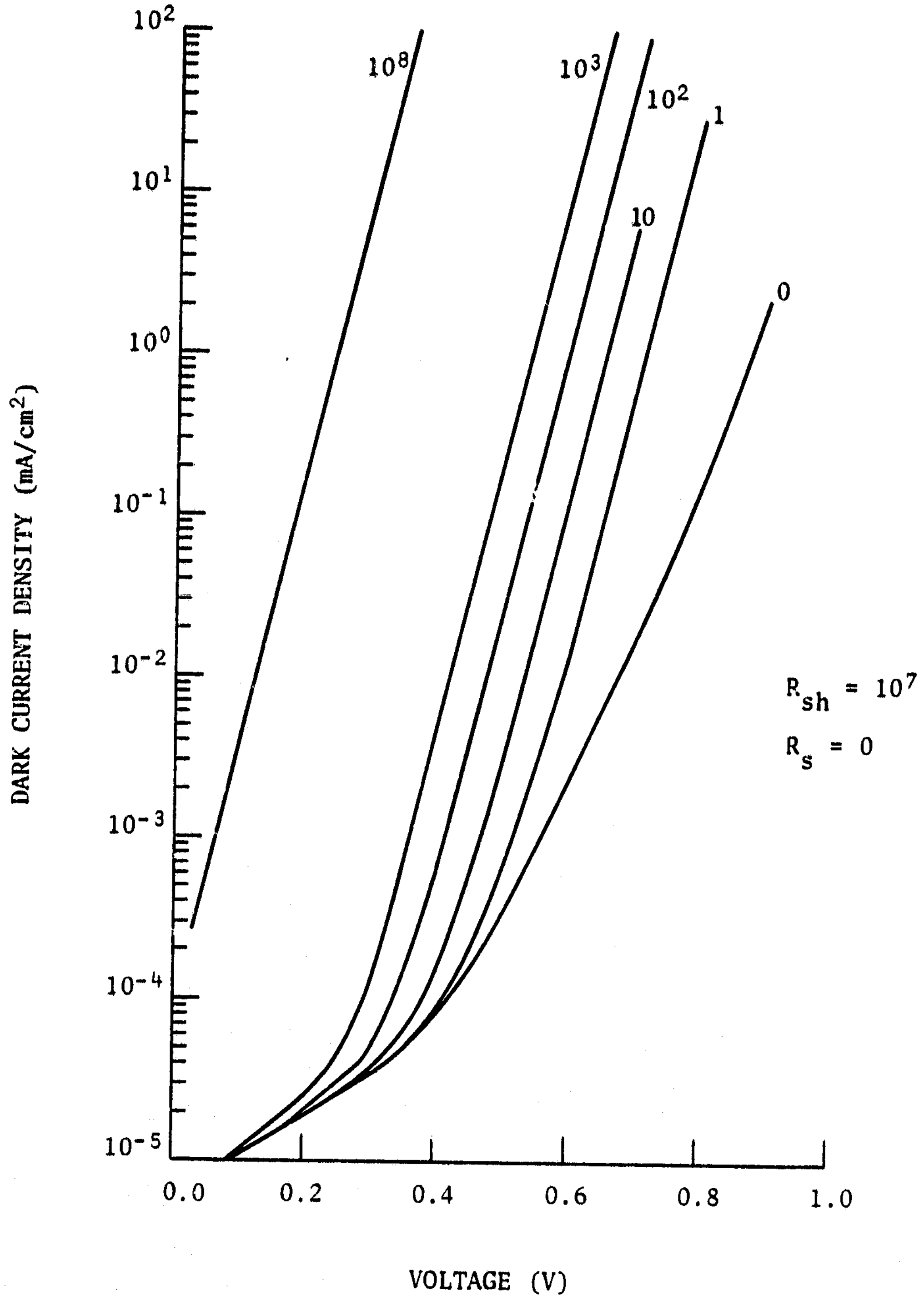

Figure 12. Dark current vs. voltage for various Schottky defects; $\phi_{bn} = 0.75$, $\alpha = \alpha_o(10^{-8})$.

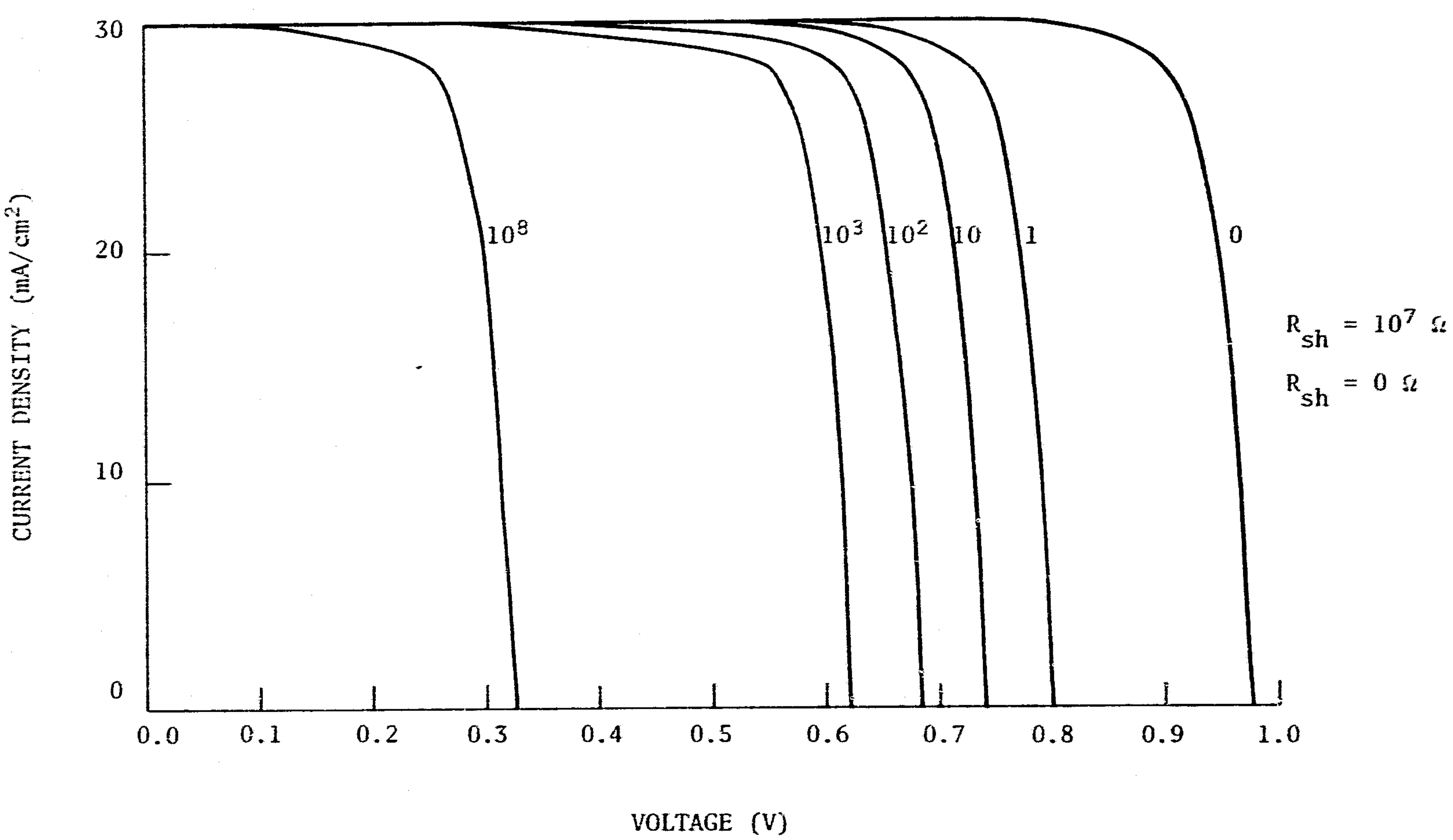

Figure 13. Illuminated current voltage curves for various values of α_o; $\phi_{bn} = 0.75$, $\alpha = \alpha_o(10^{-8})$.

In order to see how equations (24) and (23) are related, we can expand equation (24) in a Taylor's series about $IR_s = 0$ to obtain

$$I = f(V) + f'(V)IR_s + f''(V)\frac{(IR_s)^2}{2!} + \ldots \tag{25}$$

For IR_s positive and much less than one, we can write

$$IR_s << 1 \text{ and } f(IR_s) \approx 0$$

Hence, equations (23) and (24) simplify to the same form of

$$I = f(V) \tag{26}$$

For large values of the current (high illumination), the product of $I_{sc}R_s$ is no longer small and the current voltage relation obtained from equation (23) is no longer representative of the dark current. However, the relation determined by equation (23) can be used to estimate the series resistance R_s. For large values of the illumination, the open-circuit voltage (V_{oc}) and the short circuit current (I_{sc}) values will increase; for large values of the product $I_{sc}R_s$ the exponential term in equation (19) will dominate, and we may write equation (23) in the form

$$I_{sc} = I_o\, e^{\frac{qV_{oc}}{KT}} - I_o\, e^{\frac{qI_{sc}R_s}{KT}}$$

which can be expressed as

$$V_{oc} - I_{sc}R_s = \frac{KT}{q} \ln\left[1 + \frac{I_{sc}}{I_o}\, e^{-\frac{qI_{sc}R_s}{KT}}\right] \tag{27}$$

Now for large values of the product $I_{sc}R_s$ the right-hand side of equation (27) will be zero and we have

$$R_s = \frac{V_{oc}}{I_{sc}} \tag{28}$$

where V_{oc}, I_{sc} are large.

The effect of series resistance on the dark current voltage curves is illustrated in the figure 14. This resistance effect is characterized by a sharp bending of the curve to the right (illuminated dark-current method used to obtain data). Note that for large voltages the series resistance is the voltage divided by the current. Hence, the dark current data appears to be an impractical method for estimating small series resistance effects. However, large series resistance

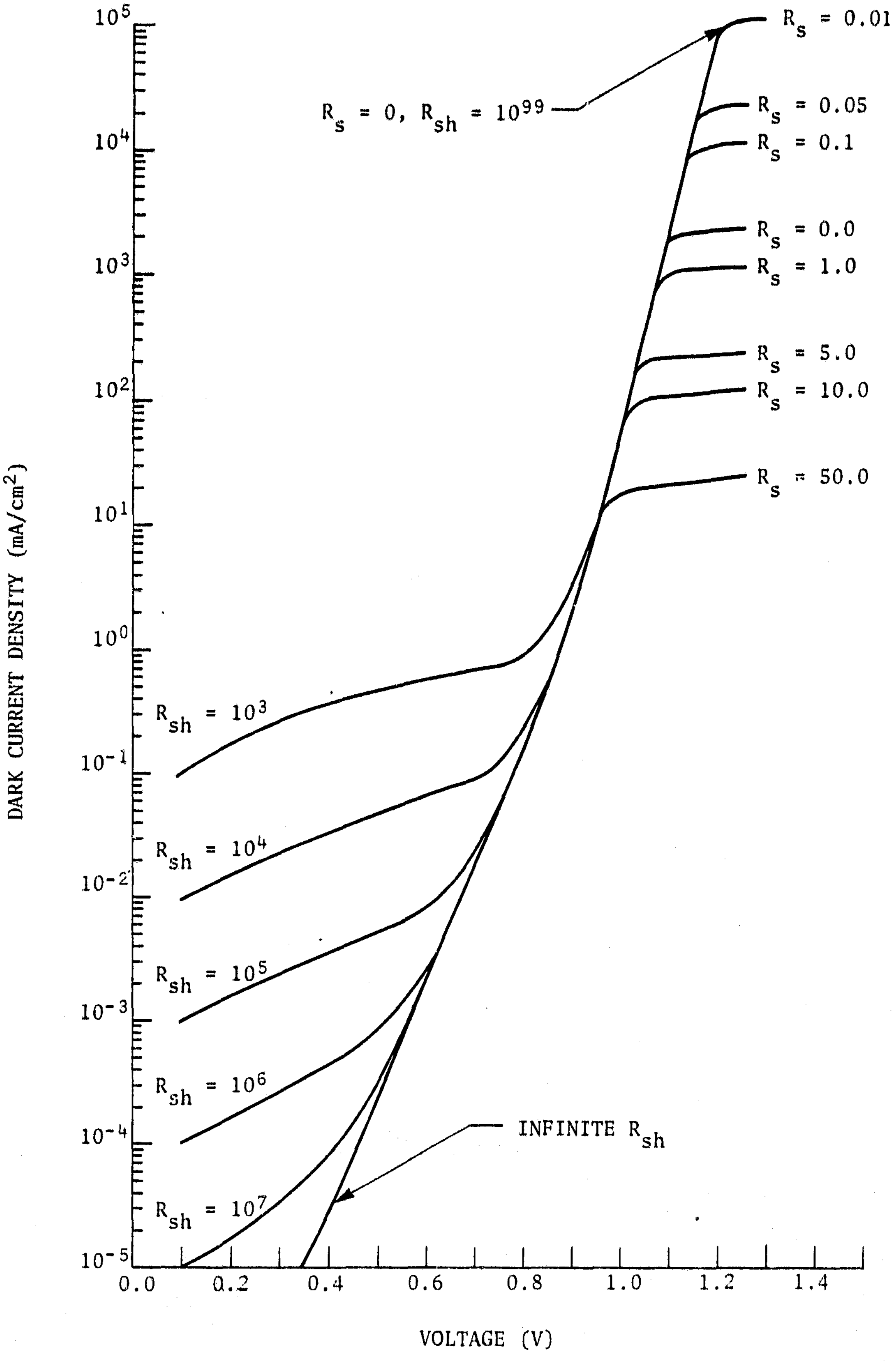

Figure 14. P_n function model dark current curves for various shunt and series resistances.

effects, $R_s \geq 50\Omega$, can be estimated from these bending limits.

For small values of the voltage and for small values of the product IR_S, the $qv/2KT$ exponential term will dominate in equation (23) and we can write the approximate relation

$$I = \beta_o e^{qv/2KT} + \frac{V}{R_{sh}} \tag{29}$$

where $\beta_o = I_1/\sqrt{V_o}$ is obtained from equation (19). Let (I_1^*, V_1^*), (I_2^*, V_2^*) denote two values of the dark current voltage obtained from the dark current curve for two different low voltages. Then equation (29) implies that

$$R_{sh} = \frac{fV_2 - V_1}{fI_2 - I_1} \tag{30}$$

where $f = \exp\left[\frac{q(V_1 - V_2)}{2KT}\right]$. The approximate relation (30) can be applied to the theoretical data of figure 14 to estimate the shunt resistance effects. The shunt resistance is characterized by a bending of the dark-current voltage curve to the left. Along this left branch the relation (30) can be utilized to approximate the shunt resistance.

Figures 15 and 16 illustrate the effect of a doping density change on the dark current and illuminated current-voltage relationships. Figures 17 and 18 illustrate the effect of Schottky defects on the dark current voltage and illuminated current voltage curves. Both of these parameter changes produce a similar type of current voltage change. The Schottky type defect change produces a larger reduction in the open-circuit voltage. This type of behavior, illustrated in figures 15 through 16, has been observed in solar cells that have been exposed to high temperatures over a long period of time. Additional testing should be performed on these cells to determine if the reduction in the open-circuit voltage is due to this Schottky type defect, reduction in the doping density, or to a combination of these events.

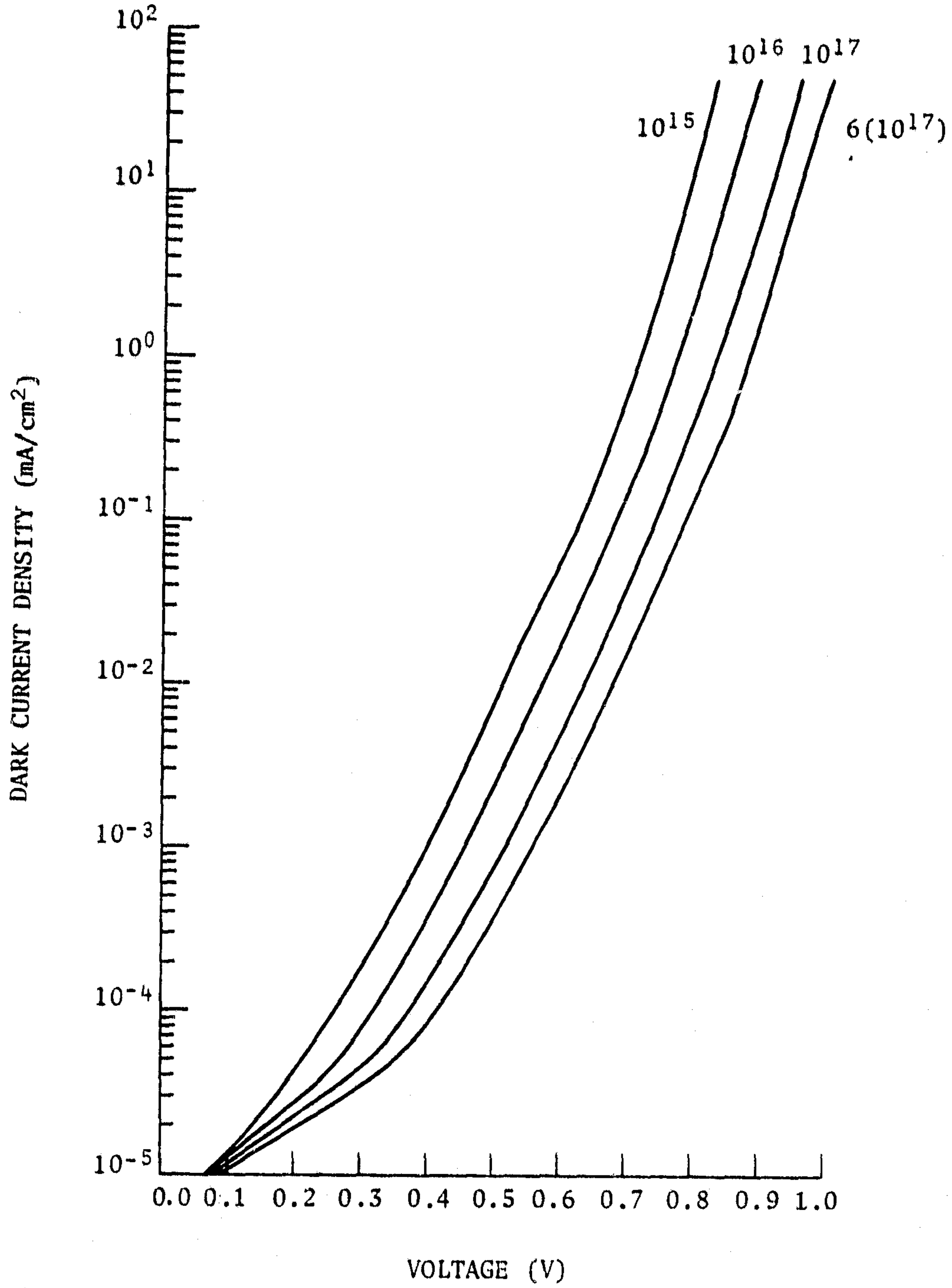

Figure 15. Dark current voltage curves for various doping densities N_d.

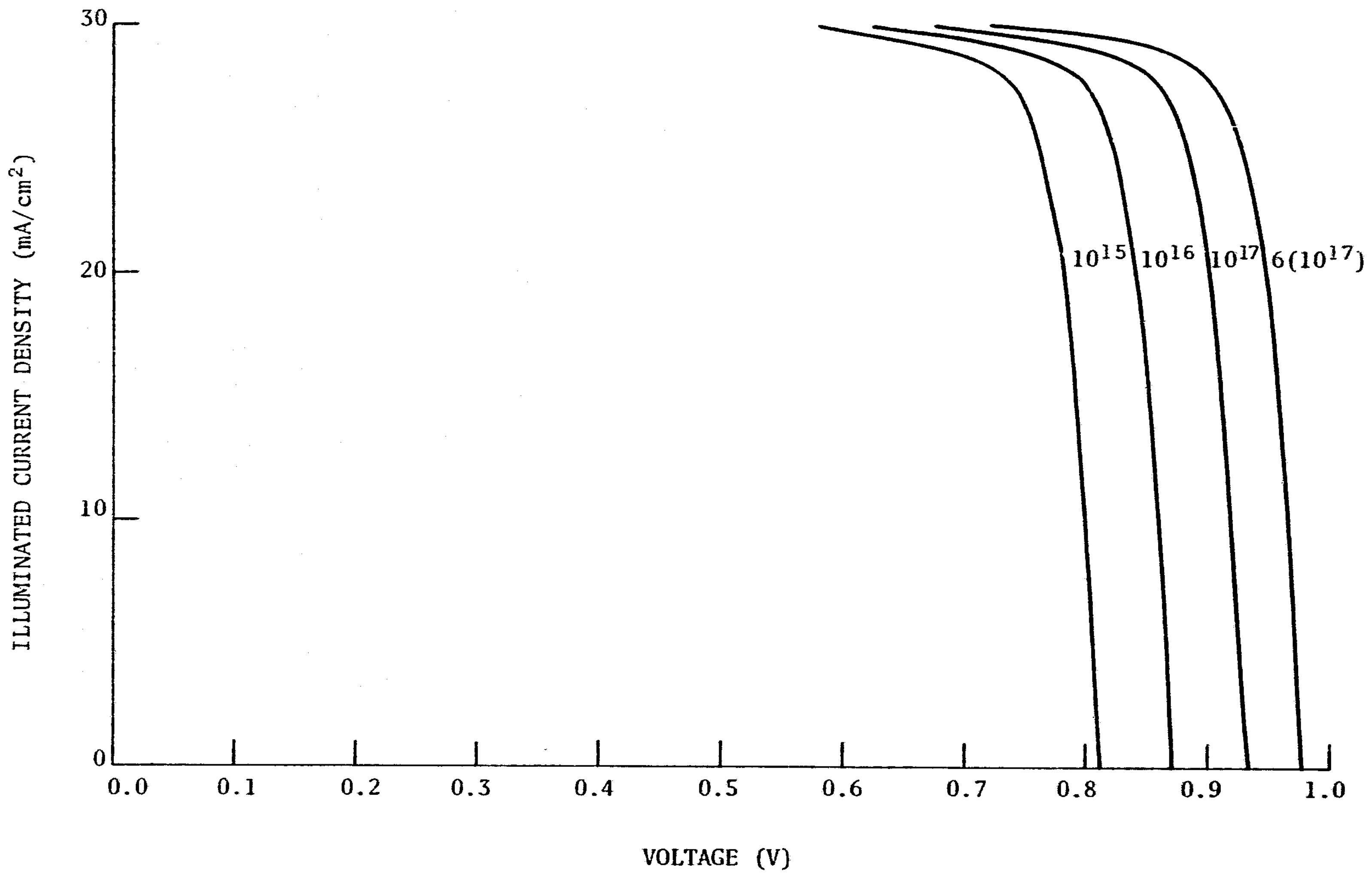

Figure 16. Illuminated current voltage curves for various doping densities N_d.

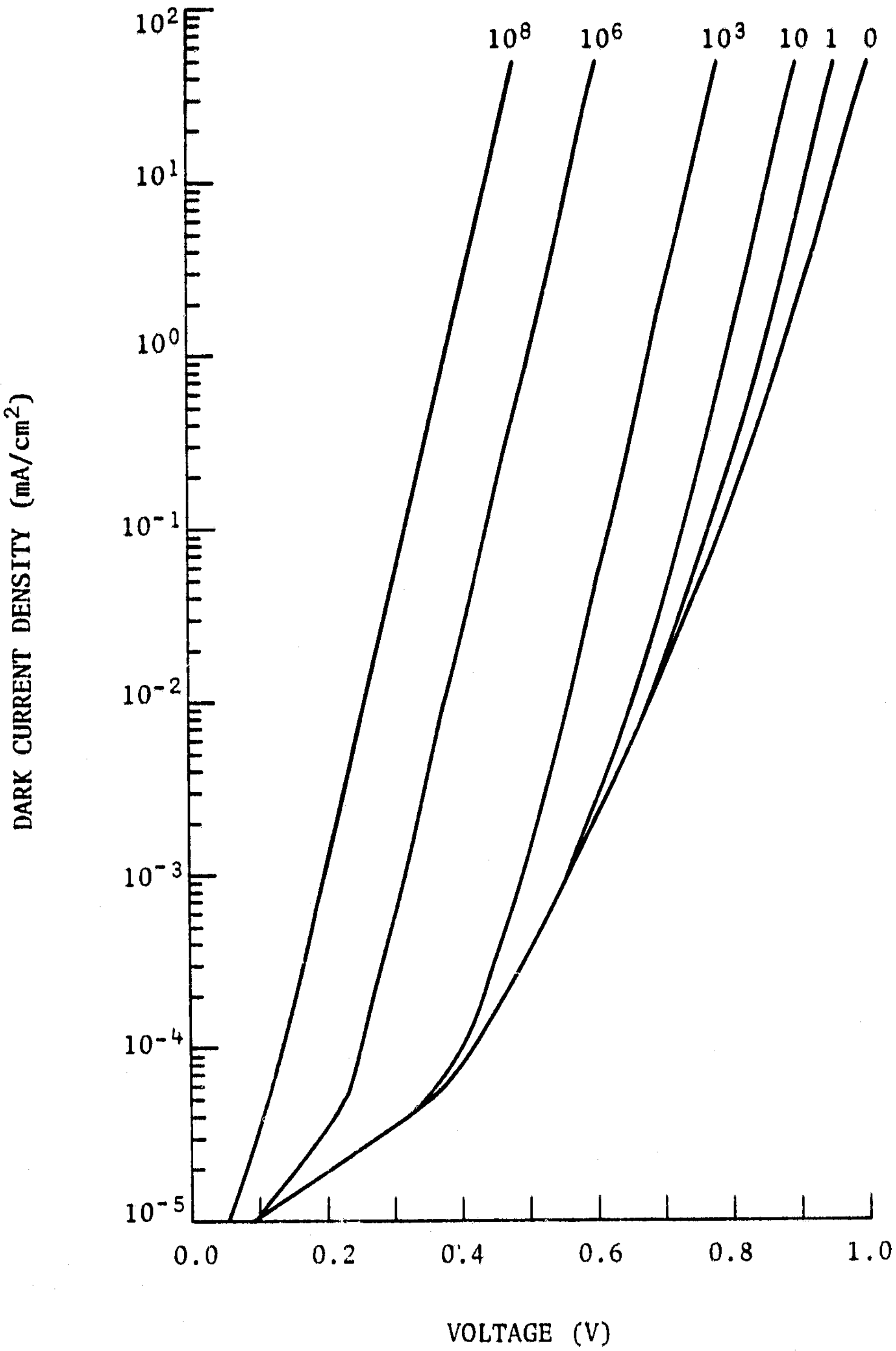

Figure 17. Dark current voltage curves for various values of number of defects α_o.

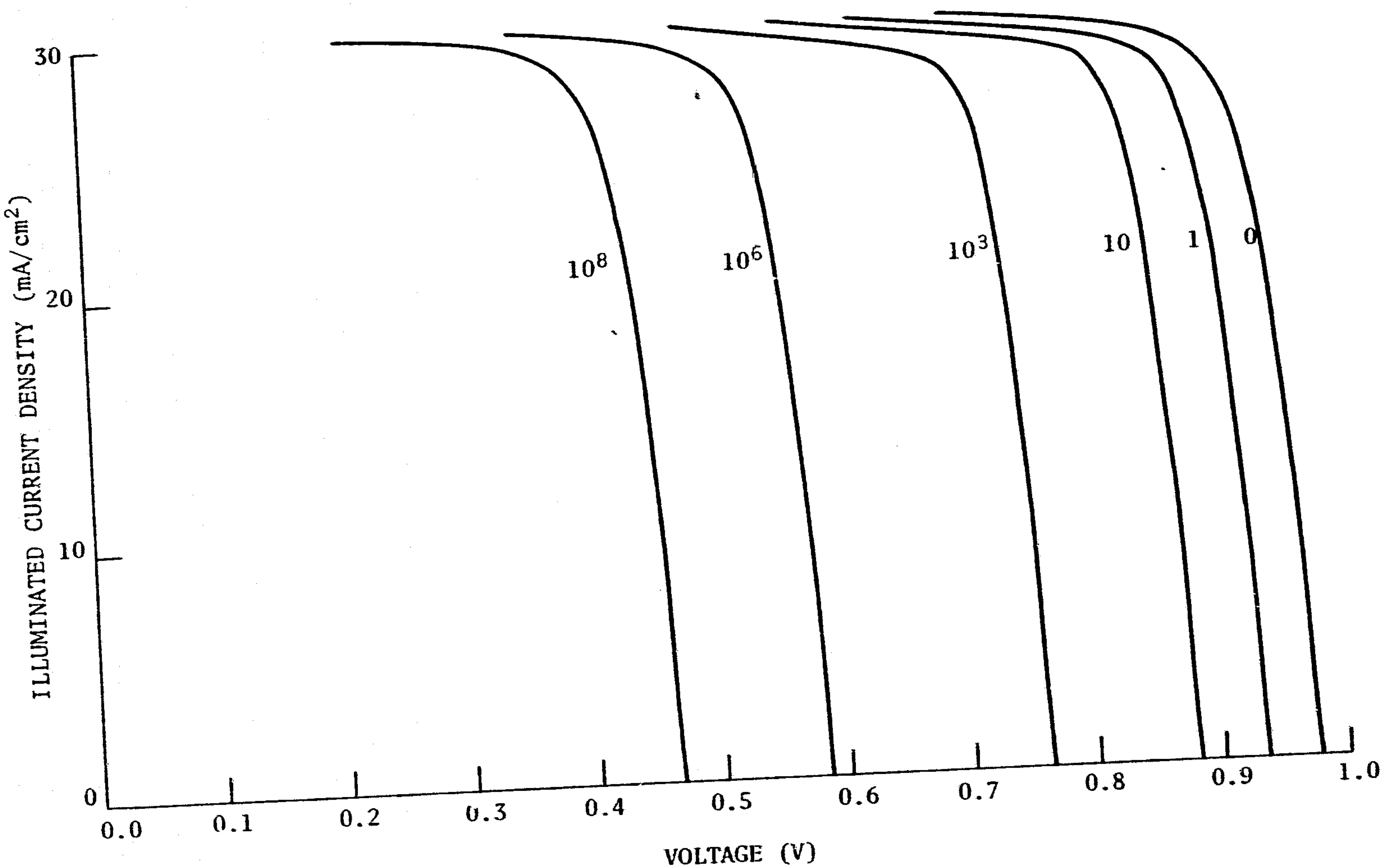

Figure 18. Illuminated current voltage curves for various values of number of defects σ_o.

A MODEL FOR THE CHEMICAL KINETICS OF ANNEALING

The following is a simple model for the annealing mechanism of GaAs solar cells. Here it is assumed that the radiation damage consists mainly of gallium vacancies V_{Ga}, and gallium interstitials Ga_i. (Chemical kinetics of the annealing process have been studied in refs. 20 to 25.) We postulate the following reaction kinetics:

$$
\begin{aligned}
&Ga_{Ga} \underset{k_2}{\overset{k_1}{\rightleftarrows}} V_{Ga} + Ga_i \\
&I_{Ga} \underset{k_4}{\overset{k_3}{\rightleftarrows}} V_{Ga} + I_i \\
&2V_{Ga} \underset{k_6}{\overset{k_5}{\rightleftarrows}} (V_{Ga})_2 \\
&Ga_{Ga} + V_{Ga} \underset{k_8}{\overset{k_7}{\rightleftarrows}} (V_{Ga})_2 + Ga_i \\
&I_{Ga} + V_{Ga} \underset{k_{10}}{\overset{k_9}{\rightleftarrows}} (V_{Ga})_2 + I_i \\
&I_i + V_{Ga} \underset{k_{12}}{\overset{k_{11}}{\rightleftarrows}} V_{Ga}I_i
\end{aligned}
\tag{31}
$$

We let

$Y_1 = [Ga_{Ga}]$ = concentration of Ga atoms on Ga sites (cm^{-3}),

$Y_2 = [V_{Ga}]$ = concentration of Ga vacancies (cm^{-3}),

$Y_3 = [Ga_i]$ = concentration of Ga interstitials (cm^{-3}),

$Y_4 = [I_{Ga}]$ = concentration of impurities on Ga sites (cm^{-3}),

$Y_5 = [I_i]$ = concentration of impurity interstitials (cm^{-3}),

$Y_6 = [(V_{Ga})_2]$ = concentration of divacancies (cm^{-3}),

$Y_7 = [V_{Ga}I_I]$ = concentration of vacancies bound to impurities (cm^{-3}),

and the chemical kinetics associated with the above reaction equations can be expressed:

$$\frac{dy_1}{dt} = -k_1y_1 + k_2y_2y_3 - k_7y_1y_2 + k_8y_6y_3$$

$$\frac{dy_2}{dt} = k_1y_1 - k_2y_2y_3 + k_3y_4 - k_4y_2y_5 - 2k_5y_2{}^2 + 2k_6y_6 - k_7y_1y_2$$
$$+ k_8y_6y_3 - k_9y_2y_4 + k_{10}\, y_6y_5 + k_{12}y_7 - k_{11}y_2y_5$$

$$\frac{dy_3}{dt} = k_1y_1 - k_2y_2y_3 + k_7y_1y_2 - k_8y_6y_3$$

$$\frac{dy_4}{dt} = -k_3y_4 + k_4y_2y_5 - k_9y_2y_4 + k_{10}y_5y_6 \tag{32}$$

$$\frac{dy_5}{dt} = k_3y_4 - k_4y_2y_5 + k_9y_2y_4 - k_{10}y_5y_6 - k_{11}y_2y_5 + k_{12}y_7$$

$$\frac{dy_6}{dt} = k_5y_2^2 - k_6y_6 \quad k_7y_1y_2 - k_8y_3y_6 + k_9y_2y_4 - k_{10}y_5y_6$$

$$\frac{dy_7}{dt} = k_{11}y_2y_5 - k_{12}y_7$$

Associated with the above equations are the mass balancing relations

$$\frac{d}{dt}(y_1 + y_3) = 0$$

$$\frac{d}{dt}(y_4 + y_5 + y_7) = 0$$

$$\frac{d}{dt}(y_3 + y_5 - y_2 - 2y_6) = 0$$

If we assume the initial conditions $y_{10} = N_\ell$ and $y_{40} = N_A$, then $y_{20} = y_{30} = y_{50} = y_{60} = y_{70} = 0$ and the above mass balancing relations imply

$$\begin{aligned} y_1 + y_3 &= N_\ell \\ y_4 + y_5 + y_7 &= N_A \\ y_3 + y_5 &= y_2 + 2y_6 \end{aligned} \tag{33}$$

In the above equations it is assumed that

$$k_1 = \dot{\phi}\sigma_1 = [2.5(10^7)](10^{-22})$$

$$k_3 = \dot{\phi}\sigma_3$$

$$k_7 = \dot{\phi}\sigma_7/N_\ell$$

$$k_9 = \dot{\phi}\sigma_9/N_\ell$$

are radiation-dependent reaction coefficients. The remaining reaction coefficients are assumed to be temperature dependent and can be expressed in terms of the Arrhenius expressions:

$$k_2 = \frac{1}{N_\ell} \nu_2 \exp(-E_2/KT)$$

$$k_4 = \frac{1}{N_\ell} \nu_4 \exp(-E_4/KT)$$

$$k_6 = \nu_6 \exp(-E_6/KT)$$

$$k_5 = (6.0)(k_6)\exp(+1.15/KT)$$

$$k_8 = \nu_8 \exp(-E_8/KT)$$

$$k_{10} = \nu_{10} \exp(-E_{10}/KT)$$

$$k_{11} = \frac{1}{N_\ell} \nu_{11} \exp(-E_{11}/KT)$$

$$k_{12} = \nu_{12} \exp(-E_{12}/KT)$$

At equilibrium, the mass balance relations (33) must hold. In addition, we may choose any four independent equations from equations (32). We then obtain the following system of equilibrium equations:

$$y_1 + y_3 = N_\ell$$

$$y_4 + y_5 + y_7 = N_A$$

$$y_3 + y_5 - y_2 - 2y_6 = 0$$

$$-k_1 y_1 + k_2 y_2 y_3 - k_7 y_1 y_2 + k_8 y_6 y_3 = 0$$

$$k_5 y_2^2 - k_6 y_6 + k_7 y_1 y_2 - k_8 y_3 y_6 + k_9 y_2 y_4 - k_{10} y_5 y_6 = 0$$

$$-k_3 y_4 + k_4 y_2 y_5 - k_9 y_2 y_4 + k_{10} y_6 y_5 = 0$$

$$k_{11} y_2 y_5 - k_{12} y_7 = 0$$

Solving this system of nonlinear equations for various values of temperature gives the results presented in table 3.

Table 3. Results from equilibrium equations.

```
K1= 2.50000E-15 K2= 3.28139E-29 K3= 2.50000E-15 K4= 3.28139E-29
K5= 3.28139E-29 K6= 3.23348E-32 K7= 3.28139E-29 K8= 5.40091E-24
K9= 3.28139E-29 K10= 1.34650E-16 K11= 1.12613E-37 K12= 3.28139E-29

E2= 7.20000E-01 E4= 7.20000E-01 E5= 7.20000E-01 E6= 1.75000E+00 E7= 7.20000E-01
E8= 1.40000E+00 E9= 7.20000E-01 E10= 8.30000E-01 E12= 7.20000E-01
V2= 1.00000E+12 V4= 1.00000E+12 V5= 1.00000E+12 V6= 1.00000E+13 V7= 1.00000E+12
V8= 1.00000E+12 V9= 1.00000E+12 V10= 1.09098E+05 V12= 1.00000E+12


TEMP= 2.00000E+02 Na= 2.00000E+17 Ni= 2.22000E+22
Y1=[Ga Ga]= 2.160371400E+22          Y2=[ V Ga ]= 5.960163678E+20
Y3=[Ga i] = 5.962960009E+20          Y4=[ I  Ga]= 8.944653000E+13
Y5=[I i ] = 9.773473842E+04          Y6=[(VGa)2]= 1.348165044E+17
Y7=[VGa[i]= 1.999105535E+17


TEMP= 2.00000E+02 Na= 5.00000E+17 Ni= 2.22000E+22
Y1=[Ga Ga]= 2.159864220E+22          Y2=[ V Ga ]= 6.010881687E+20
Y3=[Ga i] = 6.013578029E+20          Y4=[ I  Ga]= 2.217320350E+14
Y5=[I   ] = 2.422761189E+05          Y6=[(VGa)2]= 1.348170226E+17
Y7=[VGa[i]= 4.997782680E+17


TEMP= 2.00000E+02 Na= 2.00000E+18 Ni= 2.22000E+22
Y1=[Ga Ga]= 2.159610629E+22          Y2=[ V Ga ]= 6.036240803E+20
Y3=[Ga i] = 6.038937149E+20          Y4=[ I  Ga]= 3.832069600E+14
Y5=[I i ] = 9.650349242E+05          Y6=[(VGa)2]= 1.348172737E+17
Y7=[VGa[i]= 1.999116793E+18


TEMP= 2.00000E+02 Na= 4.00000E+18 Ni= 2.22000E+22
Y1=[Ga Ga]= 2.159568363E+22          Y2=[ V Ga ]= 6.040467310E+20
Y3=[Ga i] = 6.043163651E+20          Y4=[ I  Ga]= 1.765179560E+15
Y5=[I i ] = 1.928719971E+06          Y6=[(VGa)2]= 1.348173126E+17
Y7=[VGa[i]= 3.998234820E+18

K1= 2.50000E-15 K2= 1.39180E-25 K3= 2.50000E-15 K4= 1.39180E-25
K5= 1.39180E-25 K6= 5.40091E-23 K7= 1.39180E-25 K8= 6.10905E-17
K9= 1.39180E-25 K10= 2.04611E-12 K11= 1.12613E-37 K12= 1.39180E-25

E2= 7.20000E-01 E4= 7.20000E-01 E5= 7.20000E-01 E6= 1.75000E+00 E7= 7.20000E-01
E8= 1.40000E+00 E9= 7.20000E-01 E10= 8.30000E-01 E12= 7.20000E-01
V2= 1.00000E+12 V4= 1.00000E+12 V5= 1.00000E+12 V6= 1.00000E+13 V7= 1.00000E+12
V8= 1.00000E+12 V9= 1.00000E+12 V10= 1.09098E+05 V12= 1.00000E+12


TEMP= 2.50000E+02 Na= 2.00000E+17 Ni= 2.22000E+22
Y1=[Ga Ga]= 2.219999996E+22          Y2=[ V Ga ]= 1.221000000E+13
Y3=[Ga i] = 4.173600000E+13          Y4=[ I  Ga]= 2.000000000E+17
Y5=[I i ] = 1.846040640E+06          Y6=[(VGa)2]= 1.478340394E+13
Y7=[VGa[i]= 1.823760425E+07


TEMP= 2.50000E+02 Na= 5.00000E+17 Ni= 2.22000E+22
Y1=[Ga Ga]= 2.219999996E+22          Y2=[ V Ga ]= 1.221000000E+13
Y3=[Ga i] = 4.173600000E+13          Y4=[ I  Ga]= 5.000000000E+17
Y5=[I i ] = 1.863332336E+06          Y6=[(VGa)2]= 1.477993345E+13
Y7=[VGa[i]= 1.840843424E+07


TEMP= 2.50000E+02 Na= 2.00000E+18 Ni= 2.22000E+22
Y1=[Ga Ga]= 2.219999996E+22          Y2=[ V Ga ]= 1.221000000E+13
Y3=[Ga i] = 4.173600000E+13          Y4=[ I  Ga]= 2.000000000E+18
Y5=[I i ] = 1.950917513E+06          Y6=[(VGa)2]= 1.475497809E+13
Y7=[VGa[i]= 1.927371519E+07
```

(continued)

Table 3. (continued).

```
TEMP= 2.50000E+02 Na= 4.00000E+18 NI= 2.22000E+22
Y1=[Ga Ga]= 2.219999996E+22            Y2=[ V Ga ]= 1.221000000E+13
Y3=[Ga I] = 4.173600000E+13            Y4=[ I  Ga]= 4.000000000E+18
Y5=[I I ] = 2.059528664E+06            Y6=[(VGa)2]= 1.478339940E+13
Y7=[VGaI I]= 2.034671822E+07

K1= 2.50000E-15 K2= 3.64688E-23 K3= 2.50000E-15 K4= 3.64688E-23
K5= 3.64688E-23 K6= 4.07745E-17 K7= 3.64688E-23 K8= 3.07930E-12
K9= 3.64688E-23 K10= 1.25529E-09 K11= 1.12613E-37 K12= 3.64688E-23

E2= 7.20000E-01 E4= 7.20000E-01 E5= 7.20000E-01 E6= 1.75000E+00 E7= 7.20000E-01
E8= 1.40000E+00 E9= 7.20000E-01 E10= 8.30000E-01 E12= 7.20000E-01
V2= 1.00000E+12 V4= 1.00000E+12 V5= 1.00000E+12 V6= 1.00000E+13 V7= 1.00000E+12
V8= 1.00000E+12 V9= 1.00000E+12 V10= 1.09098E+05 V12= 1.00000E+12


TEMP= 3.00000E+02 Na= 2.00000E+17 NI= 2.22000E+22
Y1=[Ga Ga]= 2.219999999E+22            Y2=[ V Ga ]= 1.221000000E+13
Y3=[Ga I] = 1.265400000E+13            Y4=[ I  Ga]= 2.000000000E+17
Y5=[I I ] = 4.570003520E+05            Y6=[(VGa)2]= 2.519872858E+11
Y7=[VGaI I]= 1.723050164E+04


TEMP= 3.00000E+02 Na= 5.00000E+17 NI= 2.22000E+22
Y1=[Ga Ga]= 2.219999999E+22            Y2=[ V Ga ]= 1.221000000E+13
Y3=[Ga I] = 1.265400000E+13            Y4=[ I  Ga]= 5.000000000E+17
Y5=[I I ] = 8.814711319E+05            Y6=[(VGa)2]= 2.512709553E+11
Y7=[VGaI I]= 3.323452535E+04


TEMP= 3.00000E+02 Na= 2.00000E+18 NI= 2.22000E+22
Y1=[Ga Ga]= 2.219999999E+22            Y2=[ V Ga ]= 1.221000000E+13
Y3=[Ga I] = 1.265400000E+13            Y4=[ I  Ga]= 2.000000000E+18
Y5=[I I ] = 2.909518961E+06            Y6=[(VGa)2]= 2.521027834E+11
Y7=[VGaI I]= 1.127152553E+05


TEMP= 3.00000E+02 Na= 4.00000E+18 NI= 2.22000E+22
Y1=[Ga Ga]= 2.219999999E+22            Y2=[ V Ga ]= 1.221000000E+13
Y3=[Ga I] = 1.265400000E+13            Y4=[ I  Ga]= 4.000000000E+18
Y5=[I I ] = 5.804561570E+06            Y6=[(VGa)2]= 2.520636770E+11
Y7=[VGaI I]= 2.188521457E+05

K1= 2.50000E-15 K2= 1.94675E-21 K3= 2.50000E-15 K4= 1.94675E-21
K5= 1.94675E-21 K6= 6.44028E-13 K7= 1.94675E-21 K8= 7.03273E-09
K9= 1.94675E-21 K10= 1.23038E-07 K11= 1.12613E-37 K12= 1.94675E-21

E2= 7.20000E-01 E4= 7.20000E-01 E5= 7.20000E-01 E6= 1.75000E+00 E7= 7.20000E-01
E8= 1.40000E+00 E9= 7.20000E-01 E10= 8.30000E-01 E12= 7.20000E-01
V2= 1.00000E+12 V4= 1.00000E+12 V5= 1.00000E+12 V6= 1.00000E+13 V7= 1.00000E+12
V8= 1.00000E+12 V9= 1.00000E+12 V10= 1.09098E+05 V12= 1.00000E+12


TEMP= 3.50000E+02 Na= 2.00000E+17 NI= 2.22000E+22
Y1=[Ga Ga]= 2.220000000E+22            Y2=[ V Ga ]= 1.221000000E+06
Y3=[Ga I] = 0.000000000E+00            Y4=[ I  Ga]= 2.000000000E+17
Y5=[I I ] = 5.076370518E+06            Y6=[(VGa)2]= 8.885952728E+07
Y7=[VGaI I]= 3.585463554E-04


TEMP= 3.50000E+02 Na= 5.00000E+17 NI= 2.22000E+22
Y1=[Ga Ga]= 2.220000000E+22            Y2=[ V Ga ]= 1.221000000E+06
Y3=[Ga I] = 0.000000000E+00            Y4=[ I  Ga]= 5.000000000E+17
Y5=[I I ] = 5.078727457E+06            Y6=[(VGa)2]= 8.881943047E+07
```

Table 3. (continued).

```
Y7=[VGa[i]= 3.587128271E-04

TEMP= 3.50000E+02 Na= 2.00000E+18 Ni= 2.22000E+22
Y1=[Ga Ga]= 2.220000000E+22          Y2=[ V Ga ]= 1.221000000E+06
Y3=[Ga i] = 0.000000000E+00          Y4=[ I  Ga]= 2.000000000E+18
Y5=[I i ] = 5.076794581E+06          Y6=[(VGa)2]= 8.885895454E+07
Y7=[VGa[i]= 3.505763072E-04

TEMP= 3.50000E+02 Na= 4.00000E+18 Ni= 2.22000E+22
Y1=[Ga Ga]= 2.220000000E+22          Y2=[ V Ga ]= 1.221000000E+06
Y3=[Ga i] = 0.000000000E+00          Y4=[ I  Ga]= 4.000000000E+18
Y5=[I i ] = 5.072571999E+06          Y6=[(VGa)2]= 8.894054086E+07
Y7=[VGa[i]= 3.502780643E-04

K1= 2.50000E-15 K2= 3.84461E-20 K3= 2.50000E-15 K4= 3.84461E-20
K5= 3.84461E-20 K6= 9.07385E-10 K7= 3.84461E-20 K8= 2.32399E-06
K9= 3.84461E-20 K10= 3.83276E-06 K11= 1.12613E-37 K12= 3.84461E-20

E2= 7.20000E-01 E4= 7.20000E-01 E5= 7.20000E-01 E6= 1.75000E+00 E7= 7.20000E-01
E8= 1.40000E+00 E9= 7.20000E-01 E10= 8.30000E-01 E12= 7.20000E-01
V2= 1.00000E+12 V4= 1.00000E+12 V5= 1.00000E+12 V6= 1.00000E+13 V7= 1.00000E+12
V8= 1.00000E+12 V9= 1.00000E+12 V10= 1.09098E+05 V12= 1.00000E+12

TEMP= 4.00000E+02 Na= 2.00000E+17 Ni= 2.22000E+22
Y1=[Ga Ga]= 2.219999999E+22          Y2=[ V Ga ]= 1.221000000E+13
Y3=[Ga i] = 1.221000000E+13          Y4=[ I  Ga]= 1.999999999E+17
Y5=[I i ] = 6.685946510E+07          Y6=[(VGa)2]= 3.665900648E+08
Y7=[VGa[i]= 2.391183229E+03

TEMP= 4.00000E+02 Na= 5.00000E+17 Ni= 2.22000E+22
Y1=[Ga Ga]= 2.219999999E+22          Y2=[ V Ga ]= 1.221000000E+13
Y3=[Ga i] = 1.221000000E+13          Y4=[ I  Ga]= 4.999999998E+17
Y5=[I i ] = 1.670884486E+08          Y6=[(VGa)2]= 3.665921790E+08
Y7=[VGa[i]= 5.975804554E+03

TEMP= 4.00000E+02 Na= 2.00000E+18 Ni= 2.22000E+22
Y1=[Ga Ga]= 2.219999999E+22          Y2=[ V Ga ]= 1.221000000E+13
Y3=[Ga i] = 1.221000000E+13          Y4=[ I  Ga]= 1.999999999E+18
Y5=[I i ] = 6.682090866E+08          Y6=[(VGa)2]= 3.666065569E+08
Y7=[VGa[i]= 2.389804284E+04

TEMP= 4.00000E+02 Na= 4.00000E+18 Ni= 2.22000E+22
Y1=[Ga Ga]= 2.219999999E+22          Y2=[ V Ga ]= 1.221000000E+13
Y3=[Ga i] = 1.221000000E+13          Y4=[ I  Ga]= 3.999999999E+18
Y5=[I i ] = 1.336306997E+09          Y6=[(VGa)2]= 3.666262211E+08
Y7=[VGa[i]= 4.779210955E+04

K1= 2.50000E-15 K2= 3.91288E-19 K3= 2.50000E-15 K4= 3.91288E-19
K5= 3.91288E-19 K6= 2.55227E-07 K7= 3.91288E-19 K8= 2.11612E-04
K9= 3.91288E-19 K10= 5.56033E-05 K11= 1.12613E-37 K12= 3.91288E-19

E2= 7.20000E-01 E4= 7.20000E-01 E5= 7.20000E-01 E6= 1.75000E+00 E7= 7.20000E-01
E8= 1.40000E+00 E9= 7.20000E-01 E10= 8.30000E-01 E12= 7.20000E-01
V2= 1.00000E+12 V4= 1.00000E+12 V5= 1.00000E+12 V6= 1.00000E+13 V7= 1.00000E+12
V8= 1.00000E+12 V9= 1.00000E+12 V10= 1.09098E+05 V12= 1.00000E+12

TEMP= 4.50000E+02 Na= 2.00000E+17 Ni= 2.22000E+22
Y1=[Ga Ga]= 2.220000000E+22          Y2=[ V Ga ]= 1.221000000E+12
Y3=[Ga i] = 1.332000000E+12          Y4=[ I  Ga]= 2.000000000E+17
```

Table 3. (concluded).


```
Y5=[I + ] = 4.5082146 31E+07          Y6=[(VGa)2]= 3.797226704E+07
Y7=[VGa(+]= 1.591230712E+01


TEMP= 4.50000E+02 Na= 5.00000E+17 Ni= 2.22000E+22
Y1=[Ga Ga]= 2.220000000E+22           Y2=[ V Ga ]= 1.221000000E+12
Y3=[Ga +] = 1.332000000E+12           Y4=[ I  Ga]= 4.999999999E+17
Y5=[I + ] = 1.131605924E+08           Y6=[(VGa)2]= 3.797406036E+07
Y7=[VGa(+]= 3.976503429E+01


TEMP= 4.50000E+02 Na= 2.00000E+18 Ni= 2.22000E+22
Y1=[Ga Ga]= 2.220000000E+22           Y2=[ V Ga ]= 1.221000000E+12
Y3=[Ga +] = 1.332000000E+12           Y4=[ I  Ga]= 2.000000000E+18
Y5=[I + ] = 4.524498966E+08           Y6=[(VGa)2]= 3.798359636E+07
Y7=[VGa(+]= 1.589925014E+02


TEMP= 4.50000E+02 Na= 4.00000E+18 Ni= 2.22000E+22
Y1=[Ga Ga]= 2.219999999E+22           Y2=[ V Ga ]= 1.221000000E+13
Y3=[Ga +] = 1.221000000E+13           Y4=[ I  Ga]= 3.999999992E+18
Y5=[I + ] = 8.371183475E+09           Y6=[(VGa)2]= 4.105686131E+07
Y7=[VGa(+]= 2.941663620E+04

K1= 2.50000E-15 K2= 2.50387E-18 K3= 2.50000E-15 K4= 2.50387E-18
K5= 2.50387E-18 K6= 2.32399E-05 K7= 2.50387E-18 K8= 7.81604E-03
K9= 2.50387E-18 K10= 4.72468E-04 K11= 1.12613E-37 K12= 2.50387E-18

E2= 7.20000E-01 E4= 7.20000E-01 E5= 7.20000E-01 E6= 1.75000E+00 E7= 7.20000E-01
E8= 1.40000E+00 E9= 7.20000E-01 E10= 8.30000E-01 E12= 7.20000E-01
V2= 1.00000E+12 V4= 1.00000E+12 V5= 1.00000E+12 V6= 1.00000E+13 V7= 1.00000E+12
V8= 1.00000E+12 V9= 1.00000E+12 V10= 1.09098E+05 V12= 1.00000E+12


TEMP= 5.00000E+02 Na= 2.00000E+17 Ni= 2.22000E+22
Y1=[Ga Ga]= 2.219999999E+22           Y2=[ V Ga ]= 1.221000000E+13
Y3=[Ga +] = 1.221000000E+13           Y4=[ I  Ga]= 1.999999982E+17
Y5=[I + ] = 1.832072327E+09           Y6=[(VGa)2]= 7.060073436E+06
Y7=[VGa(+]= 1.006631931E+03


TEMP= 5.00000E+02 Na= 5.00000E+17 Ni= 2.22000E+22
Y1=[Ga Ga]= 2.219999999E+22           Y2=[ V Ga ]= 1.221000000E+13
Y3=[Ga +] = 1.221000000E+13           Y4=[ I  Ga]= 4.999999954E+17
Y5=[I + ] = 4.581651092E+09           Y6=[(VGa)2]= 7.061621729E+06
Y7=[VGa(+]= 2.516014353E+03


TEMP= 5.00000E+02 Na= 2.00000E+18 Ni= 2.22000E+22
Y1=[Ga Ga]= 2.219999999E+22           Y2=[ V Ga ]= 1.221000000E+13
Y3=[Ga +] = 1.221000000E+13           Y4=[ I  Ga]= 1.999999982E+18
Y5=[I + ] = 1.830648167E+10           Y6=[(VGa)2]= 7.069364697E+06
Y7=[VGa(+]= 1.005300703E+04


TEMP= 5.00000E+02 Na= 4.00000E+18 Ni= 2.22000E+22
Y1=[Ga Ga]= 2.219999999E+22           Y2=[ V Ga ]= 1.221000000E+13
Y3=[Ga +] = 1.221000000E+13           Y4=[ I  Ga]= 3.999999963E+18
Y5=[I + ] = 3.655956003E+10           Y6=[(VGa)2]= 7.079687851E+06
Y7=[VGa(+]= 2.007668762E+04
```

A more realistic set of chemical equations is

$$
\begin{aligned}
&Ga_{Ga} \underset{k_2}{\overset{k_1}{\rightleftarrows}} V_{Ga} + Ga_i \\
&As_{As} \underset{k_4}{\overset{k_3}{\rightleftarrows}} V_{As} + As_i \\
&V_{Ga} + I_{Ga} \underset{k_6}{\overset{k_5}{\rightleftarrows}} V_{Ga} I_{Ga} \\
&2V_{Ga} \underset{k_8}{\overset{k_7}{\rightleftarrows}} (V_{Ga})_2 \\
&2V_{As} \underset{k_{10}}{\overset{k_9}{\rightleftarrows}} (V_{As})_2 \\
&Ga_{Ga} + V_{Ga} \underset{k_{12}}{\overset{k_4}{\rightleftarrows}} (V_{Ga})_2 + Ga_i
\end{aligned}
\tag{35}
$$

Let [ ] denote "concentration of" in units of cm^{-3}, then for

$y_1 = [Ga_{Ga}]$ = gallium on Ga sites

$y_2 = [V_{Ga}]$ = vacancies on Ga sites

$y_3 = [Ga_i]$ = gallium interstitials

$y_4 = [As_{As}]$ = arsenic on As sites

$y_5 = [V_{As}]$ = vacancies on As sites

$y_6 = [As_i]$ = arsenic interstitials

$y_7 = [I_{Ga}]$ = impurity on Ga site

$y_8 = [V_{Ga} I_{Ga}]$ = vacancy-impurity complex

$y_9 = [(V_{Ga})_2]$ = gallium divacancy

$y_{10} = [(V_{As})_2]$ = arsenic divacancy

we have the following chemical kinetics:

$$\frac{dy_1}{dt} = -k_1y_1 - k_{11}y_1y_2 + k_2y_2y_3 + k_{12}y_9y_3$$

$$\frac{dy_2}{dt} = k_1y_1 - k_2y_2y_3 - k_5y_2y_7 + k_6y_8 - 2k_7y_2^2 + 2k_8y_9 - k_{11}y_1y_2 + k_{12}y_9y_3$$

$$\frac{dy_3}{dt} = k_1y_1 - k_2y_2y_3 + k_{11}y_1y_2 - k_{12}y_9y_3$$

$$\frac{dy_4}{dt} = -k_3y_4 + k_4y_5y_6$$

$$\frac{dy_5}{dt} = k_3y_4 - k_4y_5y_6 - 2k_9y_5^2 + 2k_{10}y_{10}$$

$$\frac{dy_6}{dt} = k_3y_4 - k_4y_5y_6$$

$$\frac{dy_7}{dt} = -k_5y_2y_7 + k_6y_8$$

$$\frac{dy_8}{dt} = k_5y_2y_7 - k_6y_8$$

$$\frac{dy_9}{dt} = k_7y_2^2 - k_8y_9 + k_{11}y_1y_2 - k_{12}y_9y_3$$

$$\frac{dy_{10}}{dt} = k_9y_5^2 - k_{10}y_{10}$$

The mass balance associated with the above equations implies that

$$y_1 + y_3 = N_\ell$$

$$y_4 + y_6 = N_\ell$$

$$y_4 + y_5 + 2y_{10} = N_\ell$$

$$y_1 + y_2 + 2y_9 + y_8 = N_\ell$$

$$y_7 + y_8 = N_a$$

where we have assumed the initial conditions $y_1(0) = N_\ell$, $y_4(0) = N_\ell$, $y_7(0) = N_a$, and all other $y_i(0) = 0$. This produces the equilibrium equations:

$$y_1 + y_3 = N_\ell$$

$$y_4 + y_6 = N_\ell$$

$$y_1 + y_2 + 2y_9 + y_8 = N_\ell$$

$$y_4 + y_5 + 2y_{10} = N_\ell$$

$$y_7 + y_8 = N_a$$

$$-k_1y_1 - k_{11}y_1y_2 + k_2y_2y_3 + k_{12}y_3y_9 = 0$$

$$-k_7{y_2}^2 + k_8y_9 - k_{11}y_1y_2 + k_{12}y_3y_9 = 0$$

$$-k_3y_4 + k_4y_5y_6 = 0$$

$$-k_9{y_5}^2 + k_{10}y_{10} = 0$$

$$-k_5y_2y_7 + k_6y_8 = 0$$

with the reaction coefficients given by:

$$k_1 = \sigma_1 \dot{\phi} = (10^{-22}) [2.5(10^7)] \text{ sec}^{-1}$$

$$k_2 = \sigma_2\nu_2 \exp(-E_2/KT) \text{ cm}^3\text{sec}^{-1}$$

$$k_3 = \sigma_3\dot{\phi} \text{ sec}^{-1}$$

$$k_4 = \sigma_4\nu_4 \exp(-E_4/KT) \text{ cm}^3\text{sec}^{-1}$$

$$k_5 = \sigma_5\nu_5 \exp(-E_5/KT) \text{ cm}^3\text{sec}^{-1}$$

$$k_6 = \sigma_6\nu_6 \exp(-E_6/DT) \text{ sec}^{-1}$$

$$k_7 = \sigma_7\sigma_7 \exp(-E_7/KT) \text{ cm}^3\text{sec}^{-1}$$

$$k_8 = \sigma_8\nu_8 \exp(-E_8/KT) \text{ sec}^{-1}$$

$$k_9 = \sigma_9\nu_9 \exp(-E_9/KT) \text{ cm}^3\text{sec}^{-1}$$

$$k_{10} = \sigma_{10}\nu_{10} \exp(-E_{10}/KT) \text{ sec}^{-1}$$

$$k_{11} = \sigma_{11}\nu_{11} \exp(-E_{11}/KT) \ \mathrm{cm^3sec^{-1}}$$

$$k_{12} = \sigma_{12}\nu_{12} \exp(-E_{12}/KT) \ \mathrm{cm^3sec^{-1}}$$

The results of a parametric study of the equilibrium equations are given in table 4, and a graph of results is illustrated in figure 19.

Table 4. Results of a parametric study of the equilibrium equations.

```
K1= 2.50000E-15 K2= 1.39180E-25 K3= 2.50000E-15 K4= 1.39180E-25
K5= 1.39180E-25 K6= 5.40091E-23 K7= 1.39180E-25 K8= 6.10905E-17
K9= 1.39180E-25 K10= 2.04611E-12 K11= 1.12613E-37 K12= 1.39180E-25

E2= 7.20000E-01 E4= 7.20000E-01 E5= 7.20000E-01 E6= 1.75000E+00 E7= 7.20000E-01
E8= 1.40000E+00 E9= 7.20000E-01 E10= 8.30000E-01 E12= 7.20000E-01
V2= 1.00000E+12 V4= 1.00000E+12 V5= 1.00000E-12 V6= 1.00000E+13 V7= 1.00000E+12
V8= 1.00000E+12 V9= 1.00000E+12 V10= 1.09099E+05 V12= 1.00000E+12


TEMP= 2.50000E+02 Na= 2.00000E+17 NI= 2.22000E+22
Y1=[Ga Ga]= 2.219979864E+22           Y2=[ V Ga ]= 1.954640625E+15
Y3=[Ga i] = 2.013571120E+17           Y4=[ As As]= 2.219972089E+22
Y5=[V As] = 1.428680143E+15           Y6=[ As i ]= 2.791106100E+17
Y7=[I Ga] = 3.970576548E+04           Y8=[VGaIGa]= 2.000000000E+17
Y9=[(VGa)2]= 2.572755764E+13          Y10=[(VAs)2]= 1.388409043E+17


TEMP= 2.50000E+02 Na= 5.00000E+17 NI= 2.22000E+22
Y1=[Ga Ga]= 2.219949859E+22           Y2=[ V Ga ]= 7.915878468E+14
Y3=[Ga i] = 5.014136216E+17           Y4=[ As As]= 2.219972089E+22
Y5=[V As] = 1.428680143E+15           Y6=[ As i ]= 2.791106100E+17
Y7=[I Ga] = 2.451102003E+05           Y8=[VGaIGa]= 5.000000000E+17
Y9=[(VGa)2]= 3.675365377E+12          Y10=[(VAs)2]= 1.388409043E+17


TEMP= 2.50000E+02 Na= 2.00000E+18 NI= 2.22000E+22
Y1=[Ga Ga]= 2.219800022E+22           Y2=[ V Ga ]= 1.993664063E+14
Y3=[Ga i] = 1.999780903E+18           Y4=[ As As]= 2.219972089E+22
Y5=[V As] = 1.428680143E+15           Y6=[ As i ]= 2.791106100E+17
Y7=[I Ga] = 3.892857564E+06           Y8=[VGaIGa]= 2.000000000E+18
Y9=[(VGa)2]= 1.987744990E+10          Y10=[(VAs)2]= 1.388409043E+17


TEMP= 2.50000E+02 Na= 4.00000E+18 NI= 2.22000E+22
Y1=[Ga Ga]= 2.219599963E+22           Y2=[ V Ga ]= 9.966152344E+13
Y3=[Ga i] = 4.000370427E+18           Y4=[ As As]= 2.219972089E+22
Y5=[V As] = 1.428680143E+15           Y6=[ As i ]= 2.791106100E+17
Y7=[I Ga] = 1.557481756E+07           Y8=[VGaIGa]= 4.000000000E+18
Y9=[(VGa)2]= 2.483322300E+09          Y10=[(VAs)2]= 1.388409043E+17

K1= 2.50000E-15 K2= 3.64688E-23 K3= 2.50000E-15 K4= 3.64688E-23
K5= 3.64688E-23 K6= 4.07745E-17 K7= 3.64688E-23 K8= 3.07830E-12
K9= 3.64688E-23 K10= 1.25529E-09 K11= 1.12613E-37 K12= 3.64688E-23

E2= 7.20000E-01 E4= 7.20000E-01 E5= 7.20000E-01 E6= 1.75000E+00 E7= 7.20000E-01
E8= 1.40000E+00 E9= 7.20000E-01 E10= 8.30000E-01 E12= 7.20000E-01
V2= 1.00000E+12 V4= 1.00000E+12 V5= 1.00000E+12 V6= 1.00000E+13 V7= 1.00000E+12
V8= 1.00000E+12 V9= 1.00000E+12 V10= 1.09098E+05 V12= 1.00000E+12


TEMP= 3.00000E+02 Na= 2.00000E+17 NI= 2.22000E+22
Y1=[Ga Ga]= 2.219979990E+22           Y2=[ V Ga ]= 7.605234375E+12
Y3=[Ga i] = 2.000956603E+17           Y4=[ As As]= 2.219999478E+22
Y5=[V As] = 2.913500691E+14           Y6=[ As i ]= 5.223438000E+15
Y7=[I Ga] = 2.940254389E+10           Y8=[VGaIGa]= 1.999999706E+17
Y9=[(VGa)2]= 3.062035944E+08          Y10=[(VAs)2]= 2.466086300E+15


TEMP= 3.00000E+02 Na= 5.00000E+17 NI= 2.22000E+22
Y1=[Ga Ga]= 2.219949932E+22           Y2=[ V Ga ]= 3.039492188E+12
Y3=[Ga i] = 5.006776546E+17           Y4=[ As As]= 2.219999478E+22
Y5=[V As] = 2.913500691E+14           Y6=[ As i ]= 5.223438000E+15
Y7=[I Ga] = 1.839231476E+11           Y8=[VGaIGa]= 4.999998161E+17
Y9=[(VGa)2]= 1.845243037E+07          Y10=[(VAs)2]= 2.466086300E+15
```

(continued)

Table 4. (continued).

```
TEMP= 3.00000E-02 Na= 2.00000E+18 NI= 2.22000E+22
Y1=[Ga Ga]= 2.219799913E+22           Y2=[ V Ga ]= 7.605234375E+11
Y3=[Ga I] = 2.000874087E+18           Y4=[ As As]= 2.219999478E+22
Y5=[V As] = 2.913500691E+14           Y6=[ As I ]= 5.223438000E+15
Y7=[I Ga] = 2.940250499E+12           Y8=[VGaIGa]= 1.999997060E+18
Y9=[(VGa)2]= 2.890976543E+05          Y10=[(VAs)2]= 2.466086300E+15

TEMP= 3.00000E-02 Na= 4.00000E+18 NI= 2.22000E+22
Y1=[Ga Ga]= 2.219599919E+22           Y2=[ V Ga ]= 3.802888184E+11
Y3=[Ga I] = 4.000811160E+18           Y4=[ As As]= 2.219999478E+22
Y5=[V As] = 2.913500691E+14           Y6=[ As I ]= 5.223438000E+15
Y7=[I Ga] = 1.176014661E+13           Y8=[VGaIGa]= 3.999988240E+18
Y9=[(VGa)2]= 2.783669040E+07          Y10=[(VAs)2]= 2.466086300E+15

K1= 2.50000E-15 K2= 1.94675E-21 K3= 2.50000E-15 K4= 1.94675E-21
K5= 1.94675E-21 K6= 6.44028E-13 K7= 1.94675E-21 K8= 7.03273E-09
K9= 1.94675E-21 K10= 1.23038E-07 K11= 1.12613E-37 K12= 1.94675E-21

E2= 7.20000E-01 E4= 7.20000E-01 E5= 7.20000E-01 E6= 1.75000E+00 E7= 7.20000E-01
E8= 1.40000E+00 E9= 7.20000E-01 E10= 8.30000E-01 E12= 7.20000E-01
V2= 1.00000E+12 V4= 1.00000E+12 V5= 1.00000E+12 V6= 1.00000E+13 V7= 1.00000E+12
V8= 1.00000E+12 V9= 1.00000E+12 V10= 1.09098E+05 V12= 1.00000E+12

TEMP= 3.50000E-02 Na= 2.00000E+17 NI= 2.22000E+22
Y1=[Ga Ga]= 2.219979979E+22           Y2=[ V Ga ]= 1.423921875E+11
Y3=[Ga I] = 2.002128083E+17           Y4=[ As As]= 2.219999967E+22
Y5=[V As] = 8.712279903E+13           Y6=[ As I ]= 3.272280000E+14
Y7=[I Ga] = 4.635857357E+14           Y8=[VGaIGa]= 1.995364143E+17
Y9=[(VGa)2]= 1.141262422E+05          Y10=[(VAs)2]= 1.200977710E+14

TEMP= 3.50000E+02 Na= 5.00000E+17 NI= 2.22000E+22
Y1=[Ga Ga]= 2.219950266E+22           Y2=[ V Ga ]= 5.732109375E+10
Y3=[Ga I] = 4.973447835E+17           Y4=[ As As]= 2.219999967E+22
Y5=[V As] = 8.712279903E+13           Y6=[ As I ]= 3.272280000E+14
Y7=[I Ga] = 2.869130656E+15           Y8=[VGaIGa]= 4.971308693E+17
Y9=[(VGa)2]= 6.847574529E+04          Y10=[(VAs)2]= 1.200977710E+14

TEMP= 3.50000E+02 Na= 2.00000E+18 NI= 2.22000E+22
Y1=[Ga Ga]= 2.219804360E+22           Y2=[ V Ga ]= 1.457091797E+10
Y3=[Ga I] = 1.956397474E+18           Y4=[ As As]= 2.219999967E+22
Y5=[V As] = 8.712279903E+13           Y6=[ As I ]= 3.272280000E+14
Y7=[I Ga] = 4.440042067E+16           Y8=[VGaIGa]= 1.955599579E+18
Y9=[(VGa)2]= 1.085310993E+02          Y10=[(VAs)2]= 1.200977710E+14

TEMP= 3.50000E+02 Na= 4.00000E+18 NI= 2.22000E+22
Y1=[Ga Ga]= 2.219617101E+22           Y2=[ V Ga ]= 7.444262695E+09
Y3=[Ga I] = 3.828991039E+18           Y4=[ As As]= 2.219999967E+22
Y5=[V As] = 8.712279903E+13           Y6=[ As I ]= 3.272280000E+14
Y7=[I Ga] = 1.701958395E+17           Y8=[VGaIGa]= 3.829804161E+18
Y9=[(VGa)2]= 2.282524843E+04          Y10=[(VAs)2]= 1.200977710E+14

K1= 2.50000E-15 K2= 3.84461E-20 K3= 2.50000E-15 K4= 3.84461E-20
K5= 3.84461E-20 K6= 9.07385E-10 K7= 3.84461E-20 K8= 2.32399E-06
K9= 3.84461E-20 K10= 3.83276E-06 K11= 1.12613E-37 K12= 3.84461E-20

E2= 7.20000E-01 E4= 7.20000E-01 E5= 7.20000E-01 E6= 1.75000E+00 E7= 7.20000E-01
E8= 1.40000E+00 E9= 7.20000E-01 E10= 8.30000E-01 E12= 7.20000E-01
V2= 1.00000E+12 V4= 1.00000E+12 V5= 1.00000E+12 V6= 1.00000E+13 V7= 1.00000E+12
V8= 1.00000E+12 V9= 1.00000E+12 V10= 1.09098E+05 V12= 1.00000E+12
```

Table 4. (continued).

```
TEMP= 4.00000E+02 Na= 2.00000E+17 NI= 2.22000E+22
Y1=[Ga Ga]= 2.21999161E+22          Y2=[ V Ga ]= 1.720500000E+10
Y3=[Ga i] = 8.390422605E+16          Y4=[ As As]= 2.219999995E+22
Y5=[V As] = 2.996591436E+13          Y6=[ As i ]= 4.817400000E+13
Y7=[I Ga] = 1.156751226E+17          Y8=[VGaIGa]= 8.432487741E+16
Y9=[(VGa)2]= 3.532525636E+03         Y10=[(VAs)2]= 9.007335546E+12

TEMP= 4.00000E+02 Na= 5.00000E+17 NI= 2.22000E+22
Y1=[Ga Ga]= 2.219985255E+22          Y2=[ V Ga ]= 9.790546875E+09
Y3=[Ga i] = 1.474451115E+17          Y4=[ As As]= 2.219999995E+22
Y5=[V As] = 2.996591436E+13          Y6=[ As i ]= 4.817400000E+13
Y7=[I Ga] = 3.533998571E+17          Y8=[VGaIGa]= 1.466001429E+17
Y9=[(VGa)2]= 6.645345256E+02         Y10=[(VAs)2]= 9.007335546E+12

TEMP= 4.00000E+02 Na= 2.00000E+18 NI= 2.22000E+22
Y1=[Ga Ga]= 2.219967941E+22          Y2=[ V Ga ]= 4.502871094E+09
Y3=[Ga i] = 3.205859270E+17          Y4=[ As As]= 2.219999995E+22
Y5=[V As] = 2.996591436E+13          Y6=[ As i ]= 4.817400000E+13
Y7=[I Ga] = 1.679560380E+18          Y8=[VGaIGa]= 3.204396205E+17
Y9=[(VGa)2]= 3.497550135E+01         Y10=[(VAs)2]= 9.007335546E+12

TEMP= 4.00000E+02 Na= 4.00000E+18 NI= 2.22000E+22
Y1=[Ga Ga]= 2.219953551E+22          Y2=[ V Ga ]= 3.107783203E+09
Y3=[Ga i] = 4.444943528E+17          Y4=[ As As]= 2.219999995E+22
Y5=[V As] = 2.996591436E+13          Y6=[ As i ]= 4.817400000E+13
Y7=[I Ga] = 3.534575680E+18          Y8=[VGaIGa]= 4.654243202E+17
Y9=[(VGa)2]= 2.079091316E+01         Y10=[(VAs)2]= 9.007335546E+12

K1= 2.50000E-15 K2= 3.91288E-19 K3= 2.50000E-15 K4= 3.91288E-19
K5= 3.91288E-19 K6= 2.55227E-07 K7= 3.91288E-19 K8= 2.11612E-04
K9= 3.91288E-19 K10= 5.56033E-05 K11= 1.12613E-37 K12= 3.91288E-19

E2= 7.20000E-01 E4= 7.20000E-01 E5= 7.20000E-01 E6= 1.75000E+00 E7= 7.20000E-01
E8= 1.40000E+00 E9= 7.20000E-01 E10= 8.30000E-01 E12= 7.20000E-01
V2= 1.00000E+12 V4= 1.00000E+12 V5= 1.00000E+12 V6= 1.00000E+13 V7= 1.00000E+12
V8= 1.00000E+12 V9= 1.00000E+12 V10= 1.09098E+05 V12= 1.00000E+12

TEMP= 4.50000E+02 Na= 2.00000E+17 NI= 2.22000E+22
Y1=[Ga Ga]= 2.219999323E+22          Y2=[ V Ga ]= 2.095125000E+10
Y3=[Ga i] = 6.769944644E+15          Y4=[ As As]= 2.219999999E+22
Y5=[V As] = 1.101578537E+13          Y6=[ As i ]= 1.287600000E+13
Y7=[I Ga] = 1.937758477E+17          Y8=[VGaIGa]= 6.224152258E+15
Y9=[(VGa)2]= 6.004206404E+04         Y10=[(VAs)2]= 8.539385555E+11

TEMP= 4.50000E+02 Na= 5.00000E+17 NI= 2.22000E+22
Y1=[Ga Ga]= 2.219998946E+22          Y2=[ V Ga ]= 1.345875000E+10
Y3=[Ga i] = 1.053879542E+16          Y4=[ As As]= 2.219999999E+22
Y5=[V As] = 1.101578537E+13          Y6=[ As i ]= 1.287600000E+13
Y7=[I Ga] = 4.898917614E+17          Y8=[VGaIGa]= 1.010823862E+16
Y9=[(VGa)2]= 1.634937591E+04         Y10=[(VAs)2]= 8.539385555E+11

TEMP= 4.50000E+02 Na= 2.00000E+18 NI= 2.22000E+22
Y1=[Ga Ga]= 2.219997945E+22          Y2=[ V Ga ]= 6.902812500E+09
Y3=[Ga i] = 2.054801210E+16          Y4=[ As As]= 2.219999999E+22
Y5=[V As] = 1.101578537E+13          Y6=[ As i ]= 1.287600000E+13
Y7=[I Ga] = 1.979056231E+18          Y8=[VGaIGa]= 2.094376876E+16
Y9=[(VGa)2]= 2.259172766E+03         Y10=[(VAs)2]= 8.539385555E+11
```

Table 4. (concluded).

```
TEMP= 4.50000E+02 Na= 4.00000E+18 Ni= 2.22000E+22
Y1=[Ga Ga]= 2.21999709E+22           Y2=[ V Ga ]= 4.87359375E+09
Y3=[Ga i] = 2.91035836E+16           Y4=[ As As]= 2.21999999E+22
Y5=[V As] = 1.10157853E+13           Y6=[ As i ]= 1.28760000E+13
Y7=[I Ga] = 3.97033481E+18           Y8=[VGaIGa]= 2.96651862E+16
Y9=[(VGa)2]= 8.01617600E+02          Y10=[(VAs)2]= 8.53938555E+11

K1= 2.50000E-15 K2= 2.50387E-18 K3= 2.50000E-15 K4= 2.50387E-18
K5= 2.50387E-18 K6= 2.32399E-05 K7= 2.50387E-18 K8= 7.81604E-03
K9= 2.50387E-18 K10= 4.72468E-04 K11= 1.12613E-37 K12= 2.50387E-18

E2= 7.20000E-01 E4= 7.20000E-01 E5= 7.20000E-01 E6= 1.75000E+00 E7= 7.20000E-01
E8= 1.40000E+00 E9= 7.20000E-01 E10= 8.30000E-01 E12= 7.20000E-01
V2= 1.00000E+12 V4= 1.00000E+12 V5= 1.00000E+12 V6= 1.00000E+13 V7= 1.00000E+12
V8= 1.00000E+12 V9= 1.00000E+12 V10= 1.09098E+05 V12= 1.00000E+12


TEMP= 5.00000E+02 Na= 2.00000E+17 Ni= 2.22000E+22
Y1=[Ga Ga]= 2.21999995E+22           Y2=[ V Ga ]= 4.71750000E+10
Y3=[Ga i] = 4.64854903E+14           Y4=[ As As]= 2.22000000E+22
Y5=[V As] = 4.50843093E+12           Y6=[ As i ]= 4.88400000E+12
Y7=[I Ga] = 1.09988610E+17           Y8=[VGaIGa]= 1.01138938E+15
Y9=[(VGa)2]= 6.19662994E+05          Y10=[(VAs)2]= 1.09156772E+11


TEMP= 5.00000E+02 Na= 5.00000E+17 Ni= 2.22000E+22
Y1=[Ga Ga]= 2.21999987E+22           Y2=[ V Ga ]= 1.72050000E+10
Y3=[Ga i] = 1.28832368E+15           Y4=[ As As]= 2.22000000E+22
Y5=[V As] = 4.50843093E+12           Y6=[ As i ]= 4.88400000E+12
Y7=[I Ga] = 4.99074878E+17           Y8=[VGaIGa]= 9.25121240E+14
Y9=[(VGa)2]= 6.71242974E+04          Y10=[(VAs)2]= 1.09156772E+11


TEMP= 5.00000E+02 Na= 2.00000E+18 Ni= 2.22000E+22
Y1=[Ga Ga]= 2.21999981E+22           Y2=[ V Ga ]= 1.22100000E+10
Y3=[Ga i] = 1.81536773E+15           Y4=[ As As]= 2.22000000E+22
Y5=[V As] = 4.50843093E+12           Y6=[ As i ]= 4.88400000E+12
Y7=[I Ga] = 1.99737243E+18           Y8=[VGaIGa]= 2.62756204E+15
Y9=[(VGa)2]= 3.01976177E+04          Y10=[(VAs)2]= 1.09156772E+11


TEMP= 5.00000E+02 Na= 4.00000E+18 Ni= 2.22000E+22
Y1=[Ga Ga]= 2.21999969E+22           Y2=[ V Ga ]= 7.21500000E+09
Y3=[Ga i] = 3.07216462E+15           Y4=[ As As]= 2.22000000E+22
Y5=[V As] = 4.50843093E+12           Y6=[ As i ]= 4.88400000E+12
Y7=[I Ga] = 3.99689303E+18           Y8=[VGaIGa]= 3.10697044E+15
Y9=[(VGa)2]= 8.40465293E+03          Y10=[(VAs)2]= 1.09156772E+11
```

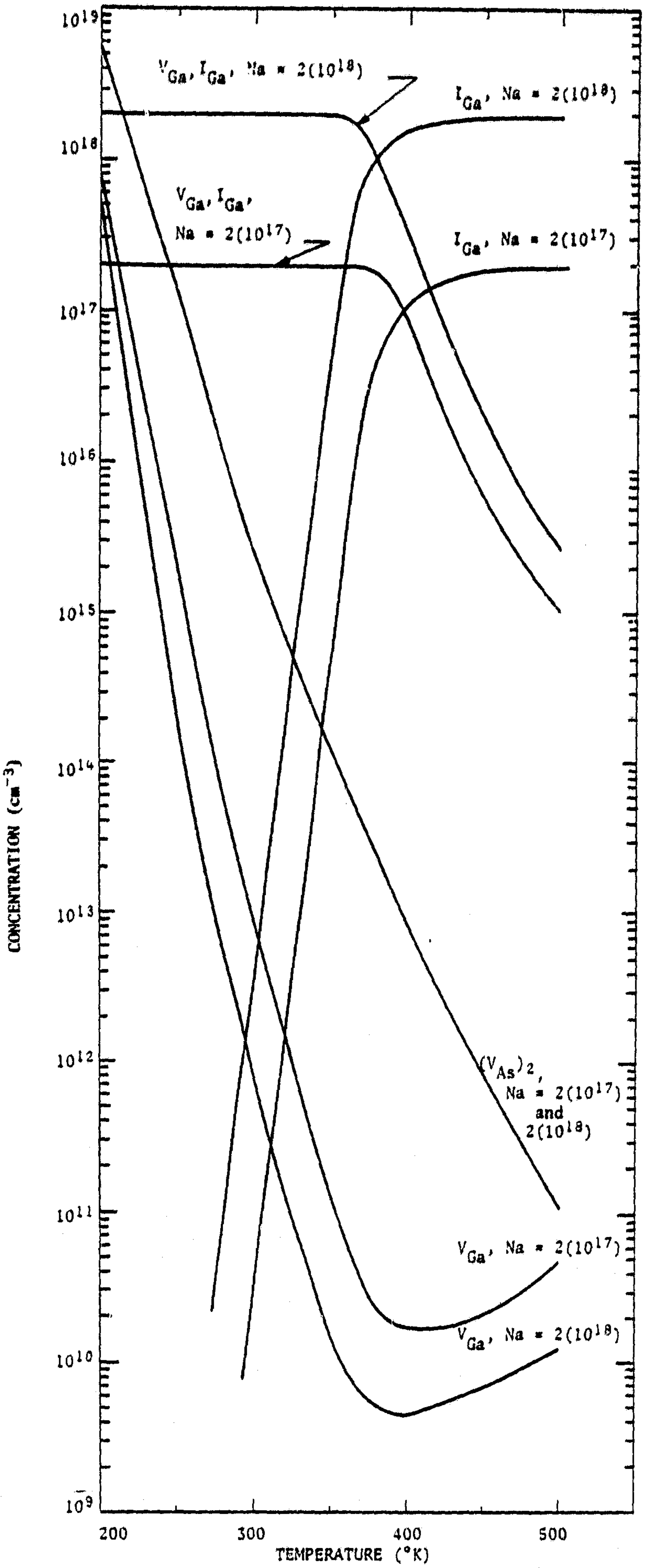

Figure 19. Equilibrium values vs. temperature.

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